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# Theoretical Study of In-plane Heterojunctions of Transition-metal Dichalcogenides and their Applications for Low-power Transistors

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# Theoretical Study of In-plane Heterojunctions of transition-metal Dichalcogenides and their Applications for Low-power Transistors

Thèse de doctorat de l'Université Paris-Saclay  
préparée à Université Paris-Sud

École doctorale n°575 : Electrical, Optical, Bio : Physics and Engineering  
(EOBE)  
Spécialité : Electronique et optoélectronique, nano et microtechnologies

Thèse présentée et soutenue à Orsay, le 14 décembre 2018 par

**Jean CHOUKROUN**

Composition du Jury :

|  |                    |
|--|--------------------|
| <b>M. Yann-Michel NIQUET</b><br>Ingénieur-chercheur, CEA, INAC, Grenoble           | Rapporteur         |
| <b>M. Raphaël CLERC</b><br>Professeur, CNRS, Laboratoire Hubert Curien, St Etienne | Rapporteur         |
| <b>M. Philippe DOLLFUS</b><br>Directeur de recherche, CNRS, C2N, Orsay             | Directeur de thèse |
| <b>M. Marco PALA</b><br>Chargé de recherche, CNRS, C2N, Orsay                      | Co-encadrant       |
| <b>M. Frédéric ANIEL</b><br>Professeur, CNRS, C2N, Orsay                           | Président          |
| <b>M. Bernard PLAÇAIS</b><br>Directeur de Recherche, CNRS, ENS-LPA, Paris          | Examineur          |







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*Bures-sur-Yvette, December 14<sup>th</sup> 2018*

**Jean Choukroun**



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# Abstract

The invention of the transistor in 1947 is arguably one of the most important advances in technology in the history of mankind. From single transistors came integrated circuits, and finally microprocessors in 1971 based on the traditional MOSFET architecture.

The number of transistors per microprocessor increased following Moore's law, nowadays reaching the tens of billions. However, this scaling of traditional, silicon-based MOSFET seems to be reaching its conclusion: with billions of transistors crammed into a single chip, the dissipated heat actually impedes device performance and a scaling of the power supply is therefore badly needed to remedy this issue. However, due to the working mechanism at the very core of MOSFETs, which prevents further decrease of the supply voltage of these transistors without affecting performance, this power supply scaling won't come.

New architectures such as the TFET could bring a solution to this issue: thanks to their reliance on band-to-band tunneling, TFETs can perform at very low supply voltages and are amongst the most promising avenues for transistor technology beyond the age of the silicon-based MOSFET.

New materials could also take part in this transistor revolution: since the experimental isolation of graphene in 2004 by Geim and Novoselov, research interest in 2D materials has soared, motivated by the incredible electronic and mechanical properties of the single-layer carbon material. Dozens of 2D materials were since discovered and fabricated, and among them, transition metal dichalcogenide monolayers (TMDs) are some of the most commonly studied to this day. Thanks to their semiconducting nature and direct band gaps ranging from 1 to 2 eV, they hold potential in electronics and photonics.

Moreover, when under appropriate strains, their band alignment can result in broken-gap configurations which could be used in the case of TFETs to circumvent the traditionally low currents observed due to the tunneling mechanism they rely upon.

In this work, TMDs based in-plane heterojunctions are investigated thanks to an atomistic tight-binding approach, some of which are observed to lead to a broken-gap configuration (namely  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$ ). Their potential for use in tunnel field-effect transistors is subsequently evaluated via quantum transport computations based on this atomistic tight-binding model as well as the non-equilibrium Green's function theory. N-type TFETs based on these in-plane heterojunctions are shown to yield high ON currents ( $I_{ON} > 10^3 \mu\text{A}/\mu\text{m}$ ) and extremely low subthreshold swings ( $SS < 5 \text{ mV/dec}$ ) at low supply voltages ( $V_{DD} = 0.3 \text{ V}$ ). Innovative device architectures allowed by the 2D nature of these materials are also proposed, and shown to enhance performance even further.



# Résumé

## A - Introduction

L'invention du transistor en 1947 est sans aucun doute l'une des plus grandes avancées technologiques de l'histoire de l'humanité. Vinrent ensuite les circuits intégrés, puis les microprocesseurs, (basés sur des transistors de type MOSFET) et pouvant contenir aujourd'hui des dizaines de milliards de transistors.

Néanmoins, la miniaturisation des MOSFETs lancée dans les années 70 semble à bout de souffle: le mécanisme de fonctionnement au cœur même des MOSFET empêche aujourd'hui la diminution de leur tension d'alimentation pourtant nécessaire pour réduire la consommation (voir Figure R 1), entraînant un échauffement pouvant fortement dégrader les performances des composants.

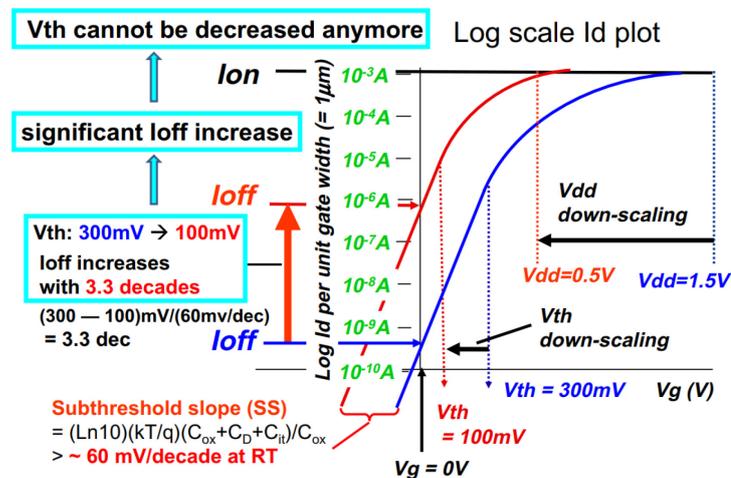
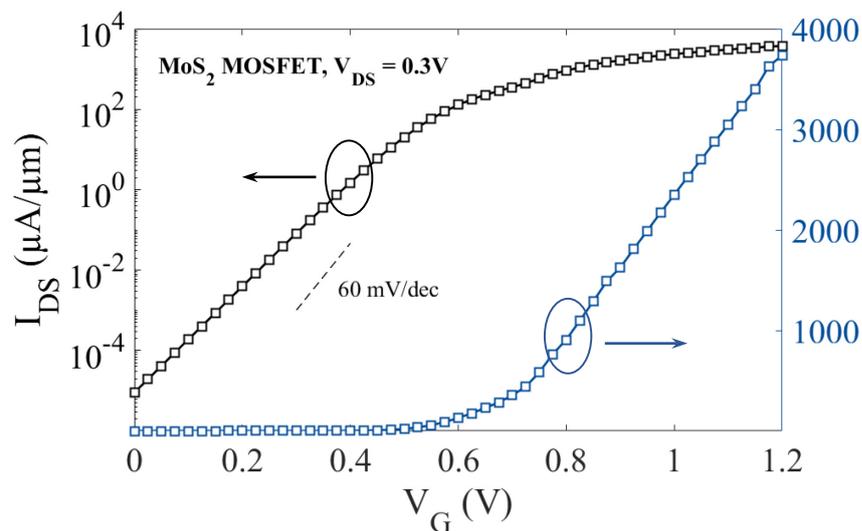


Figure R 1. (haut) Caractéristique  $I_D - V_G$  d'un MOSFET à inversion type-n à  $V_{DS} = 0.3 \text{ V}$  et (bas) augmentation de  $I_{OFF}$  induite par une diminution de la tension d'alimentation.

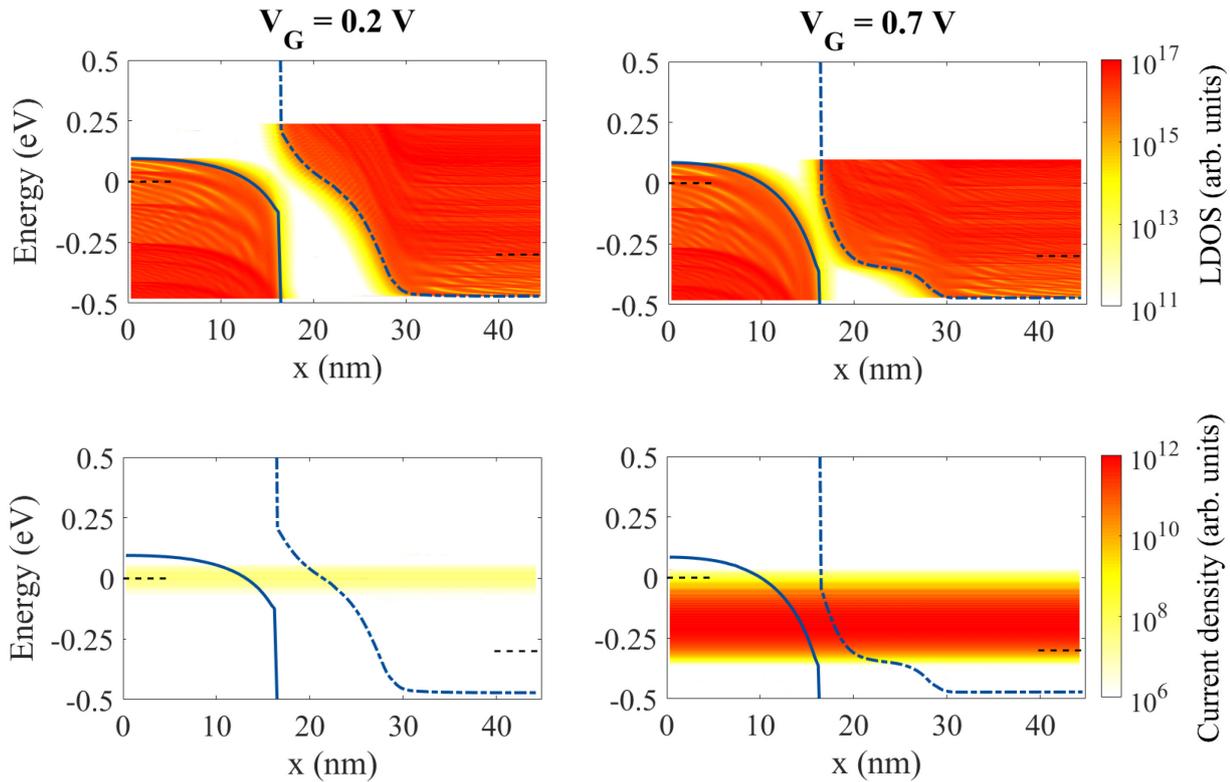


Figure R 2. (haut) LDOS dans un TFET  $\text{WSe}_2\text{-MoS}_2$  (contraint) à l'état OFF (gauche) et ON (droite). La courbe bleue pleine (pointillée) représente la CB la plus basse (VB la plus haute), et les lignes noires pointillées le niveau de Fermi dans les contacts. (bas) Densité de courant dans le même dispositif.

De nouvelles architectures telles que le TFET pourraient donc apporter une alternative au MOSFET silicium. Grâce à son mode de fonctionnement (effet tunnel bande-à-bande, voir Figure R 2), le TFET peut présenter une pente sous-seuil bien plus raide, et donc un  $SS$  (augmentation de  $V_G$  nécessaire pour augmenter le courant d'un facteur 10) plus faible que le MOSFET (dont la limite théorique est de 60 mV/dec) : une très légère augmentation de  $V_G$  peut suffire pour passer de l'état OFF à l'état ON.

Ainsi, le TFET peut en principe fonctionner à des tensions d'alimentation bien plus faibles que les MOSFETs traditionnels, ce qui en fait un candidat de choix pour succéder au MOSFET silicium. Néanmoins, du fait que leur fonctionnement repose sur l'effet tunnel bande à bande, les TFETs présentent un inconvénient de taille : de faibles courants ON, limitant leurs applications possibles.

Du point de vue des matériaux, les matériaux 2D dont la notoriété est en constante augmentation depuis l'observation expérimentale du graphène en 2004, pourraient également être une alternative viable au silicium. De par leur épaisseur monoatomique, la plupart de ces matériaux présentent des propriétés novatrices, qu'elles soient électroniques ou mécaniques. Des applications variées en nanoélectronique, optoélectronique, spintronique, science des matériaux mais aussi conversion et stockage d'énergie par exemple, leur sont promises. Parmi ces matériaux 2D, les monocouches de dichalcogénures de métaux de transitions (TMDs) -des semi-conducteurs à bande interdite directe d'environ 1 à 2 eV- possèdent un fort potentiel pour l'électronique et la photonique.

De plus, dans le cas de contraintes appropriées, les hétérojonctions de TMDs peuvent conduire un alignement de bandes présentant un « broken-gap ». Cette configuration ( $E_{VB-source} > E_{CB-drain}$  pour un TFET type n) permettrait de surpasser les limites habituelles du TFET, à savoir de faibles courants, limités par l'effet tunnel sur lequel ces dispositifs reposent.

Dans ce travail de thèse, le potentiel de diverses hétérojonctions planaires de TMDs dans le cadre de TFETs est donc étudié en détail, au moyen d'une approche liaisons fortes couplée à des simulations de transport balistique quantique basées sur la théorie des fonctions de Green hors-équilibre.

## B - Modèles et méthodes

Les TMDs étudiés sont les suivants : MoS<sub>2</sub>, MoSe<sub>2</sub>, MoTe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub> et WTe<sub>2</sub>. Leur agencement atomique respecte une maille hexagonale séparée en trois niveaux (chalcogène, métal, chalcogène – voir Figure R 3).

Ils sont modélisés via un modèle liaisons fortes basé sur le modèle développé par Fang et al. [1]. Ce modèle prend en compte les contributions de 11 orbitales atomiques : les 5 orbitales  $d$  du métal de transition, et les 3 orbitales  $p$  du chalcogène ( $3 \times 2$  puisque deux atomes de chalcogène dans la cellule unitaire des TMDs). La réponse des matériaux à une contrainte mécanique, et l'évolution de leurs propriétés en résultant, est également modélisée. Les couplages aux premiers et seconds voisins sont pris en compte, ainsi que le couplage partiel aux troisièmes voisins pour plus de précision.

Afin d'utiliser ce modèle dans le cadre de notre étude de transport électronique, un changement de base était nécessaire. Le modèle fut donc reconstruit pour s'accommoder à nos besoins : en résulte le modèle schématisé en Figure R 5.

La cellule unitaire considérée est représentée en rouge (jaune pour celle du modèle initial), et les Hamiltoniens  $\mathbf{H}_{n,m}$  et  $\mathbf{T}_{i,j}$  résultant des couplages considérés y sont également représentés. A partir de ces Hamiltoniens  $22 \times 22$ , les propriétés électroniques du TMD peuvent être calculées, comme le montre la structure de bandes présentée en Figure R 4.

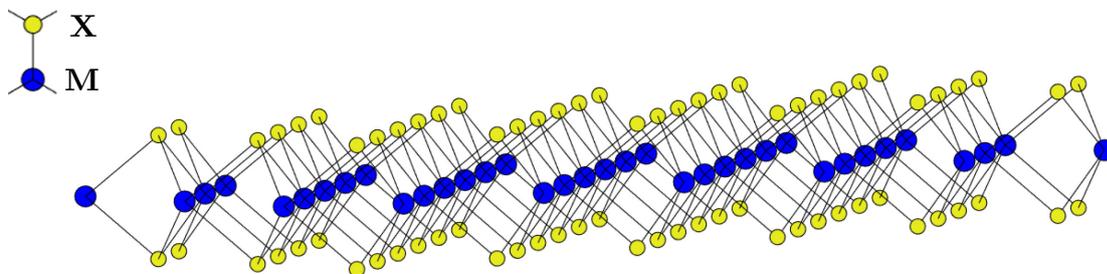


Figure R 3. Représentation « de côté » d'un TMD, mettant en avant la structure de ces matériaux, composée de trois couches distinctes.

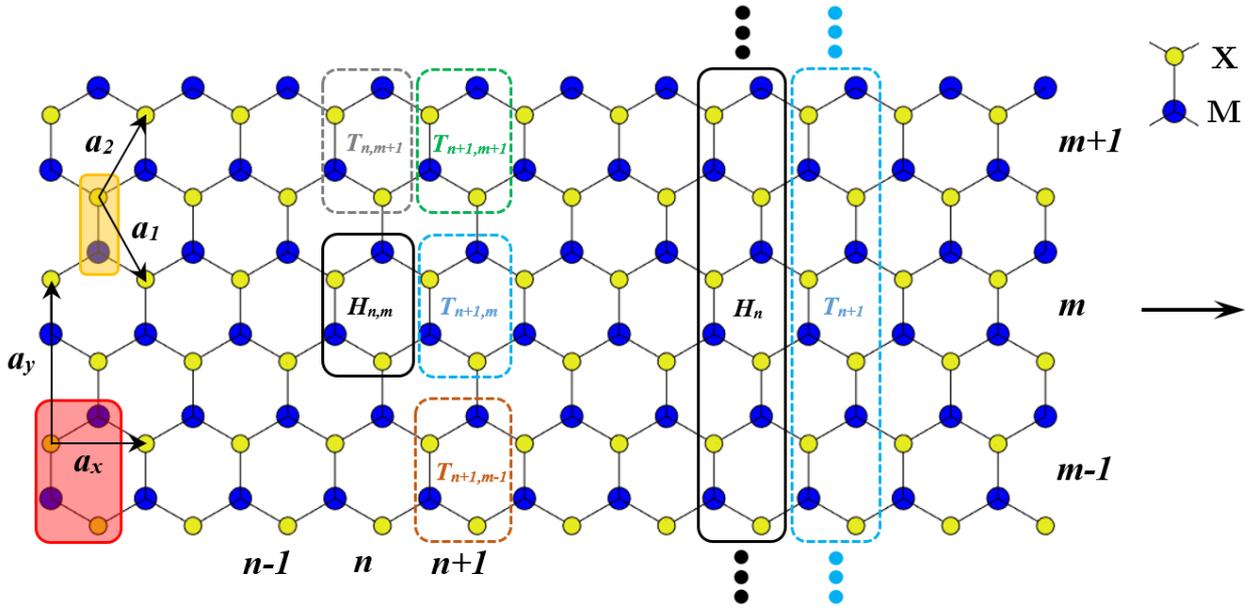


Figure R 5. Représentation de la structure des TMDs (vue de dessus) ainsi que du modèle TB utilisé. La zone rouge (jaune) représente la cellule unitaire (celle du modèle original),  $H_{n,m}$  est l'Hamiltonien d'une cellule unitaire, et  $T_{i,j}$  est l'Hamiltonien représentant le couplage de la maille (i,j) avec la maille (n,m). Les Hamiltoniens de couche  $H_n$  et  $T_{n+1}$  seront utilisés dans le modèle de transport basé sur les NEGF.

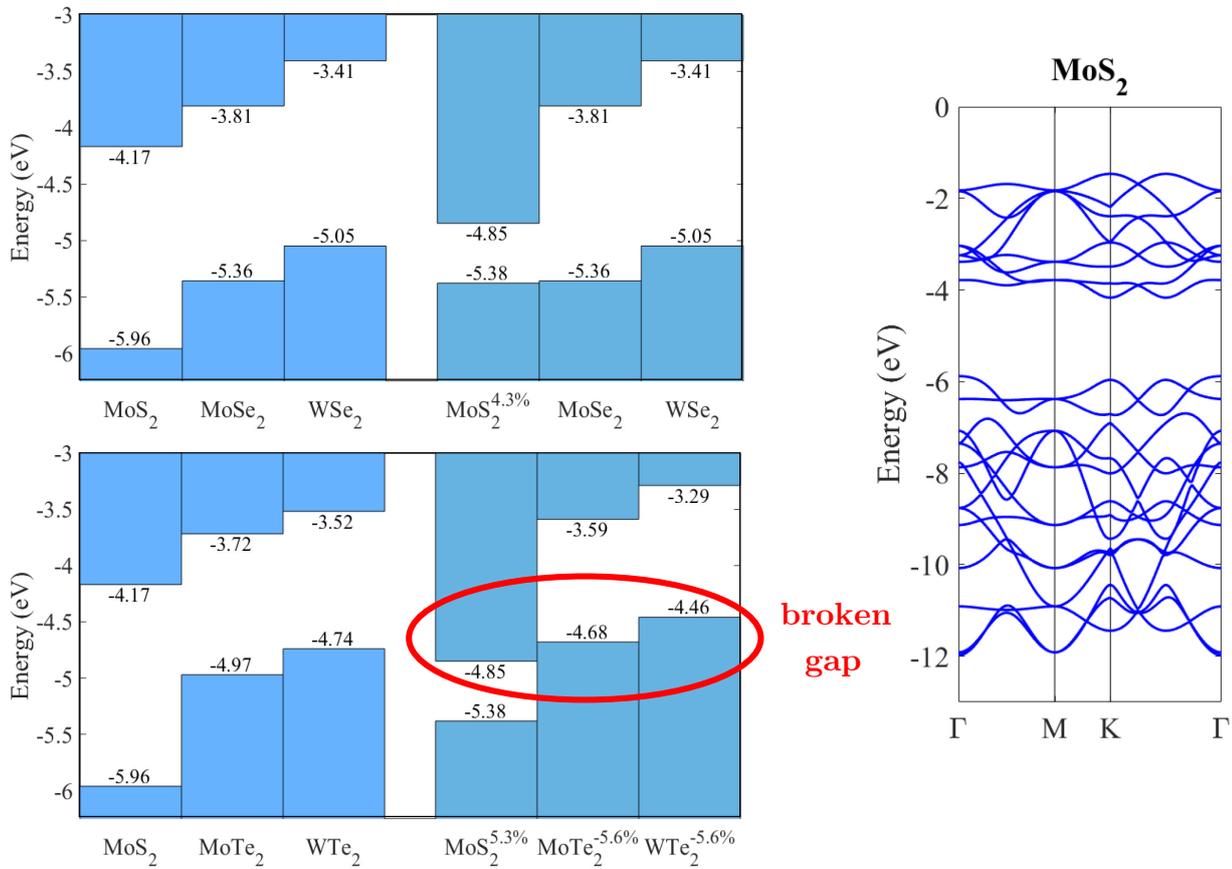


Figure R 4. (gauche) Alignement de bandes des TMDs considérés dans leur forme relaxée et contrainte (les contraintes appliquées sont celles nécessaires à l'obtention d'un accord de maille entre les TMDs considérés). L'existence d'un broken-gap dans les hétérojonctions MoS<sub>2</sub>/MoTe<sub>2</sub> et MoS<sub>2</sub>/WTe<sub>2</sub> est mise en évidence. Le niveau du vide est de 0 eV. (droite) Structure de bandes du MoS<sub>2</sub> obtenue via le modèle TB.

Les TMDs considérés n'ayant pas tous le même paramètre de maille, les matériaux de part et d'autre d'une hétérojonction seront soumis à des contraintes mécaniques.

Les alignements de bandes des TMDs sous leur forme relaxée et contrainte (auquel cas les contraintes appliquées sont celles nécessaires à l'obtention d'un accord de maille entre les TMDs considérés) sont présentées en Figure R 4, et mettent en exergue l'existence d'un broken-gap dans le cas des hétérojonctions  $\text{MoTe}_2/\text{MoS}_2$  et  $\text{WTe}_2/\text{MoS}_2$ .

Une approche basée sur la théorie des fonctions de Green hors-équilibre est utilisée pour modéliser le transport électronique dans des dispositifs basés sur ces hétérostructures.

Cette approche consiste à séparer le dispositif en trois zones distinctes : deux contacts semi-infinis (source et drain), et une zone « device ». La fonction de Green du dispositif peut ensuite être déterminée à partir du Hamiltonien de la zone device ainsi que de son couplage avec les contacts source et drain.

$$G(E) = ((E + i0^+)I - H_D - \Sigma_L - \Sigma_R)^{-1} \quad (R1)$$

Pour ce faire, il est néanmoins nécessaire de décrire la zone device comme une succession de couches identiques suivant la direction du transport, ce qui justifie le changement de base opéré dans le cadre du modèle TB. Les matrices  $H_n$  et  $T_{n+1}$  (voir Figure R 5) sont donc créées à partir des  $H_{n,m}$  et  $T_{i,j}$  présentés précédemment comme suit

$$H_n(k_y) = H_{n,m} + T_{n,m+1} \cdot e^{i \cdot k_y \cdot a_y} + T_{n,m-1} \cdot e^{-i \cdot k_y \cdot a_y} \quad (R2)$$

$$T_{n+1}(k_y) = T_{n+1,m} + T_{n+1,m-1} \cdot e^{-i \cdot k_y \cdot a_y} + T_{n+1,m+1} \cdot e^{i \cdot k_y \cdot a_y} \quad (R3)$$

A partir de cette fonction de Green, les paramètres liés au transport dans le dispositif (telles que la charge, le courant, la densité d'états ...) peuvent ensuite être calculés. Afin d'assurer une résolution optimale, cette approche NEGF est couplée de façon auto-cohérente avec la résolution de l'équation de Poisson.

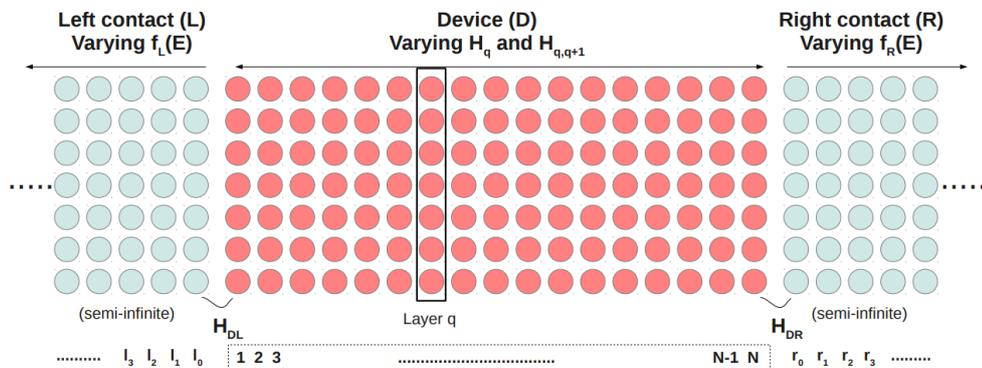


Figure R 6. Division du système en trois zones, chacune subdivisée en couches successives identiques

## C - Résultats

Les dispositifs étudiés sont composés d'une couche de  $\text{SiO}_2$  de 3.35 nm d'épaisseur sur laquelle l'hétérojonction de TMD repose. Cette hétérojonction est séparée de la top-gate par une couche d'oxyde de forte permittivité (high- $\kappa$ ) d'EOT = 1.34 nm. Les contacts sont dopés de manière électrostatique par des « backgates » (possibilité offerte par la nature 2D des matériaux utilisés), plutôt que par un dopage chimique traditionnel et invasif. La source et le drain sont de longueurs respectives  $L_S = 16.8$  nm et  $L_D = 10.05$  nm, et la longueur du canal est variable selon les dispositifs. Une différence de potentiel  $V_{DS}$  est appliquée entre les contacts source et drain, fixant ainsi les énergies de Fermi dans les contacts à  $\mu_S = 0$  et  $\mu_D = -eV_{DS}$ . Les performances visées par les dispositifs sont un rapport ON/OFF élevé ( $> 10^7$ ) et un  $SS$  faible ( $< 30$  mV/dec), assurant une transition OFF-ON ne nécessitant qu'une faible augmentation de  $V_G$ . La source est composée d'un TMD (autre que  $\text{MoS}_2$  et  $\text{WS}_2$ ), et  $\text{MoS}_2$  est utilisé dans le canal comme dans le drain.

### C.1 - TFET standard

Le potentiel des hétérojonctions de TMDs présentées en Figure R 4 dans le cadre de TFETs standard est étudiée. Leurs caractéristiques  $I_D - V_G$  sont comparées en Figure R 7, et l'importance de l'alignement de bandes résultant de l'hétérojonction est mise en exergue. Les hétérojonctions présentant une configuration broken-gap ( $\text{MoTe}_2/\text{MoS}_2$  et  $\text{WTe}_2/\text{MoS}_2$ ) présentent des performances bien plus élevées que les autres dispositifs ( $SS < 8$  mV/dec et  $I_{ON} > 10^3 \mu\text{A}/\mu\text{m}$ ).

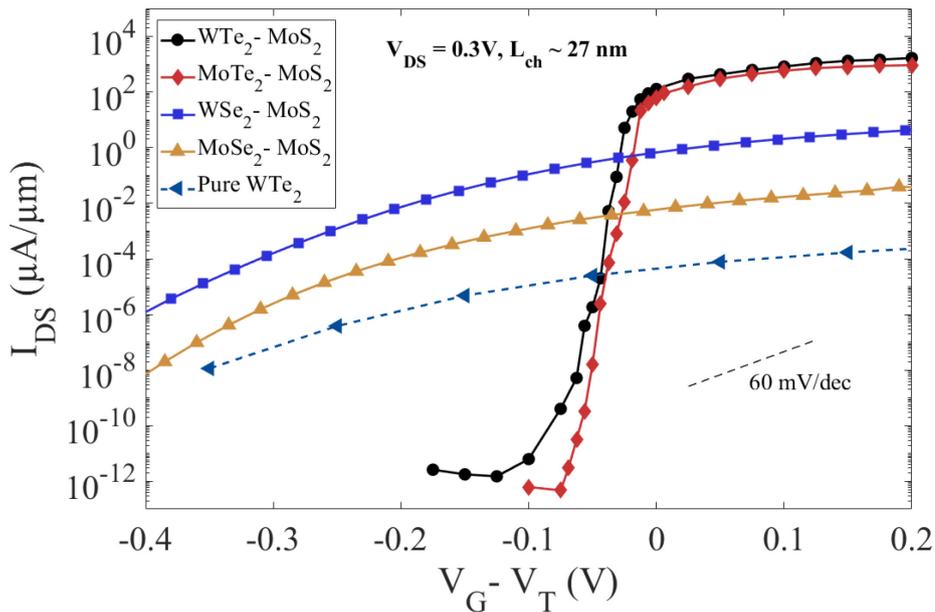


Figure R 7. Caractéristiques  $I_D - V_G$  des quatre hétérojonctions considérées, ainsi que d'un TFET homojonction  $\text{WTe}_2$  à  $V_{DS} = 0.3$  V et  $L_{ch} = 27$  nm. L'influence de l'alignement de bandes résultant de l'hétérojonction sur les performances (aussi bien  $SS$  que  $I_{ON}$ ) est mise en évidence.

Les dispositifs basés sur ces hétérojonctions sont donc étudiés plus en détail (influence de la longueur des contacts, du canal, des tensions appliquées aux « backgates ») afin d'optimiser leurs performances. Il en ressort notamment qu'une longueur de canal  $> 20$  nm est nécessaire afin de minimiser  $SS$  et de maximiser le courant ON, comme le montre Figure R 8, mais aussi que les tensions appliquées aux backgates influencent  $I_{ON}$  ainsi que  $SS$ .

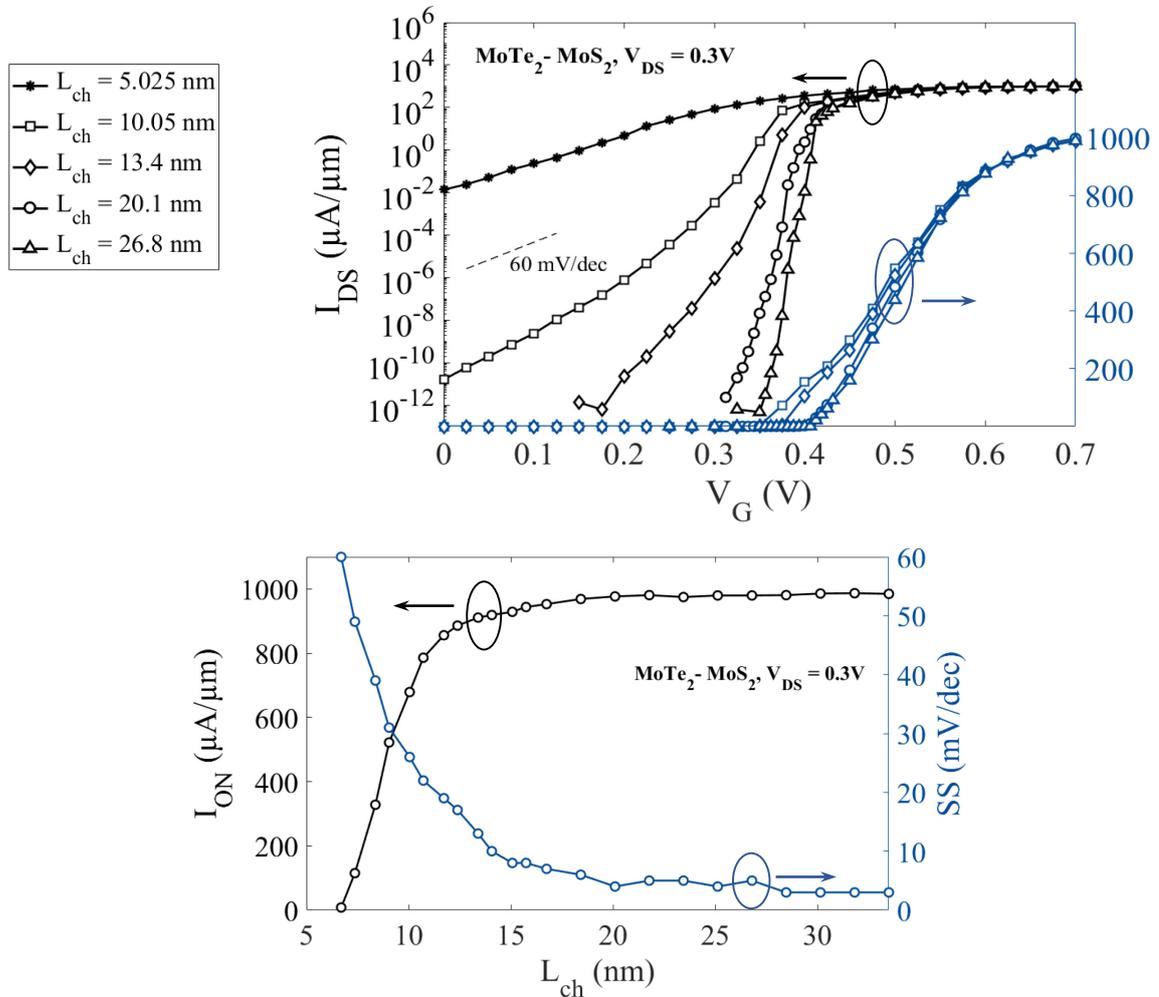


Figure R 8. (haut)  $I_D$ - $V_G$  du TFET MoTe<sub>2</sub>/MoS<sub>2</sub> à  $V_{DS} = 0.3$  V pour  $L_{ch}$  allant de 5 nm à 27 nm. (bas) Influence directe de  $L_{ch}$  sur  $SS$  et  $I_{ON}$  pour le même dispositif.

## C.2 - DBE-TFET

A partir de l'étude de l'influence des tensions appliquées aux « backgates » sur les performances des dispositifs présentés en C.1, l'idée d'une nouvelle architecture nous est venue : le DBE-TFET (Drain-backgate-enhanced TFET).

Dans ces dispositifs, la backgate drain est polarisée par rapport à la « top-gate » et un métal présentant une fonction de travail différente est utilisée, afin que  $V_{BG-D} = V_G$  et  $W_{BG-D} = W_{CG} - \Delta W$ . En fixant  $\Delta W$  à une valeur appropriée, les performances des dispositifs peuvent être fortement améliorées (voir Figure R 9).

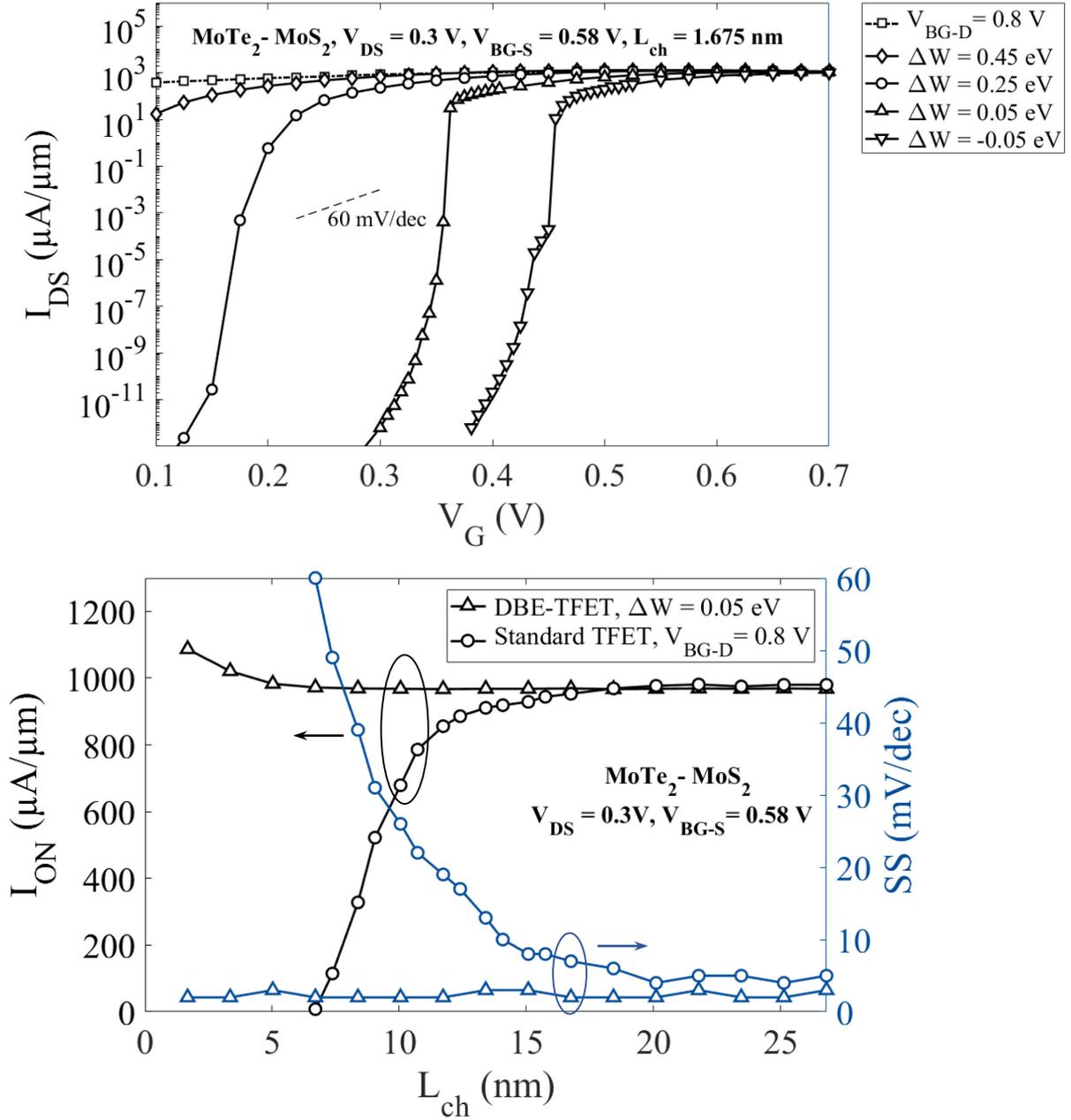


Figure R 9. (haut)  $I_D$ - $V_G$  d'un DBE-TFET  $\text{MoTe}_2/\text{MoS}_2$  à différents  $\Delta W$  à  $V_{DS} = 0.3$  V et  $L_{ch} = 1.675$  nm. L'  $I_D$ - $V_G$  d'un TFET  $\text{MoTe}_2/\text{MoS}_2$  standard est aussi représentée pour comparaison. (bas) Influence directe de  $L_{ch}$  sur  $SS$  et  $I_{ON}$  dans un DBE-TFET  $\text{MoTe}_2/\text{MoS}_2$  et un TFET standard.

Grâce à ce mécanisme, même des dispositifs comportant des canaux très courts ( $L_{ch} < 2$  nm) peuvent être réalisés, chose rendue impossible par l'effet tunnel direct source-drain présent dans les TFETs standards. Les DBE-TFETs permettent d'éliminer l'influence de la longueur de canal sur les performances du dispositif, et ont donc un avantage important par rapport aux TFETs standards.

### C.3 - UC-TFETs

Une autre architecture novatrice, basée sur les DBE-TFETs, est présentée et étudiée dans ce travail : le UC-TFET (ungated-channel TFET).

Puisque la CB du drain est contrôlée par  $V_{BG-D}$  avec précision (comme montré dans le cas des DBE-TFETs), une « top-gate » n'est pas nécessaire pour contrôler le courant. Dans un UC-TFET,  $V_{BG-D}$  est donc utilisé comme  $V_G$  le serait dans un dispositif classique.

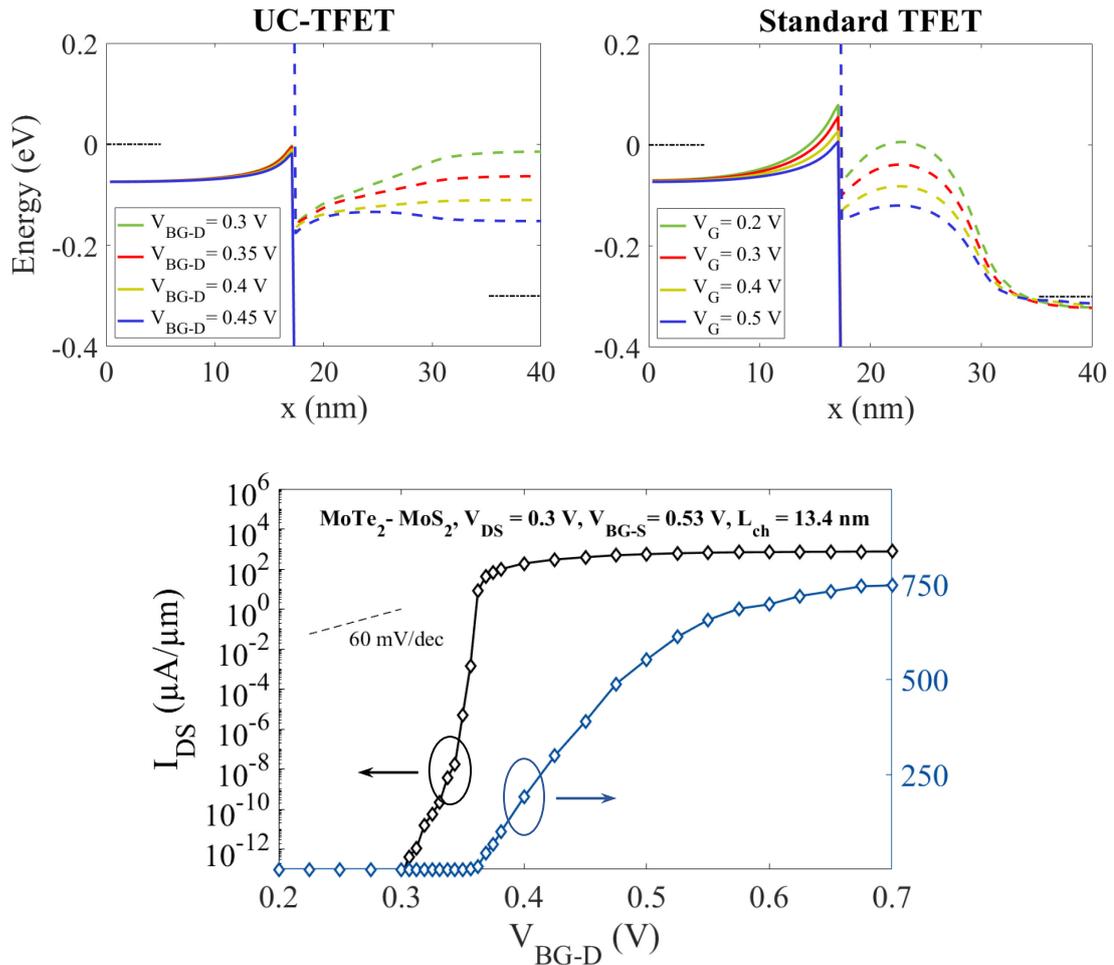


Figure R 10. (haut) Plus haute VB (lignes pleines) et plus basse CB (lignes pointillées) dans un UC-TFET et un TFET-standard lors de la transition OFF-ON.  
(bas)  $I_D$ -  $V_{BG-D}$  d'un UC-TFET  $\text{MoTe}_2/\text{MoS}_2$  à  $V_{DS} = 0.3$  V et  $L_{ch} = 13.4$  nm

Comme le montre Figure R 10, le niveau de la CB dans le drain est utilisé pour contrôler le flux de porteurs dans le dispositif. Ainsi, des performances du même ordre que celles des DBE-TFET sont obtenues, tout en éliminant la top-gate (ce qui simplifierait le processus de fabrication des transistors).

## D - Conclusion

Ce travail a mis en avant le fort potentiel des hétérojonctions planaires de TMDs dans le cadre de TFETs. En effet, sous certaines contraintes, ces hétérojonctions peuvent conduire à un broken-gap, configuration optimale pour le fonctionnement d'un TFET. Ainsi, les dispositifs basés sur ces hétérojonctions présentent des performances extrêmement élevées ( $SS < 5$  mV/dec et ON/OFF  $> 10^8$ ). De plus, deux architectures novatrices, le DBE-TFET et le UC-TFET ont été étudiées, et présentent des performances tout aussi impressionnantes. Elles permettent notamment de réaliser des dispositifs comportant un canal d'une longueur de moins de 5 nm, tout en préservant ces performances élevées.

Il est néanmoins important de rappeler que les interactions électron-phonon ne sont pas prises en compte dans ce travail, et que les performances sont donc observées dans le cas d'un transport parfait et balistique.



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# List of abbreviations

|                 |   |
|-----------------|---|
| <b>AFM</b>      | Atomic force microscopy                             |
| <b>BTBT</b>     | Band-to-band tunneling                              |
| <b>CB</b>       | Conduction band                                     |
| <b>CMOS</b>     | Complementary metal oxide semiconductor             |
| <b>CVD</b>      | Chemical vapor deposition                           |
| <b>DBE-TFET</b> | Drain-backgate-enhanced TFET                        |
| <b>DFT</b>      | Density functional theory                           |
| <b>DIBL</b>     | Drain-induced barrier lowering                      |
| <b>DITL</b>     | Drain-induced threshold lowering                    |
| <b>DOS</b>      | Density of states                                   |
| <b>FET</b>      | Field effect transistor                             |
| <b>ITRS</b>     | International technology roadmap for semiconductors |
| <b>LDOS</b>     | Local density of states                             |
| <b>LPE</b>      | Liquid phase exfoliation                            |
| <b>MBE</b>      | Molecular beam epitaxy                              |
| <b>MOSFET</b>   | Metal oxide semiconductor field effect transistor   |
| <b>NEGF</b>     | Non-equilibrium Green's function                    |
| <b>TFET</b>     | Tunnel field effect transistor                      |
| <b>TMD</b>      | Transition metal dichalcogenide                     |
| <b>TMC</b>      | Transition metal chalcogenide                       |
| <b>TMH</b>      | Transition metal halide                             |
| <b>UC-TFET</b>  | Ungated-channel TFET                                |
| <b>VB</b>       | Valence band  |
| <b>vdW</b>      | van der Waals                                       |
| <b>SCE</b>      | Short-channel effects                               |
| <b>SS</b>       | Sub-threshold swing                                 |

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# Outline

At the onset, the goal of my PhD work was to study electronic transport in nanoelectronic devices based on 2D materials and 2D material heterostructures. Important notions on nanoelectric devices and so-called 2D materials therefore need to be introduced and boiled down before delving into the actual research work I performed during the past three years.

In Chapter 1, a comprehensive history of the MOSFET, arguably the most important device in nanoelectrics, as well as its shortcomings and the limits of its scaling will be presented. One of the most promising contenders for the future of transistors -the TFET- will be discussed in detail, and the solutions it could bring to the transistor scaling issue will be outlined.

In Chapter 2, the aforementioned 2D materials will be presented, and the electronic and structural properties of a few of them will be detailed. Potential applications for these materials, as well as the main synthesis techniques used to grow and deposit them will then be discussed.

In Chapter 3, the models and methods used during my PhD work will be presented. More specifically, the tight-binding approach used to model the materials as well as the non-equilibrium Green's function formalism used to compute electronic transport through the devices and its implementation will be detailed.

Then, in Chapters 4-7, simulation results obtained for a variety of devices based on 2D materials will be presented and discussed. Among these devices are MOSFETs and TFETs, but also new device designs based on the standard TFET architecture that yield extremely promising results. In all cases, the influence of device parameters such as the materials used, channel length and more will be investigated.

Finally, a conclusion will summarize the main takeaways of this thesis work, and highlight the promising devices and results obtained. An outlook will also describe potential avenues to pursue this work further.





# Chapter 1

## Introduction to nanoelectronics

Nowadays, microprocessors are everywhere: from smartphones to traditional computers, from cars to rockets, from weighing scales to stoplights -among many other things-, they truly enable the creation of anything we consider to be “technological”. A case can therefore be made that the invention of the very building block of the microprocessor, the transistor, is one of the most important and impacting breakthroughs in human history.

### 1.1 History of transistors and nanoelectronics

In 1947 John Bardeen, William Shockley and Walter Brattain, three scientists working at Bell Telephone Laboratories, were studying the potential of germanium crystals as a replacement for the large, energy hungry, and unreliable vacuum tubes[2], [3] that were used in telecommunications to amplify voice and music. As the culmination of years of research, they finally succeeded[4]–[6] in creating the very first “point-contact” transistor, in which gold foils were deposited on a germanium crystal and successfully amplified an input signal, without the need for a lengthy heat-up time as was the case for vacuum tubes. This transistor was used in commercial products such as telephone exchanges and hearing aids as soon as 1952[2], but sensitivity to moisture and overall fragility would prevent it from being widely adopted[3], [4].



Figure 1. Left: John Bardeen, William Shockley and Walter Brattain.  
Right: the first point-contact transistor

During this time however, Schockley came up with an updated design for a transistor: the “bipolar junction” transistor. It relied on a “sandwich” NPN design and therefore on germanium doping to control current flow, and was far more robust than its point-contact counterpart[2]. This “sandwich” design was used in 1958 in the IBM 7070, the first computer based on transistors rather than vacuum tubes[4]. For their work and the invention of the transistor, Bardeen, Schockley and Brattain were awarded the Nobel Prize in 1956.

Around this time, an important shift happened in the transistor industry: instead of relying on germanium, transistor research and manufacture switched to silicon[2], [7]. Although germanium had several advantages[5], such as being less reactive than silicon, having a lower melting point which is helpful for manufacturing, as well as having superior carrier mobility, its drawbacks were too great. Its low band gap (0.67 eV compared to 1.12 eV for silicon) lead to high leakage currents, and the transistors simply did not work beyond 75°C. Another strong advantage of silicon that would be implemented later on is that its oxide ( $\text{SiO}_2$ ) can be easily grown to form an insulating layer with a high quality Si/ $\text{SiO}_2$  interface.

The first silicon transistor was reported by Texas Instruments, although Bell Telephone Laboratories had been working on similar technology for several years[5]. Silicon based electronics were thus born, and remain the dominating market force to this day. For several years, transistors were manufactured as individual components, before being assembled with other parts of the end circuit, such as resistors, capacitors diodes[2] ... However, this technique led to sprawling circuits that were challenging to assemble and increasingly unreliable[2], [5]. In 1958 Jack Kilby, an engineer at Texas Instruments, came up with a solution for this issue: create several transistors and other devices such as resistors from a single piece of semiconductor, therefore drastically reducing the size of the overall resulting circuit. The integrated circuit was born[2], [4], and Kilby was subsequently awarded the Nobel Prize in 2000 for this work.

The advent of the integrated circuit based on silicon transistors truly was the beginning of the computer revolution and, more broadly, of an electronics revolution. Since the late 1950s, radios, TVs and other consumer electronics devices based on transistors were commercialized, which only accelerated the growing interest in this technology. In 1960, John Atalla and Dawon Khang, researchers at Bell Telephone Laboratories, fabricated the first Field Effect Transistor[8] (FET), in which current flow is controlled by the electric field created by the gate. More precisely, these devices are referred to as Metal Oxide Semiconductor FETs (MOSFET), due to the materials used (metal for the gate, oxide for the insulating layer and semiconductor for the channel). Schockley and others had long anticipated[9] and worked on this transistor architecture, but never managed to fabricate it due to surface states preventing the electric fields from penetrating the semiconductor. This MOSFET architecture is the most commonly used in transistors to this day, and will be described in more detail in the next section.

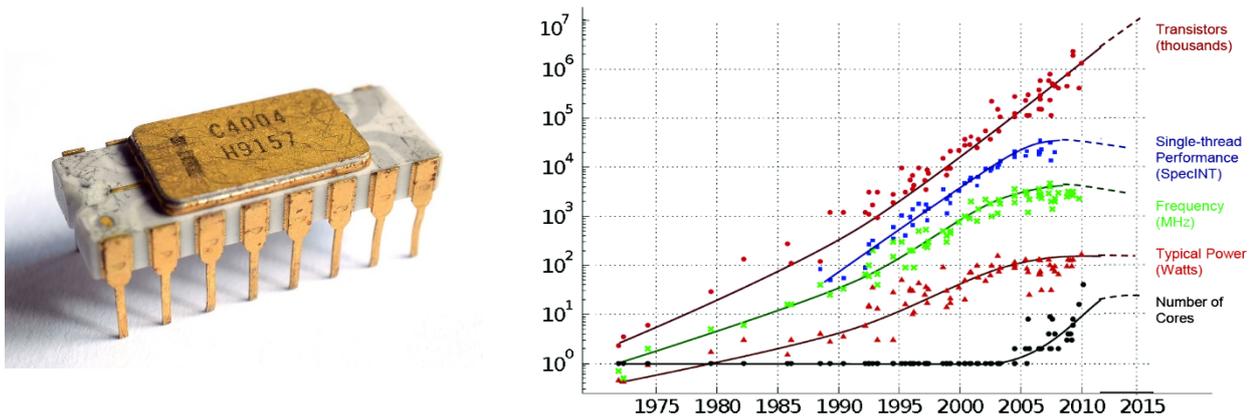


Figure 2. Left: Intel's 4004 microprocessor, composed of 2300 transistors. Right: evolution of performance indexes of microprocessors from 1971 to 2012 [10]

In 1965, Gordon Moore, then Director of R&D at Fairchild Semiconductors, published an article[11] predicting the amount of transistors in an integrated circuit would double every two years for the foreseeable future; this statement is now famously known as Moore's Law (although it has recently been slightly adapted) and ruled the industry ever since. Shortly thereafter, in 1968, Moore left Fairchild Semiconductors to form Intel Corporation, which would go on to invent the microprocessor in 1971 with its 4004 chip[12]. It was composed of 2300 transistors, had a clock speed of 108 kHz, and was as powerful as the 30-ton ENIAC computer from 1946 that filled an entire room. From there, Intel introduced new processors every couple of years which include[13] the 8086 chip in 1978 with 29 000 transistors, the 486 chip in 1989 with 1 200 000 transistors (the first generation with over 1 million transistors), or the Itanium 2 series 9000 in 2006 with 1.7 billion transistors. Since then, Intel has become the world's leading microprocessor manufacturer; however, AMD's Epyc microprocessor boasts the highest transistor count to date, with over 19.2 billion transistors[14].

So, in roughly 70 years, we have gone from large, single transistors, to packing over 19 billion transistors in areas below  $800 \text{ mm}^2$ . As far as microprocessors go, since 1971 and Intel's 4004 chip, clock speed has increased from 108 kHz in single core architecture to over 3 GHz in 32 core architectures, and the process size was reduced from  $10 \mu\text{m}$  to less than 15 nm.

The next section will focus on the device architecture that made it all possible, and that is at the core of every microprocessor used today: the MOSFET.

## 1.2 Metal Oxide Semiconductor Field-Effect Transistor (MOSFET)

As mentioned in the previous section, MOSFETs are the prevailing type of transistors used in electronics, and they have been for roughly 60 years since their initial fabrication by Bell Telephone Laboratories in 1960[8]. As its name suggests, a MOSFET is mainly composed of a metal gate, separated from a semiconductor body by a thin, insulating oxide layer, and as is the case for all FETs, the electric field created by the gate controls current flow in the device.

### 1.2.1 Working principle of a MOSFET

The working principle of an inversion mode, n-type MOSFET is shown in Figure 3 a). A semiconductor (usually silicon) makes up the body of the device, and is doped in a specific way: the source and drain region, where the electrical contacts are located, are n-doped (which means they carry excess electrons), whereas the rest of the device -and therefore the channel region, located in between the source and drain- is p-doped (which means it is lacking electrons, or has excess holes).

A constant, positive voltage  $V_{DS}$  is applied between the source and the drain, while a varying voltage  $V_G$  is applied to the gate.

In the OFF state (when no or very low voltage is applied to the gate) no current flows from source to drain due to the p character of the channel.

In the ON state however (when a high enough voltage is applied to the gate) the electric field it generates in the semiconductor, through the oxide, creates an n-type inversion channel through which electrons can flow freely from the source to the drain.

Depletion mode n-type MOSFETs have a similar working principle, with a key difference: the channel is n-doped, like the contacts. Therefore, current flows freely from the source to the drain when no gate voltage is applied, and a negative gate voltage is necessary to stop current flow through the channel.

In p-type MOSFETs,  $V_{DS}$  is negative and all doping is reversed: the contacts are p-type, the body n-type, and a negative (positive) voltage has to be applied to the gate to allow current flow in inversion (depletion) mode. In this case, the current carriers are not electrons, but holes.

When an n-type MOSFET and a p-type MOSFET operate in a complementary way, a CMOS (Complementary MOS) device is created; CMOS can be used to create inverters or NAND (Not AND) and NOR (which are the basic functions of logic operations in a circuit) and is therefore extremely useful.

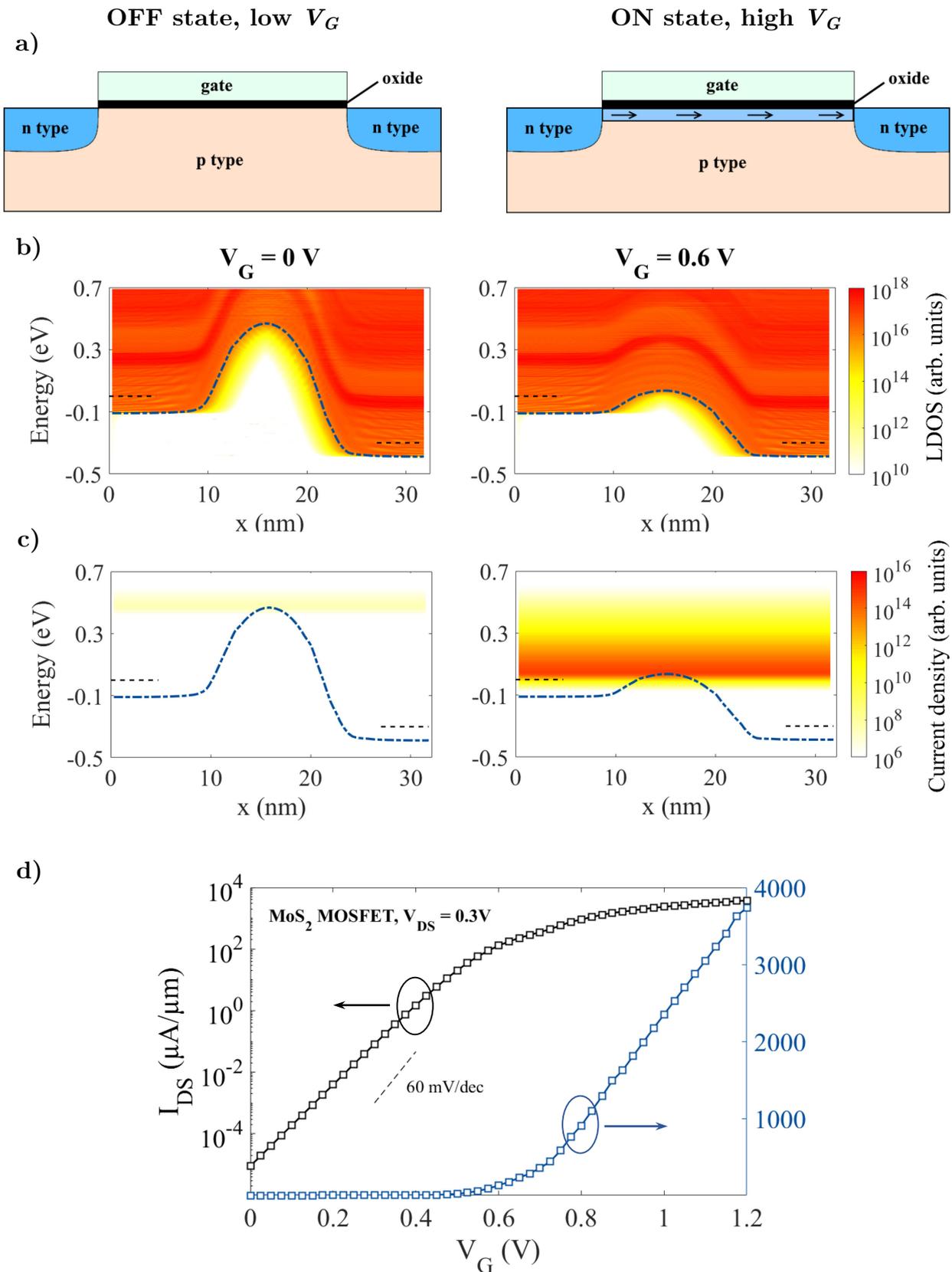


Figure 3. a) Sketch of an n-type, inversion mode MOSFET in the OFF (left) and ON state (right). b) Local density of states in a MoS<sub>2</sub> MOSFET in the OFF (left) and ON state (right). The dotted blue line represents the lowest conduction band, and the dotted black lines the Fermi levels in the source and drain. c) Current density in the same device. d) Current characteristics of the device at  $V_{DS} = 0.3$  V.

Because electrons are Fermions, their distribution along the available energy states is controlled by the Fermi-Dirac distribution given in Eq.(1)

$$n(E) = \frac{1}{e^{E-\mu/k_B T} + 1} \quad (1)$$

where  $n(E)$  is the probability that the level at energy  $E$  is occupied,  $\mu$  is the Fermi level in the device,  $k_B$  is the Boltzmann constant ( $k_B = 1,3806 \times 10^{-23}$  J.K<sup>-1</sup>) and  $T$  is the temperature in Kelvin.

As is shown in Figure 4, temperature has a high impact on the energy states that might be populated. At  $T = 0$  K, all states below the Fermi level are occupied, and all states above it are empty; as the temperature increases however, electrons gain thermal energy ( $k_B T$ ) and might leave states below  $\mu$  to populate states above it. At  $T = 500$  K for instance, electrons might populate states up to 0.25 eV above the Fermi level. However, no matter the temperature, the occupation probability at  $E = \mu$  is always 0.5.

In MOSFETs, as is the case in all other transistors, the Fermi level in the contacts in eV is dictated by the drain voltage.

$$\mu_S = 0 \quad \mu_D = -eV_{DS} \quad (2)$$

The level of the conduction band in the source and drain, while influenced by  $V_{DS}$ , also depends on the level of doping in the contacts. The height of the energy barrier imposed by the gate when  $V_G = 0$  V depends on the Fermi energy of the metal and the affinity (the bottom of the lowest conduction band compared to the vacuum level) of the material used. Therefore, only by carefully selecting the doping applied to the semiconductor, the material to use as a gate, and the drain current can a functioning MOSFET be achieved.

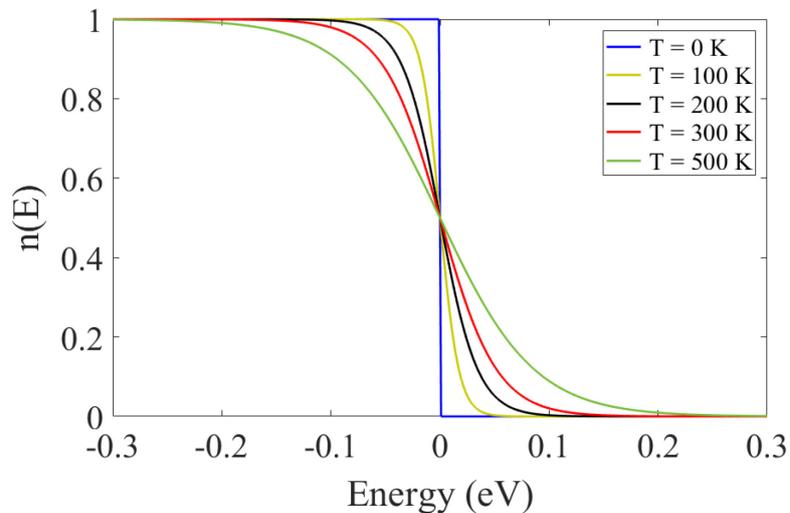


Figure 4. Fermi-Dirac distribution for  $\mu = 0$  eV at temperatures ranging from 0 to 500 K.

To characterize the performance of a transistor, several metrics are often used. The current ratio (ON/OFF) is the most prevalent.  $I_{OFF}$  is calculated either at  $V_G = V_{OFF} = 0$  V, or given a fixed value ( $10^{-5}$   $\mu\text{A}/\mu\text{m}$  for instance), in which case  $V_{OFF} = V_G(I_{OFF})$ .

The ON current,  $I_{ON}$ , is then calculated at  $V_{ON} = V_{OFF} + V_{DD}$  with  $V_{DS} = V_{DD}$ . The goal is to maximize  $I_{ON}$  while minimizing  $I_{OFF}$ , and therefore to yield a high  $I_{ON}/I_{OFF}$  ratio. The sub-threshold swing ( $SS$ ) is another important figure of merit. It describes the steepness of the current slope in the sub-threshold regime in log scale (from  $V_G = 0$  V to 0.4 V in Figure 3 d) for instance) and is calculated[15] as

$$SS = \left( \frac{\partial \log(I_{DS})}{\partial V_G} \right)^{-1} \quad (3)$$

between two fixed  $I_{DS}$  values (such as  $10^{-5}$  and  $10^{-2}$   $\mu\text{A}/\mu\text{m}$ ).  $SS$  is given in mV/dec, because it describes the increase in gate voltage necessary to increase the current ten-fold. Due to the aforementioned Fermi-Dirac distribution electrons are bound to, the thermionic effect occurring in MOSFETs entails a hard lower limit of 60 mV/dec at 300 K, as is detailed in Eq.(4)

$$SS_{MOSFET-min} = \ln(10) \times \frac{k_B T}{e} = 60 \text{ mV/dec} \quad (4)$$

Switching frequency, drain-induced barrier lowering (DIBL) and other electric characteristics have to be taken into account when designing MOSFETs, as some applications will result in strict guidelines to be followed[16]–[21].

## 1.2.2 Moore's Law and initial MOSFET scaling

As mentioned earlier, Moore's Law (stated in 1965 but slightly revised since) predicted that the amount of transistors in an integrated circuit would double roughly every two years. In order to abide by this prediction, all of the dimensions of a MOSFET had to be scaled down aggressively along the years. For instance, oxide thickness was reduced[22] from over 250 nm to roughly 15 nm between 1975 and 1990, and gate length was reduced from over 20  $\mu\text{m}$  to 1  $\mu\text{m}$  in the same timeframe, all the while making MOSFETs faster and less power-consuming. However, with such aggressive scaling, issues related to gate length and oxide thickness such as source to drain tunneling and leakage currents arose and were in part solved via the evolution of the structure of MOSFETs: first, Silicon On Insulator (SOI) MOSFETs were introduced[23], [24]. Silicon dioxide ( $\text{SiO}_2$ , same as the gate oxide) is buried in between the silicon substrate and the Si channel, and only a very thin channel of silicon is deposited above it, between the contacts.

This new structure (shown in Figure 5 a)) allowed for far lower leakage currents (and therefore lower  $I_{OFF}$ ), higher performance than regular MOSFETs at similar supply voltages[25], and for the elimination of latch-up (a specific type of short-circuit). However, the thick, buried silicon dioxide layer hampers the evacuation of the heat created by transistor operation. Nonetheless, SOI technology allowed MOSFET scaling to continue, and oxide thicknesses and channel length to be reduced even further.

In the late 1990s[26], double-gate MOSFETs (and beyond) were introduced[27], [28], as a way to enhance the electrostatic control in the channel and remedy most short-channel effects (SCE), such as carrier velocity saturation, high DIBL and others[29], [30] ... Thanks to this new structure, carriers in the whole channel could be controlled by the gates, mainly allowing for  $I_{OFF}$  reductions as well as overcoming most SCE. The FinFET[27], [28], [31], a device in which the channel is composed of a thin silicon “fin” and surrounded by several gates (shown in Figure 5 b) and c)) is the most common type of multiple-gate MOSFET. It is still currently used in the 10 nm processes of chip manufacturers such as Intel or Samsung, as it allows for shorter channels and lower  $SS$  than regular MOSFETs. In this case, specific parameters to this design such as the fin height, fin width and fin pitch in the case of multi-finger FinFETs (see Figure 5 c)), impact FinFET performance.

Another technological breakthrough that allowed the continued scaling of MOSFETs was the advent of the high- $\kappa$  dielectric[32]. Until then, only  $\text{SiO}_2$  had been used as a gate oxide, due to its inherent compatibility with silicon. However, as gate oxide thickness decreased, gate tunneling leakage currents increased and hampered device performance.

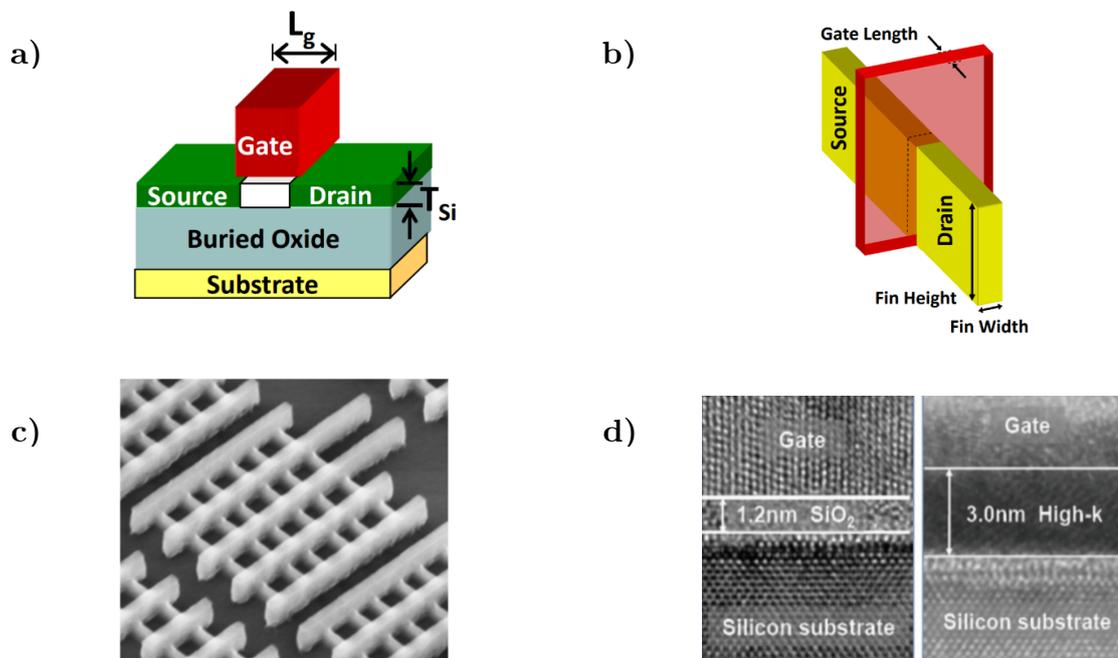


Figure 5. a) Sketch of a SOI MOSFET. b) Sketch of a FinFET. c) SEM image of a multiple-finger FinFET d) Comparison between  $\text{SiO}_2$  and a high- $\kappa$  dielectric as a gate oxide [31], [33].

So called “high- $\kappa$  materials” have a higher dielectric constant than  $\text{SiO}_2$  ( $\kappa_{\text{SiO}_2} = 3.9$ [34], [35]) and can therefore provide more capacitance for the same thickness. Thicker high- $\kappa$  dielectric layers can therefore be used to prevent gate leakage, while increasing gate control over the channel; the thickness of most oxide layers is therefore now referred to as their Equivalent Oxide Thickness (EOT), calculated as

$$EOT = t_{\text{high-}\kappa} \times \frac{\kappa_{\text{SiO}_2}}{\kappa_{\text{high-}\kappa}} \quad (5)$$

Hafnium oxide, for instance, is one of the most commonly used high- $\kappa$  dielectrics and has a  $\kappa = 20$  [33] ; a 5 nm  $\text{HfO}_2$  layer is therefore as efficient as a 1 nm  $\text{SiO}_2$  layer in terms of gate capacitance, but reduces gate leakage currents up to a factor of  $10^4$  thanks to a thicker insulating stack.

Several other techniques and designs (such as the use of strained silicon[36], [36]–[38], or a silicon-germanium alloy[39], [40] in the channel for instance) were theorized and put into use over the years, but are not detailed here for concision purposes.

Through the years and the technological nodes, from 1971 and 20  $\mu\text{m}$  processes to 2018 and 7 nm processes, these various adjustments and modifications to MOSFET design allowed the industry to more or less abide by Moore’s Law.

However, as we look into the future of nanoelectronics, several fundamental issues and challenges related to the MOSFET’s mode of operation and the properties of silicon cast doubt on the possibility for this aggressive scaling trend to continue unabated. That is, unless a truly industry-changing paradigm shift occurs.

## 1.3 The power scaling challenge

The techniques mentioned in the previous section allowed for a mitigation of the negative effects that come with MOSFET scaling (SCE such as DIBL, gate leakage ...), but these effects remain an issue and a strong hindrance to further scaling[41]–[43].

The main limiting factor currently faced by the transistor industry is power scaling: thanks to the downsizing of MOSFETs, more transistors can be crammed into a smaller area with each generation, which allows for higher performing microprocessors for instance. However, in doing so, the power dissipated by unit area vastly increases and can prevent the transistors from operating properly. A scaling in dissipated power per transistor is therefore badly needed, but has eluded the industry for over a decade[44], [45].

In a MOSFET, the power consumption is evaluated as shown in Eq.(6), and can be broken down in two parts: dynamic power consumption (when the device is ON) and static power consumption (when the device is OFF).

$$P = \underbrace{C_L \cdot f_c \cdot V_{DD}^2}_{\text{Dynamic}} + \underbrace{I_{OFF} \cdot V_{DD}}_{\text{Static}} \quad (6)$$

Where  $V_{DD}$  is the supply voltage,  $C_L$  is the load capacitance and  $f_c$  the operating clock frequency of the device. It is plain to see that both dynamic and static power consumption are highly dependent on the supply voltage, and  $V_{DD}$  scaling is therefore the most effective way to decrease the power consumed by a CMOS circuit. However,  $V_{DD}$  scaling is easier said than done, because both the supply voltage and the threshold voltage ( $V_T$ ) are intrinsically tied to each other and to the performance of the transistor.

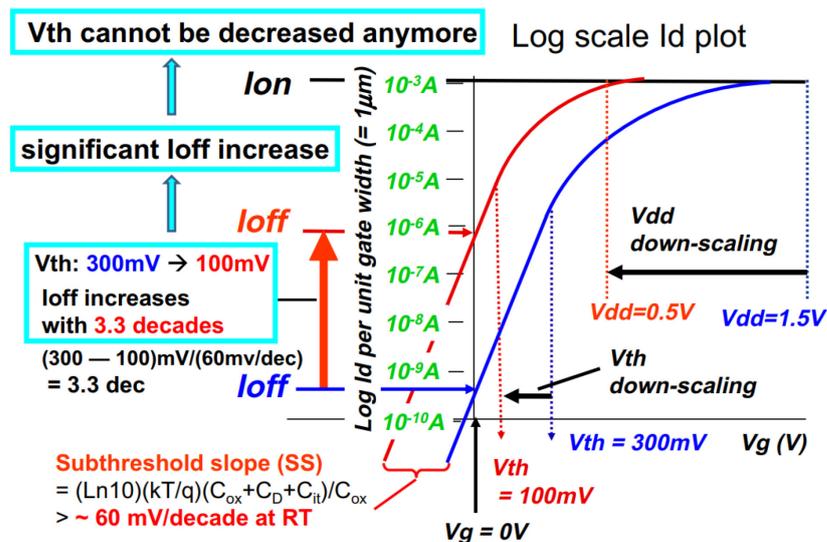


Figure 6. Increase in  $I_{OFF}$  due to a reduction of  $V_{DD}$  and  $V_T$ [43].

In order to decrease  $V_{DD}$  and maintain  $I_{ON}$ ,  $V_T$  has to be reduced. However, by decreasing  $V_T$ , the OFF current (current at  $V_G = 0$  V) is strongly increased, as shown in Figure 6. Because this is due to the high  $SS$  ( $> 60$  mV/dec) of MOSFETs, it cannot be circumvented and has kept  $V_{DD}$  scaling from keeping up with other aspects of MOSFET scaling such as channel length, oxide thickness... What's more, this inability to scale the supply voltage at the same rate as the other characteristics of the device actively hampers performance[42], [44]: the strong electric fields generated by the high supply voltage cannot be dealt with properly by the shorter channels for instance, which increases DIBL and can cause barrier breakdown.

In an effort to limit power consumption,  $V_{DD}$  has nonetheless been scaled down as much as possible, down to approximately 1 V since the mid-2000s[46]. As a result, static power consumption has accounted for over 50%[47] of the dissipated power since the 45 nm node; the bulk of the power consumed by today's transistors therefore occurs when they are turned off.

This trend obviously cannot continue, and new approaches are therefore required to pursue transistor scaling further.

Two main types of approaches are possible:

- MOSFET based on new materials: most transistors manufactured and used today are based on silicon. The use of higher mobility materials in the channel could increase device performance and allow for the use of lower supply voltages without degrading  $I_{ON}$ . Silicon-germanium alloys[39], [40], as well as III-V semiconductors[48]–[51] (such as InAs, InGaAs, GaAs...) and their heterostructures hold some potential in this regard. Another possibility is the use of 2D materials[41], [52], [53] (only one atom thick) such as graphene for instance, to take advantage of their properties and the vastly different physics their 2D structure allows. These materials and their possible applications will be detailed in Chapter 2.
- New device architectures: other kinds of FETs hold potential for power supply scaling beyond the limits of regular MOSFETs. The inability to scale  $V_{DD}$  any lower in MOSFETs originates from their gradual current increase in the sub-threshold regime; therefore, devices presenting a much steeper turn-on transition (and therefore a far lower  $SS$ ) hold potential for ultra-low power operation. While some architectures such as the piezoelectrical FET[54], [55] the electro-mechanical FET[55], [56] and the negative capacitance MOSFET based on ferroelectric gate stacks[57]–[59] have shown promise for specific applications, the Tunnel FET (TFET) has by far been the most investigated and developed concept in the last fifteen years[46], [55], [60], [61] thanks to its versatility compared to other steep-slope devices.

In the next section, the core concepts and working principle of TFETs will be discussed, as well as the advantages (and shortcomings) of this transistor design compared to traditional MOSFETs.

A quick review of the state-of-the-art in TFET technology will also be presented.

## 1.4 Tunnel Field Effect Transistor (TFET)

While MOSFETs are the prevailing types of transistor, Si-based MOSFET scaling is slowing down and seems to be reaching its limits, due to increasingly high dissipated power per unit area and the inability to provide satisfactory performance at low supply voltages. TFETs are one of the most promising avenues for ultra-low power operation identified by the international technology roadmap for semiconductors (ITRS)[16].

### 1.4.1 Working principle of a TFET

From a structural standpoint, TFETs are no different from MOSFETs. A TFET is made up of source and drain contacts separated by a channel area, over which are deposited a thin insulating layer and a gate that will control current flow. The source and drain are doped differently, unlike in the case of MOSFETs.

From an operating principle standpoint however, TFETs are vastly different from MOSFETs. They don't rely on an energy barrier to overcome, but, as their name suggests, on band-to-band-tunneling (BTBT), which frees them from the 60 mV/dec  $SS$  lower limit that constrains MOSFET technology.

The sketch of an n-type TFET and its operating principle are shown in Figure 7 (a). In an n-type TFET, the source is p-doped and the drain n-doped, while the channel is not doped (pristine material).

Just like in a MOSFET, a constant, positive supply voltage  $V_{DS}$  is applied to the source and drain and sets the Fermi energies  $\mu_S$  and  $\mu_D$ , while a varying gate voltage  $V_G$  controls current flow in the device.

In the OFF state (as shown in Figure 7 (b) and (c)) -when no or low  $V_G$  is applied-, carriers in the source valence band (VB) are contained to the source because no energy states are available to them in the channel, and because the distance to tunnel straight from the source VB to drain conduction band (CB) is too high.

In the ON state (as shown in Figure 7 (b) and (c)), the electric field generated by the high  $V_G$  brings the channel CB down into the same energy range as the source VB. Carriers are therefore able to tunnel from the source VB to the channel CB, and current can flow between the source and the drain.

In a p-type TFET, the doping is reversed: the source is n-doped while the drain is p-doped. A constant, negative  $V_{DS}$  is therefore applied to the contacts, and a highly negative gate voltage  $V_G$  is necessary to bring VB states in the channel up into the energy range of the source CB states. In this case, carriers tunnel from the source CB to the channel VB. Only lateral TFETs are discussed in this work, but vertical TFETs (in which the channel is composed of overlapping layers) are also being heavily investigated.

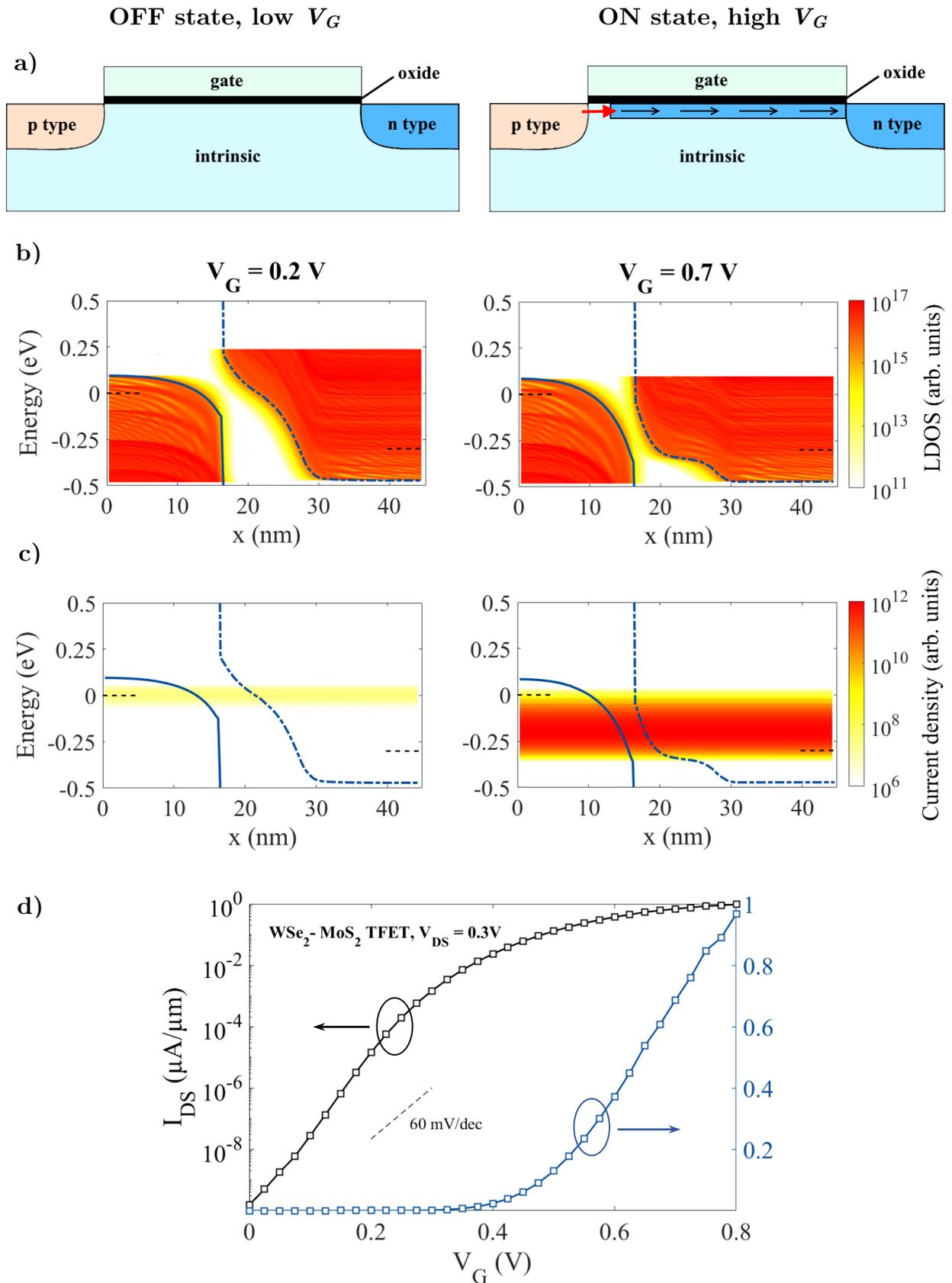


Figure 7. a) Sketch of an n-type TFET in the OFF (left) and ON state (right). b) Local density of states in a  $\text{WSe}_2$ - $\text{MoS}_2$  (strained) TFET in the OFF (left) and ON state (right). The dotted (full) blue line represents the lowest CB (highest VB), and the dotted black lines the Fermi levels in the source and drain. c) Current density in the same device. d) Current characteristics of the device at  $V_{DD} = 0.3$  V.

Much like in a CMOS device, a p-type TFET and an n-type TFET can operate in a complementary way in order to create inverters and NAND gates for instance, which are the basic functions for logic operations.

Two types of lateral TFETs can be distinguished: homojunction TFETs and heterojunction TFETs.

- In a homojunction TFET the source, channel and drain are all composed of the same material (see Figure 8 (b)). A low band gap is therefore needed, as it is directly correlated to the length of the depletion region (the length through which the carriers will tunnel). If the band gap is too low however, a true OFF state will never be reached; finding the appropriate material is therefore very challenging.
- In a heterojunction TFET, at least two different materials are used. Most often, one material is used in the source, and the other in the channel and drain, thus creating an interface where the tunneling will occur. With this heterojunction approach, each material's individual band gap does not matter anymore; rather, the band alignment of those materials compared to one another is the most important parameter. For instance, in the case of an n-type TFET, using a material with a high VB in the source and another with a low CB in the channel and drain will be highly beneficial, as this favorable band alignment (known as a staggered gap) will reduce the length of the depletion region to be tunneled. These heterojunction devices are however more challenging to simulate and produce, due to the strains and lattice reconstructions imposed by the interface.

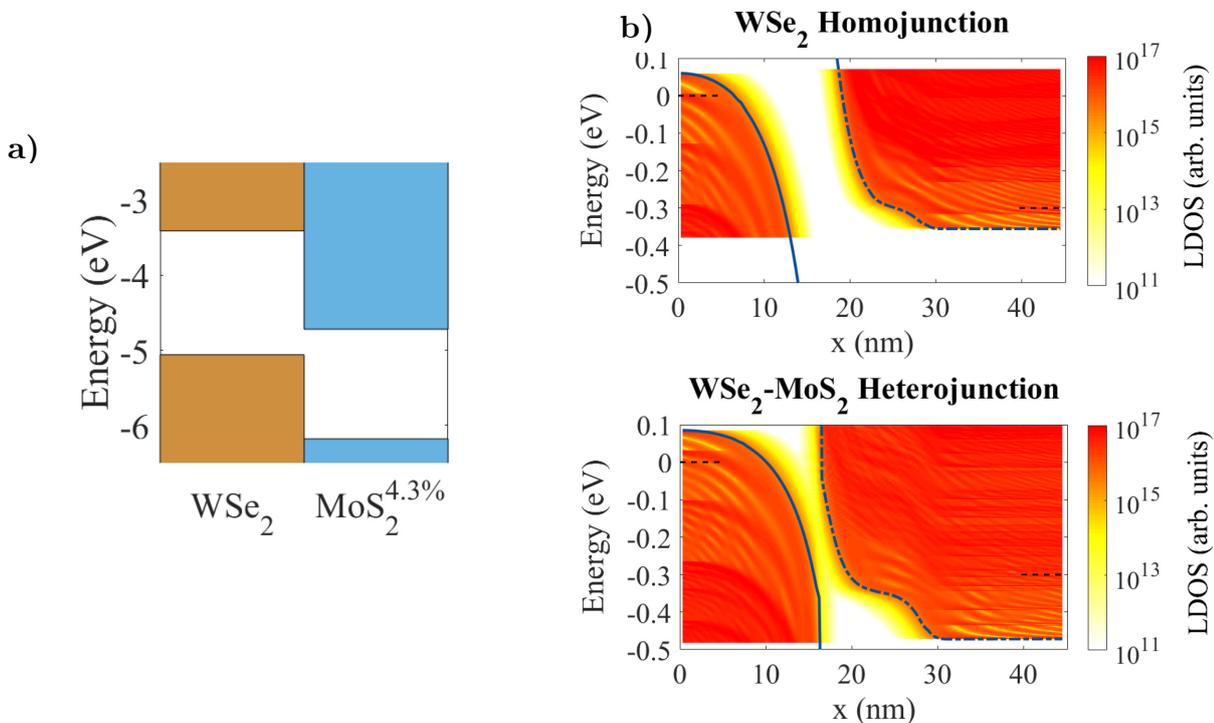


Figure 8. a) Band alignment for WSe<sub>2</sub> and MoS<sub>2</sub> (under a 4.3% tensile strain). b) LDOS of a WSe<sub>2</sub> homojunction TFET in the ON state; the depletion region is roughly 10 nm long. c) LDOS of a WSe<sub>2</sub>-MoS<sub>2</sub> (strained) heterojunction TFET in the ON state; the depletion region is less than 5 nm long.

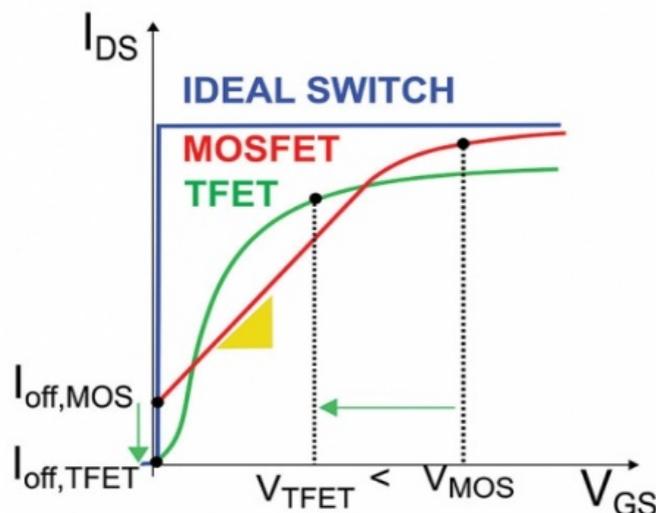


Figure 9. Typical current characteristic for a TFET (green), a MOSFET (red), and an ideal switch (blue).

Thanks to their BTBT injection mechanism (rather than the thermionic injection found in MOSFETs), TFETs have no lower limit for  $SS$ : because the carriers come from the top of the source VB, the band gap of the source material acts as an energy filtering mechanism and cuts the tail of the Fermi-Dirac distribution.

Theoretically, a properly designed TFET could therefore go from a fully OFF state ( $I_{DS} \leq 10^{-5} \mu\text{A}/\mu\text{m}$ ) to a fully ON state ( $I_{DS} \geq 10^3 \mu\text{A}/\mu\text{m}$ ) with less than a 0.1 V increase in gate voltage; to perform the same transition, a perfect 60 mV/dec MOSFET would require at least a 0.5 V increase. However, because TFETs rely on tunneling through a bandgap of finite (real space) thickness, the maximum currents they can yield are often lower than that of similar MOSFETs.

Typical current characteristics for a MOSFET and a TFET are shown in Figure 9 and exemplify the typical behavior of each device: MOSFETs switch gradually from the OFF to the ON state but yield high ON current, while TFETs present a much steeper slope in the sub-threshold regime and yield lower current, but reach saturation at lower gate voltages. Finally, an ideal switch would go from a fully OFF state to a fully ON state with only an infinitesimal increase in  $V_G$ , and would yield extremely high  $I_{ON}$ .

Now that the operating principle and main characteristics of the TFET have been introduced, I will briefly discuss the history the device, and its current state-of-the-art.

## 1.4.2 History and current state of the TFET

The origin of the TFET can be traced back to 1978, when Quinn *et al.* [62] proposed to modify a MOSFET with a highly degenerate p-doped source. Later, in 1992[63], this design was realized based on GaAs, and named the surface tunnel transistor (STT) and was reported to exhibit transistor characteristics at room temperature. In the following years, TFETs based on silicon, SOI substrates, and InGaAs on InP substrates were reported[64]–[66]; however, in those early days the focus of TFETs wasn't their potentially low  $SS$ , but the possibility to control negative differential resistance (NDR) via the gate.

It was not until 2004 that discussion about the low- $SS$  potential of TFETs started to gain traction[67]–[70] and ushered new interest in these devices. Since then, and due to the foreshadowing of the end of Si MOSFET scaling due to power consumption issues, interest in TFETs (along other steep-slope devices) has been growing rapidly.

By 2010, sub-60 mV/dec TFETs based on Si[71]–[73], Ge[74] and carbon nanotubes (CNT)[67], [75] had been reported.

Since its invention, the TFET structure has, much like the MOSFET structure before it, been tuned and modified to enhance device performance. Multiple-gate TFETs such as double-gate TFETs[76]–[78] and gate-all-around (GAA) TFETs[78], [79] have been reported to strongly enhance performance, namely increasing  $I_{ON}$  while decreasing  $I_{OFF}$  and  $V_T$ . In order to more precisely control the bands along the devices, structures such as dual material gates[80] (the gate material changes depending on the position along transport direction) and dual gate oxides[81] (the gate oxide changes depending on the position along transport direction) have been investigated.

In the last ten years, homojunction TFETs based on a wide variety of materials have been investigated: from Si[71], [72], [82], [83], Ge[74], GeSn[84], strained SiGe[85] to III-V semiconductors such as InGaAs[86], [87] and InAs[88], [89], some of which yielded relatively high ON currents and sub-thermal  $SS$ . The same cannot be said of heterojunction TFETs based on III-V semi-conductors such as AlGaSb/InAs[90], InAsSb/GaSb[91], InAs/GaSb[92], and others; these tend to achieve very high ON currents in exchange for  $SS$  far beyond 60 mV/dec.

More recently, theoretical studies of TFETs based on 2D materials have multiplied, due to the high interest garnered by those materials since the isolation of graphene in 2004[93]. Due to their one-atom thick structure, 2D materials have a host of advantages compared to their bulk counterparts; they are for instance free of dangling bonds and have a lower concentration of traps and roughness at the interface, which favor  $SS$ [94]–[96].

Vertical TFETs based on 2D materials such as graphene[97], [98] and transition metal dichalcogenides have been reported[99]–[101], some of which have shown potential for extremely low-power operation ( $V_{DD} < 0.1$  V) thanks to sub-20 mV/dec  $SS$  and high  $I_{ON}$ .

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Many lateral TFETs based on 2D materials have also been reported. Transition metal dichalcogenides, thanks to their direct band gap, are the most commonly used materials, and have shown great promise via low  $SS$  and relatively high  $I_{ON}$  both in homojunction[102], [103] and heterojunction TFETs[104]–[106]. Promising performance has also been reported for TFETs based on few-layer phosphorene[107],  $\text{Bi}_2\text{Se}_3$  [108], and carbon nanotubes[109], [110] for instance.

Thanks to the unique advantages they offer compared to Si-based MOSFETs, for which the end of scaling is rapidly approaching, TFETs are uniquely positioned to take up the mantle and enable ultra-low power operation in nanoelectronics.

For this reason, TFETs are one of the hottest topics in transistor research today, and are at the center of this work.

# Chapter 2

## Introduction to 2D materials

### 2.1 History and characteristics of 2D materials

The first experimental isolation of graphene (by Geim and Novoselov in 2004[93]) and the subsequent demonstration of its extremely attractive properties ushered the golden age of 2D material research in all areas of physics; from condensed matter research to material science, mechanical engineering and nanoelectronics just to name a few.

Graphene suddenly became of extremely high interest, as can attest the exponential growth of the number of studies about graphene (shown in Figure 10), and even though the initial excitement over graphene has somewhat steadied over the past couple of years, it will most likely find its way into industrial use. However, the excitement ignited by graphene extended to all 2D materials, of which many were discovered and isolated in the following years.

While hexagonal boron nitride (h-BN) and transition metal dichalcogenides (TMDs) are the most commonly studied of those materials, research focused on many others such as silicene, germanene, black phosphorus and group-III mono-chalcogenides for instance, is being pursued in order to report and classify their properties.

The term “2D material” is quite vague considering the breadth of the properties of the materials classified as such. Some of them are semi-metals, some are insulators, some are semiconductors (with narrow to wide band gaps), some exhibit in-plane anisotropy[111]–[113] while others do not ... The one thing all 2D materials have in common is weak interlayer bonding due to van der Waals interactions, and strong intralayer covalent bonding. This weak interlayer bonding allows (in most cases) for mechanical exfoliation of a few layers or even a single layer -via the scotch tape method used to isolate graphene in 2004 for instance-; many research teams are therefore able to access 2D materials and study their properties.

From their atomic thickness also come several traits found across many 2D materials:

- Flexibility and elastic properties: most 2D materials exhibit exceptionally high mechanical properties. In 2008, a Young’s modulus of 1 TPa and a breaking strength of 130 GPa were reported for graphene[114], while a similar study on MoS<sub>2</sub> reported a Young’s modulus above 200 GPa and a breaking strength of 27 GPa[115] which remains remarkable.

In-plane strains exceeding 20% are required to break those materials, making them extremely promising for potential use in flexible electronics for instance.

- Possibility of creating heterostructures with clean interfaces: their atomic thickness allows 2D materials to be either combined in-plane or stacked out-of plane in order to create heterostructures. By doing so, it is possible to drastically modify the properties of the structure, or protect it from its environment; for instance, the encapsulation of an air-sensitive material between two h-BN layers helps prevent degradation. In the case of in-plane heterojunctions, the absence of the out-of-plane dangling bonds[46] found in bulk materials allows for a much cleaner interface with far fewer traps and defects.

Due to the breadth of those properties, applications spaces for 2D materials are extremely broad and the main areas of focus of current academic research are therefore to classify those materials, determine the limits of their performance, and develop the growth and deposition techniques needed to integrate them in future devices. For instance, although the electron mobility is extremely high in graphene, the absence of a band gap prevents its use for logic applications, and the relatively low mobility in TMDs make them poor candidates for MOSFET technology. There is therefore a necessity to study those materials and determine the best possible use of their properties, while avoiding their inherent setbacks; once the appropriate application will have been determined, the tall order of scaling up and maturing the resulting technology will remain.

In this chapter, I will present the crystal structure and electronic properties of several 2D materials, before briefly outlining some of their potential applications in nanoelectronics and optoelectronics and the state of the art deposition and growth techniques related to them.

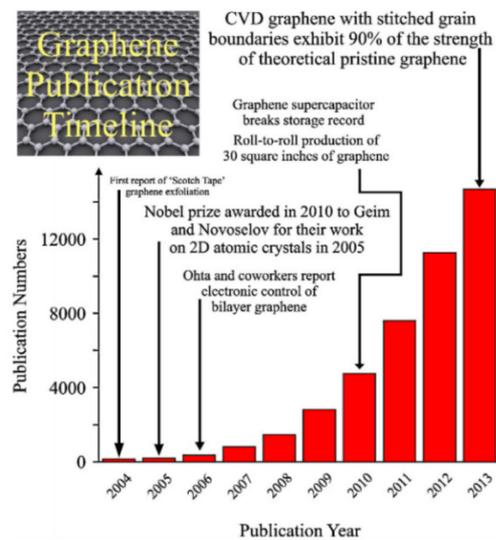


Figure 10. Number of publications about graphene per year, from 2004 to 2013, from [116].

## 2.2 Properties of 2D materials

### 2.2.1 Graphene

As mentioned above, graphene is the origin of today's interest in 2D materials. This can be attributed to the fact that many of its properties are best in class: unparalleled mechanical stiffness, strength and elasticity, as well as supreme electrical and thermal conduction[52]. However, some of its inherent drawbacks, such as the absence of a band gap, will force technology to adapt to graphene and complicate its integration.

#### 2.2.1.1 Crystal structure

Graphene is a one-atom-thick sheet of honeycomb arranged  $sp^2$  hybridized carbon atoms with a lattice constant of  $a_G = 2.46 \text{ \AA}$ , which itself can be divided in two sublattices. The C-C bonds are separated by an angle of  $120^\circ$ , and have a length of  $d_{C-C} = 1.42 \text{ \AA}$ [117].

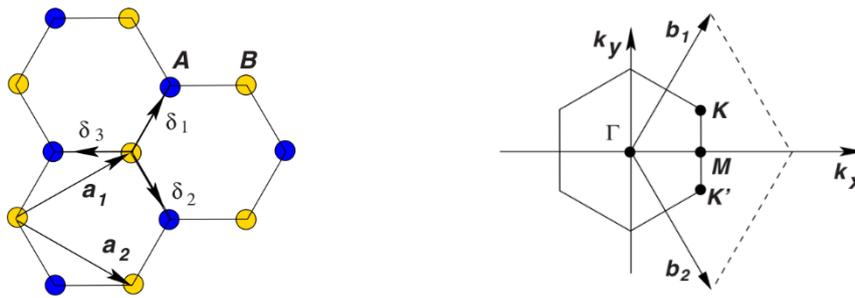


Figure 11. Left : Lattice arrangement of graphene in which  $a_{1,2}$  are the lattice unit vectors and  $\delta_{1,2,3}$  are the nearest neighbor vectors. Right : first Brillouin zone of graphene[118].

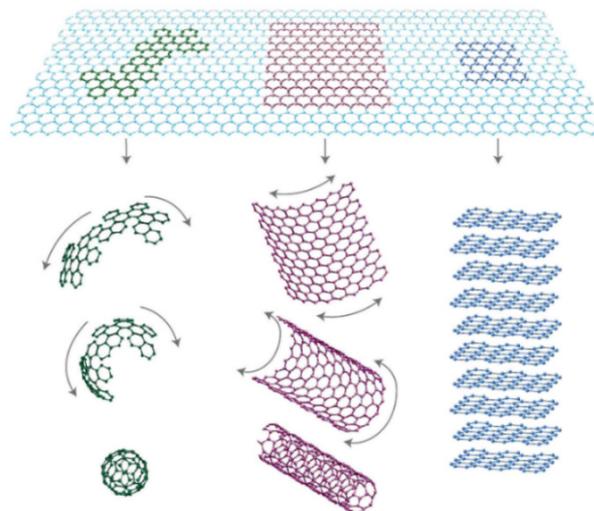


Figure 12. Graphene (top) and related structures: fullerene (left), carbon nanotube (center) and graphite (right) [119].

As presented in Figure 12, graphene is the basis for many carbon allotropes such as graphite (stack of graphene sheets), fullerenes (graphene sheet rolled up into a ball) and carbon nanotubes (graphene sheet rolled up into a tube).

Now that I have briefly described the crystal structure of graphene, I will present its electronic properties which, along with its mechanical and optical properties, make it one of the most interesting materials currently available.

### 2.2.1.2 Electronic and transport properties

Due to its atomic arrangement, the electronic dispersion of graphene presents cones at the  $K$  and  $K'$  points of the first Brillouin zone, where the valence and conduction bands meet (see Figure 13). At those wave vectors, the dispersion increases linearly with the energy, which mimics the physics of quantum electrodynamics for massless fermions. Although they move with a velocity approximately 300 times smaller than the speed of light, those electrons are therefore referred to as “massless Dirac fermions”. This behavior allows for specific rare phenomena to occur in graphene, such as the integer quantum Hall effect that was observed experimentally[120], and the possibility for Klein tunneling, a non-relativistic process in which the transmission through a potential barrier may be almost perfect and non-dependent on barrier height or length[118].

This linear dispersion allows graphene to present extremely high carrier mobility, beyond  $200\,000\text{ cm}^2.\text{V}^{-1}.\text{s}^{-1}$ [121] -compared to  $1400\text{ cm}^2.\text{V}^{-1}.\text{s}^{-1}$  in silicon- and a large critical current density of  $10^8\text{ A}.\text{cm}^{-2}$ [93]. However, the absence of a band gap induced by those Dirac cones greatly limits the potential of graphene for logic operation; without a band gap, a graphene transistor cannot be properly switched off and the resulting  $I_{ON}/I_{OFF}$  ratios are very low. With that said, high transconductance has been observed in large area graphene field effect transistors[122], which suggests they could be used for radio frequency and analog applications.

There are, however, several techniques to open up a bandgap in graphene, some of which are presented below:

- Bilayer graphene: by applying a transverse electric field to bilayer graphene (stack of two graphene layers), a band gap of width dependent on the applied voltage can be opened near the K-point [123], [124]. This band gap can span up to 250 meV, which is too low for most electronic applications.
- Graphene nanoribbons: by nanostructuring graphene into ribbons of a specific width, a band gap can be opened in graphene[118]. However, this is only possible in perfect armchair type nanoribbons for which the number of carbon dimers along the width is  $M = 3n$  or  $3n + 1$ ,  $\forall n \in \mathbb{N}$ . In this case, the width of the band gap is inversely proportional to the nanoribbon width, and extremely narrow GNRs are therefore required to obtain usable band gaps[125]. In the case of zigzag type nanoribbons, edge states prevent the opening of a band gap (see Figure 14).

However, while this behavior is observed in theory and perfect nanoribbons, edge disorder in experimental setups have shown a universal electronic behavior in graphene nanoribbons, no matter the ribbon orientation[126].

- Graphene nanomesh : by creating periodic defects in a graphene sheet, a band gap of up to 500 meV can also be opened [127]–[129]. However, controlling the exact shape and periodicity of the defects can prove challenging in an experimental setup.

Although graphene is the reason for today's tremendous interest in 2D materials, many other 2D materials exhibit interesting properties and could potentially find their use in future devices. TMDs -which I will now present- are, apart from graphene, one of the most studied class of 2D materials.

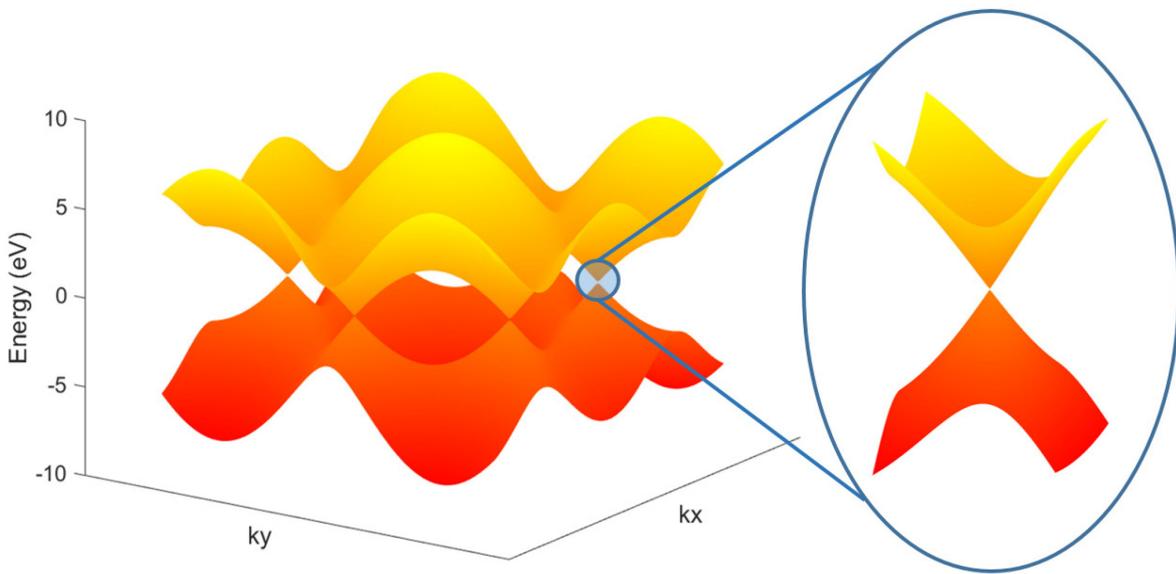


Figure 13. Electronic band structure of graphene, and zoom on one of the Dirac points.

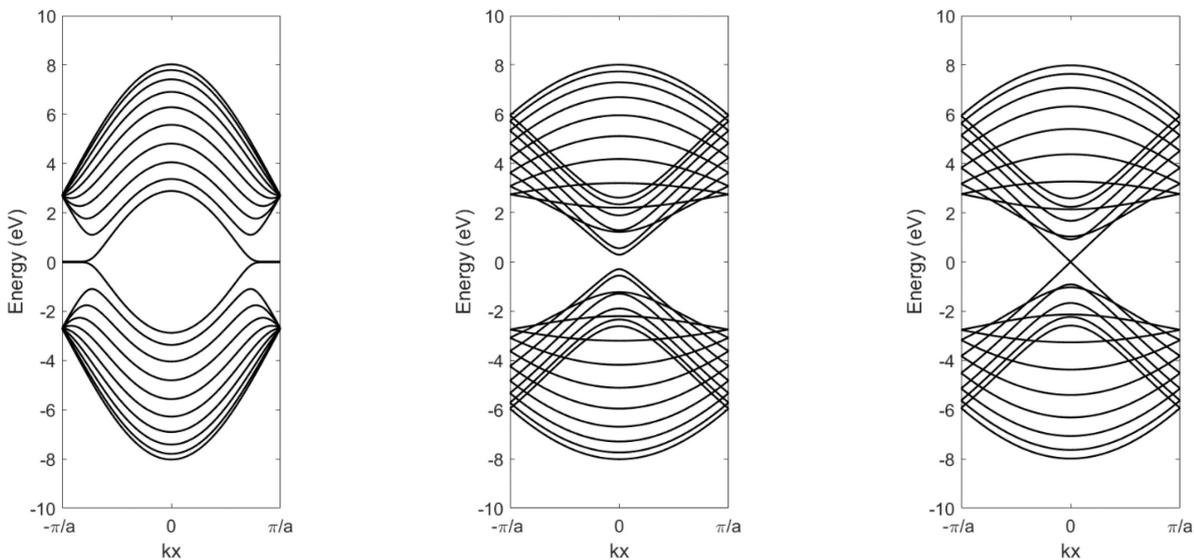


Figure 14. Electronic dispersion diagrams in  $k_y = 0$  for several types of perfect graphene nanoribbons.

Left : zigzag nanoribbon, Center : armchair nanoribbon of width  $M = 3n$  or  $3n + 1$ .

Right : armchair nanoribbon of width  $M = 3n + 2$ .

## 2.2.2 Transition Metal Dichalcogenides

TMDs are a class of materials composed of one transition metal atom for every two chalcogen atoms. Although the metal can be from groups IV, V, VI, VII or X, the TMDs garnering the most research interest are those bearing a group VI transition metal. They are of the type  $\text{MX}_2$ , and are more specifically  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ,  $\text{MoTe}_2$ ,  $\text{WS}_2$ ,  $\text{WSe}_2$  and  $\text{WTe}_2$ . Although they exist in bulk form, I am solely interested in their monolayer form; I will therefore refer to group-6 monolayer TMDs as “TMDs” from this point on.

### 2.2.2.1 Crystal structure

A TMD monolayer is actually composed of 3 separate layers : a top  $X$  layer, a middle  $M$  layer, and a bottom  $X$  layer (see Figure 15). They can exhibit three phases: hexagonal (2H), octahedral (1T), and distorted octahedral (1T'). In both octahedral phases, TMDs are semi-metallic, whereas they are semiconducting in the hexagonal phase; since the goals of my PhD project are focused on nanoelectronics applications, I will describe only the hexagonal phase of those materials. In this phase, the coordination is trigonal prismatic[130] and the chalcogen atom determines the lattice parameter of the structure -which I report in Table 1.

### 2.2.2.2 Electronic and transport properties

2H-TMDs are semiconductors with direct bands gaps ranging from 1.2 to 2 eV (as calculated by the TB model used throughout this work, which will be presented in detail later) and effective electron masses ranging from  $0.45 \times m_e$  to  $0.65 \times m_e$ [132]. Although their theoretical mobilities range from  $350 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  for  $\text{MoS}_2$  to more than  $2500 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  for  $\text{MoTe}_2$  [133], the measured experimental mobilities are far lower, in part due to the creation of a substantial Schottky barrier at the contact. For instance, a mobility of  $0.5 - 3 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  has been measured in  $\text{MoS}_2$ , and can be improved up to  $160 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  by encapsulating the monolayer in a high- $\kappa$  dielectric or a polymer electrolyte[134], [135], and mobilities up to  $50 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  were reported in  $\text{WS}_2$ [136].

| $\text{MX}_2$        | $\text{MoS}_2$ | $\text{WS}_2$ | $\text{MoSe}_2$ | $\text{WSe}_2$ | $\text{MoTe}_2$ | $\text{WTe}_2$ |
|----------------------|----------------|---------------|-----------------|----------------|-----------------|----------------|
| $a$ ( $\text{\AA}$ ) | 3.18           | 3.18          | 3.32            | 3.32           | 3.55            | 3.55           |
| $E_{gap}$ (eV)       | 1.79           | 1.95          | 1.55            | 1.65           | 1.25            | 1.23           |

Table 1. Lattice parameter (as reported in [131]) and band gap (as calculated in the DFT-validated TB model used) of the considered TMDs.

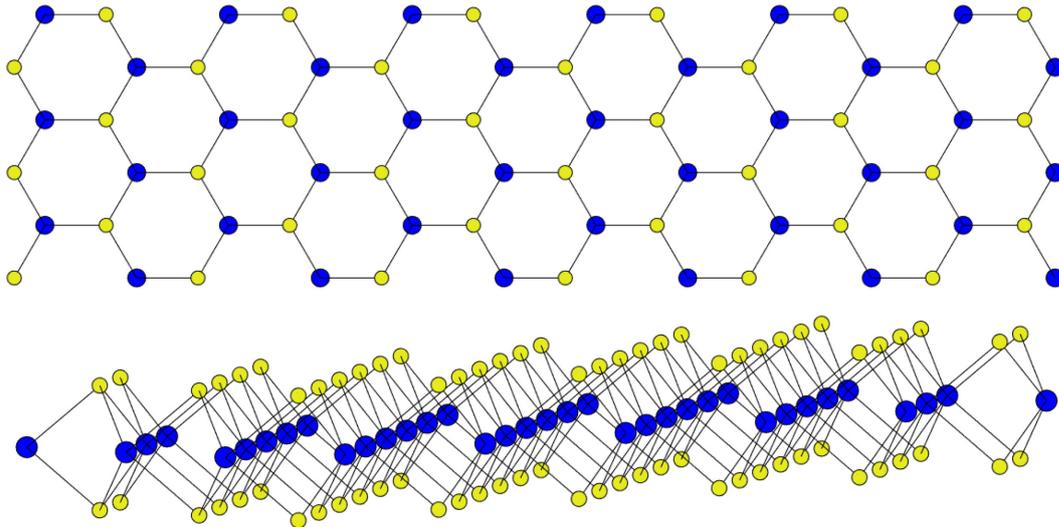


Figure 15. (top) Overhead view of a TMD monolayer in its hexagonal phase, in which yellow markers represent the chalcogen atoms and the blue markers represent the transition metal atoms. (bottom) Side view of the same TMD.

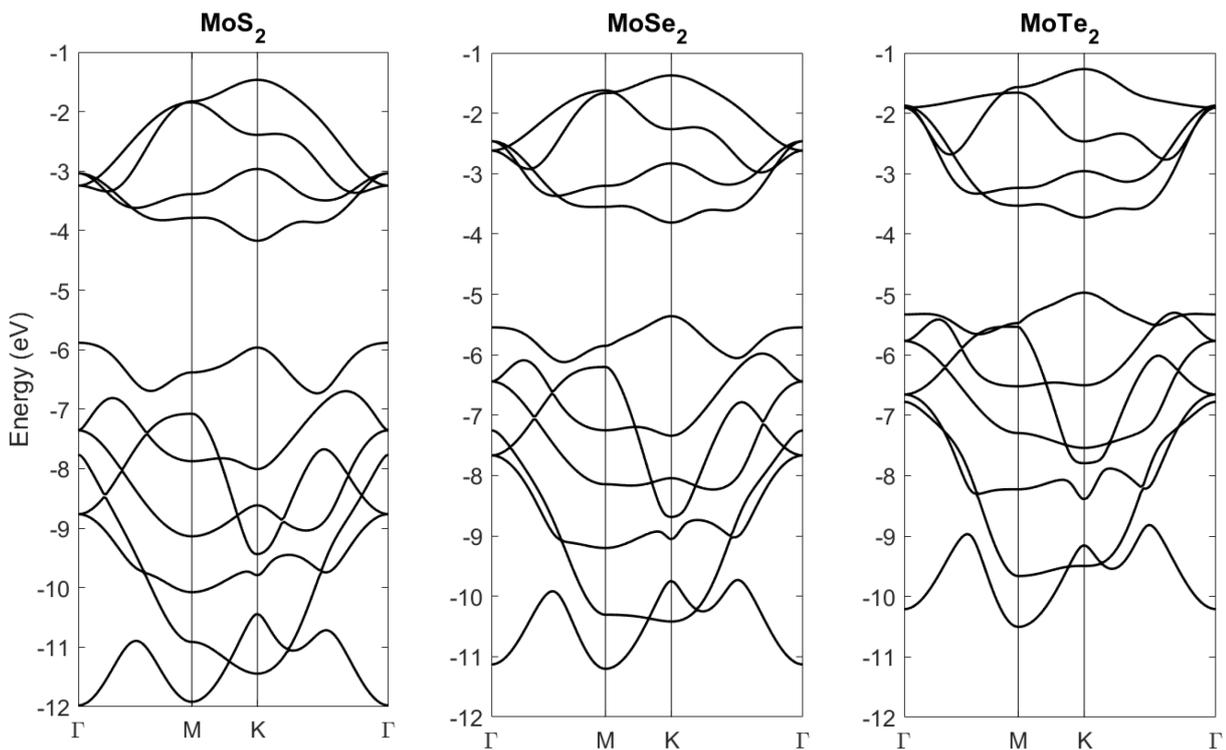


Figure 16. Electronic dispersion along the high symmetry directions of the first Brillouin zone for three of the six considered TMDs.

TMDs are the materials on which I mainly focused for this work, and ultimately, the ones used in the devices presented in the “results” section of this manuscript. However, studying other 2D materials and their properties remains interesting and can lead to novel ideas and uses. In this next part, I will therefore present a few other 2D materials.

### 2.2.3 Other 2D materials

As I mentioned in the introduction to this part, 2D materials have an incredibly broad range of properties and therefore of potential applications. Even though I did not study the following materials during my PhD work, they remain interesting and worth quickly presenting in order to present a more complete view of 2D materials. The materials discussed here are hexagonal boron nitride, silicene, germanene and phosphorene.

#### 2.2.3.1 2D hexagonal boron nitride

2D Hexagonal boron nitride (hBN) is an isomorph of graphene in which the 2 sublattices are occupied with boron and nitrogen atoms arranged in honeycomb formation. It has a lattice parameter of  $a_{h-BN} = 2.5 \text{ \AA}$  [137], which is therefore very close to that of graphene ( $a_G = 2.46 \text{ \AA}$ ). Just as is the case for graphene, h-BN layers can be stacked. hBN is an insulator, with a band gap of approximately 6 eV[137] and presents a piezoelectric effect, which enables applications in sensing and actuating. Its high thermal stability (1000 °C in air [138]), thermal conductivity ( $\kappa \sim 484 \text{ W.m}^{-1}.K^{-1}$ ) and mechanical strength (Young's modulus  $\sim 1 \text{ TPa}$ ) [139] also benefit h-BN in other applications. For instance, its layered nature makes it viable for use as a lubricant both in sintered body or in powder form[140], another example is its use for the last 30 years in the metallizing industry, where it is used as an evaporation boat for aluminum[140] Thanks to its very small lattice mismatch with graphene, h-BN has the potential to be an ideal platform for graphene electronics, but also an efficient capping layer thanks to its inert nature, protecting the structural and chemical integrity of the active layer. Many studies have investigated graphene-hBN heterostructures, whether vertical (van der Waals) or horizontal (in-plane). Several vertical graphene-hBN transistors exhibiting a strong negative differential resistance (NDR) effect[141] that can be partially controlled via the twist applied to the layers [142] have been reported for example. However, the low  $I_{ON}/I_{OFF}$  ratios and high sub-threshold swings of such devices[97], [143] present a fundamental barrier to an integrated circuit application.

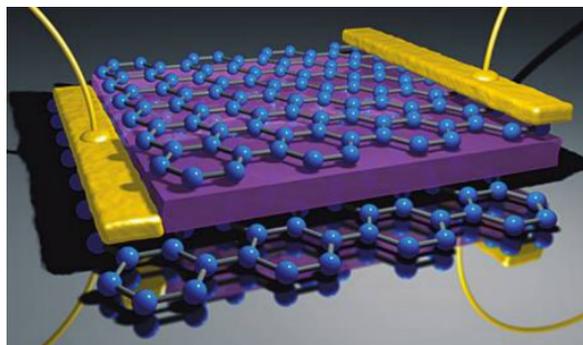


Figure 17. Vertical transistor made up of stacked hBN monolayers encapsulated between graphene contacts [97].

### 2.2.3.2 Silicene and germanene

Silicene and germanene are quasi-2D materials made up of  $sp^2$  hybridized silicon atoms arranged in a hexagonal lattice. However, contrary to graphene, this hybridization is unstable and leads to a “buckling” of the structure: the silicon/germanium atoms are shifted slightly out of plane (see Figure 18), hence the quasi-2D term.

Much like graphene, they both present a linear electronic dispersion around the  $K$  and  $K'$  points of the Brillouin zone[144]–[147] -which leads to the existence of massless Dirac Fermions along those directions-, but do not present a band gap. However, due to their buckled nature, a small tunable band gap of several tens of meV can be opened by applying a transverse electric field on the structure[148] -as is the case in graphene bilayers- or by surface adsorption[149], [150]. This ability to open a band gap, coupled with their extremely high calculated electron mobilities ( $2.57 \times 10^5 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  for silicene [151] and  $6 \times 10^5 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  for germanene [152]) makes them highly interesting for logic applications. Silicene especially, thanks to its natural compatibility with current silicon-based electronics, is being investigated for nanoelectronic applications[153], [154]. In both silicene and germanene, this band gap opening can also give rise to novel physical properties such as the quantum Hall effect due to a high spin-orbit coupling [155], which only increases their attractiveness for various applications.

Silicene and germanene have been experimentally demonstrated in 2012 and 2014 respectively, but the techniques related to their deposition are being improved upon. Silicene has for now been grown on several specific metallic substrates such as Ag(111) [156]–[160],  $\text{ZrB}_2(0001)$  and Ir(111), but its deposition remains a challenge due to its high instability in air. Germanene growth was also a challenge because of its tendency to favor  $sp^3$  hybridization rather than  $sp^2$ , and therefore give way to its hydrogenated cousin, germanane. In spite of this challenge, germanene was successfully deposited on a variety of materials ranging from metals such as Al(111)[161]–[163], Au(111)[164], [165] or Pt(111)[166], but also  $\text{MoS}_2$ , [167] or Sb[168].

Silicene and germanene, much like graphene, can also be used to create nanoribbons, either armchair or zigzag (depending on the edge type). Ab-initio studies of those nanoribbons have shown that half-metallicity[169] and giant magnetoresistance[170] can arise in those ribbons, paving the way for possible applications in spintronics.

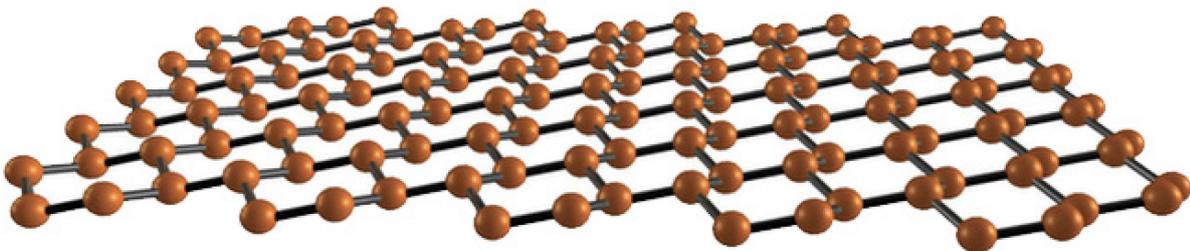


Figure 18. Lattice arrangement of silicene and germanene.

### 2.2.3.3 Phosphorene

Phosphorene is the 2D form of black phosphorus, the most stable phosphorus allotrope at room temperature, and was first isolated in 2014. Just like graphite, the layered structure of black phosphorus is held together by van der Waals forces, and allows phosphorene to be mechanically exfoliated, much like graphene[171]. Phosphorene layers share a hexagonal lattice arrangement with the other 2D materials previously mentioned, but present a high non-planarity referred to as “puckering” (shown in Figure 10) that differs from the buckling found in silicene and germanene. It has been shown[172] that black phosphorus has a direct band gap of 0.36 eV, which increases exponentially as the number of phosphorene layers decreases, reaching an appreciable value of 1 eV for a single phosphorene layer. This high dependence of the band gap on the number of layers is extremely interesting, as it would allow to tune the band gap depending on the desired application. Another interesting aspect is its reaction to electric fields: under a transverse electric field, the material turns from a semiconductor into a Dirac semi-metal with linear dispersion along the armchair direction[173], in part similar to the dispersion found in graphene for instance. Phosphorene is highly flexible and can resist stresses of up to 30% [174], [175], even though its Young modulus is one order of magnitude smaller than that of graphene. Its reaction to strain is peculiar, as the band gap experiences a direct-indirect-direct transition under axial strain before closing completely at a strain of roughly 13% [174]. Effective masses are also highly impacted by strain, allowing for yet another tuning mechanism to obtain the desired properties. Overall, significantly lower effective masses were reported in the armchair direction than in the zigzag direction, indicating that it is favored for carrier transport[174].

Due to these many interesting properties arising from its puckered structure, phosphorene is an exciting and promising candidate for electronic and optical applications [176]–[181]. Several p-type FETs based on few layer phosphorene have been studied, yielding ON currents of a few hundred mA/mm, and hole mobilities in the order of several hundred  $\text{cm}^2.\text{V}^{-1}.\text{s}^{-1}$  [171], [172], [176]. In a particular instance[171], it was used in conjunction with an  $\text{MoS}_2$  n-type FET to create the first CMOS inverter based on 2D materials.

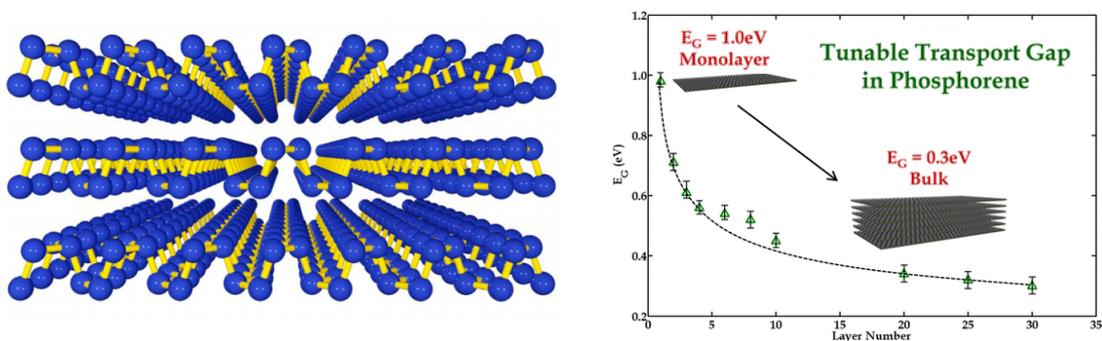


Figure 19. Left : Atomic arrangement of few layer phosphorene. Right: Evolution of its band gap with respect to the number of layers [172].

## 2.3 Atlas of 2D materials

In this part, I will present tables categorizing many known and theorized 2D materials. However, note that this list is not intended to be exhaustive, and that its goal is solely to highlight the breadth of materials being actively researched.

For each listed material, information on the band gap (its value and whether it is direct or indirect), and whether the material has been isolated experimentally (yes/no) is given. As most of these materials are still relatively new, band gap values are highly dependent on the method used to obtain them; therefore, the values mentioned here give a general indication, but **are not to be considered absolutely accurate**. Several references are given for each material, should the reader be interested in getting more information on a particular material.

Please note that neither oxides based on mentioned 2D materials (such as graphene oxide), nor layered covalent organic frameworks are listed here.

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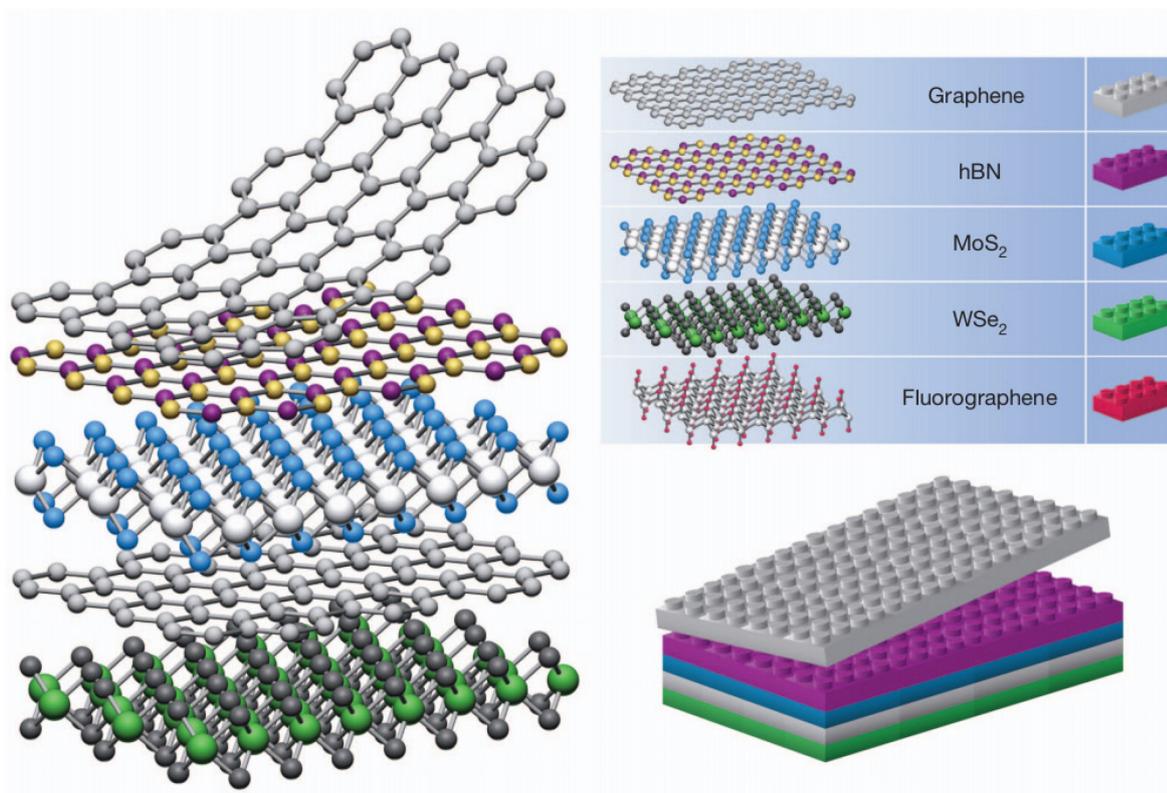


Figure 20. The “lego-like” possibilities of van der Waals heterostructures allowed by the breadth of 2D materials [182].

|               |                     | Material          | $E_G$ (eV) | Exp                 | References          |
|---------------|---------------------|-------------------|------------|---------------------|---------------------|
| Graphene-like | -ene                | Graphene          | ---        | Y                   | [119]–[121]         |
|               |                     | hBN               | 4.70 (D)   | Y                   | [137], [140], [183] |
|               |                     | Silicene          | ---        | Y                   | [144], [157], [160] |
|               |                     | Germanene         | 0.02 (D)   | Y                   | [163]–[165]         |
|               |                     | Silicon carbide   | 2.55 (D)   | Y                   | [184], [185]        |
|               |                     | Stanene           | 0.10 (D)   | Y                   | [186]–[188]         |
|               |                     | Phosphorene       | 1.88 (D)   | Y                   | [178], [179], [187] |
|               |                     | Borophene         | ---        | Y                   | [189]–[191]         |
|               |                     | Gallenene         | ---        | Y                   | [186], [192]        |
|               |                     | Antimonene        | 2.28 (I)   | Y                   | [193], [194]        |
|               |                     | Arsenene          | 2.49 (I)   | Y                   | [193], [194]        |
|               |                     | Bismuthene        | 0.55 (D)   | Y                   | [193], [195], [196] |
|               |                     | Selenene          | 0.13 (D)   | Y                   | [186], [197]        |
|               |                     | Tellurene         | 0.16 (D)   | Y                   | [186], [197]        |
|               | hydrogenated (-ane) | Graphane          | 3.56 (D)   | Y                   | [198], [199]        |
|               |                     | Silicane          | 2.26 (I)   | Y                   | [186], [200]        |
|               |                     | Germanane         | 1.16 (D)   | Y                   | [200], [201]        |
|               | halogenated         | Fluorographene    | 3.29 (D)   | Y                   | [199], [202], [203] |
|               |                     | Chlorographene    | 2.80 (D)   | Y                   | [204]–[206]         |
|               |                     | Bromographene     | 0.08 (D)   | Y                   | [205], [206]        |
|               |                     | Iodographene      | unknown    | Y                   | [205], [206]        |
|               |                     | Fluorophosphorene | ---        | N                   | [207]               |
|               |                     | Chlorophosphorene | ---        | N                   | [207]               |
|               |                     | Bromophosphorene  | ---        | N                   | [207]               |
|               |                     | Iodophosphorene   | ---        | N                   | [207]               |
|               |                     | Fluorosilicene    | 1.47 (D)   | N                   | [186], [208], [209] |
|               |                     | Chlorosilicene    | 1.97 (D)   | N                   | [186], [208], [209] |
|               |                     | Bromosilicene     | 1.95 (D)   | N                   | [186], [208], [209] |
|               |                     | Iodosilicene      | 1.19 (D)   | N                   | [186], [208], [209] |
|               |                     | Fluorogermanene   | 0.20 (D)   | N                   | [210]–[212]         |
|               |                     | Chlorogermanene   | 0.08 (D)   | N                   | [210]–[212]         |
|               | Bromogermanene      | 0.23 (D)          | N          | [210]–[212]         |                     |
|               | Iodogermanene       | 0.16 (D)          | N          | [210]–[212]         |                     |
|               | -yne                | Graphyne          | 0.50 (D)   | Y                   | [199], [213], [214] |
| Graphdiyne    |                     | 0.46 (D)          | Y          | [199], [213], [214] |                     |
| Silicyne      |                     | 0.73 (D)          | N          | [215], [216]        |                     |
| Silicidyne    |                     | 0.43 (D)          | N          | [217]               |                     |

|   | Material          | Gap (eV) | Exp      | References   |              |
|---|-------------------|----------|----------|--------------|--------------|
| Transition Metal Dichalcogenides (TMDs) | MoS <sub>2</sub>  | T        | ---      | Y            | [132], [135] |
|   |                   | H        | 2.02 (D) | Y            | [132]        |
|   | MoSe <sub>2</sub> | T        | ---      | Y            | [132], [218] |
|   |                   | H        | 1.72 (D) | Y            | [132], [185] |
|   | MoTe <sub>2</sub> | T        | ---      | Y            | [132], [219] |
|   |                   | H        | 1.28 (D) | Y            | [132], [185] |
|   | WS <sub>2</sub>   | T        | ---      | Y            | [136], [136] |
|   |                   | H        | 1.98 (D) | Y            | [115], [185] |
|   | WSe <sub>2</sub>  | T        | ---      | Y            | [185], [220] |
|   |                   | H        | 1.63 (D) | Y            | [220]        |
|   | WTe <sub>2</sub>  | T        | ---      | Y            | [113]        |
|   |                   | H        | 1.03 (D) | Y            | [113], [221] |
|   | ZrS <sub>2</sub>  | T        | 1.10 (I) | Y            | [222], [223] |
|   |                   | H        | 0.92 (I) | Y            | [222], [223] |
|   | NbS <sub>2</sub>  | T        | ---      | Y            | [224], [225] |
|   |                   | H        | ---      | Y            | [224], [225] |
|   | PdS <sub>2</sub>  | T        | 1.17 (I) | Y            | [226]        |
|   |                   | O        | 1.11 (I) | Y            | [226]        |
| TiS <sub>2</sub>                        | T                 | 1.65 (I) | Y        | [227]        |              |
|   | H                 | 1.25 (I) | Y        | [227]        |              |
| NiS <sub>2</sub>                        | T                 | ---      | Y        | [226]        |              |
|   | O                 | 0.52 (I) | Y        | [226]        |              |
| PtS <sub>2</sub>                        | T                 | ---      | Y        | [226], [228] |              |
|   | O                 | 1.75 (I) | Y        | [226], [228] |              |
| HfS <sub>2</sub>                        | T                 | 1.27 (I) | Y        | [222]        |              |
| HfSe <sub>2</sub>                       | T                 | 0.61 (I) | Y        | [222]        |              |
| Transition Metal Chalcogenides (TMCs)   | ZnS               | $\alpha$ | 2.58 (D) | Y            | [229], [230] |
|   |                   | $\beta$  | 2.57 (D) | Y            | [229], [230] |
|   | ZnSe              | $\alpha$ | 1.91 (I) | Y            | [231]        |
|   |                   | $\beta$  | 2.01 (D) | Y            | [231]        |
|   | CdS               | $\alpha$ | 1.72 (D) | Y            | [232]        |
|   |                   | $\beta$  | 1.65 (D) | Y            | [232]        |
|   | CdSe              | $\alpha$ | 1.20 (I) | Y            | [232], [233] |
|   |                   | $\beta$  | 1.30 (D) | Y            | [233], [234] |

T, H, and O refer to the tetrahedral, hexagonal and orthorhombic phases of the considered TMDs, while  $\alpha$  and  $\beta$  refer to the flat and corrugated phases of the considered TMCs.

|                                 |                 | Material          | Gap (eV) | Exp          | References |
|---------------------------------|-----------------|-------------------|----------|--------------|------------|
| Transition Metal Halides (TMHs) | MY <sub>2</sub> | CaCl <sub>2</sub> | 5.97 (I) | N            | [185]      |
|                                 |                 | CaBr <sub>2</sub> | 5.13 (I) | N            | [185]      |
|                                 |                 | MnCl <sub>2</sub> | 0.37 (D) | N            | [185]      |
|                                 |                 | MnBr <sub>2</sub> | 0.18 (I) | N            | [185]      |
|                                 |                 | FeCl <sub>2</sub> | ---      | N            | [185]      |
|                                 |                 | FeBr <sub>2</sub> | ---      | N            | [185]      |
|                                 |                 | NiCl <sub>2</sub> | 1.06 (I) | N            | [185]      |
|                                 |                 | NiBr <sub>2</sub> | 0.64 (I) | N            | [185]      |
|                                 | MY <sub>3</sub> | FeCl <sub>3</sub> | ---      | N            | [185]      |
|                                 |                 | FeBr <sub>3</sub> | ---      | N            | [185]      |
|                                 |                 | MoCl <sub>3</sub> | 0.80 (I) | N            | [235]      |
|                                 |                 | MoBr <sub>3</sub> | 0.56 (I) | N            | [235]      |
| TiCl <sub>3</sub>               |                 | 0.60**            | N        | [236]        |            |
| VCl <sub>3</sub>                |                 | 1.10**            | N        | [236]        |            |
| Semimetal Chalcogenides (SMCs)  | GaS             | 2.57 (I)          | Y        | [237], [238] |            |
|                                 | GaSe            | 2.05 (I)          | Y        | [237], [238] |            |
|                                 | GaTe            | 2.02 (I)          | Y        | [185], [237] |            |
|                                 | InS             | 2.09 (I)          | Y        | [239], [240] |            |
|                                 | InSe            | 1.70 (I)          | Y        | [239], [240] |            |
|                                 | InTe            | 1.60 (I)          | Y        | [239], [240] |            |

\*\* TiCl<sub>3</sub> and VCl<sub>3</sub> are half-metals, so the gaps mentioned only apply to one spin direction.

## 2.4 Applications of 2D materials

Thanks to their often impressive suite of mechanical, optical, thermal and electronic properties, 2D materials are being regarded as a potential paradigm shift for many industries. In this section, I will go over some of the applications for which 2D materials might be best suited. Among those technological fields are, for instance, high-frequency electronic devices, data storage, photonic and optoelectronic devices, wearable and flexible devices, sensors, and bioelectronics, just to name a few. I will try to touch on most application spaces of 2D materials, in order to highlight the breadth of possibilities and uses they offer, but this section is by no means meant to be all-encompassing.

### 2.4.1 Electronics

Electronics is one of the main areas that could be revolutionized by graphene. Indeed, the ITRS considers graphene to be among the top candidates for post-Si electronics[16]. As mentioned earlier in this manuscript, current III-V and silicon based transistor are not able to keep up with Moore's law, due to the increase in heat dissipated per unit area caused by miniaturization. Furthermore, the miniaturization of bulk devices severely impacts performance such as reducing carrier mobility in silicon when decreasing the body thickness, or causing shifts in the band gaps of semiconductors due to quantum confinement. Circumventing this issue will require a drastic change in either the materials used in nanoelectronic devices, or in the types of devices used (or even both). With its incredibly high mobility, flexibility and virtually limitless quantity, graphene could be the material that revolutionizes the nanoelectronics industry.

However, its lack of band gap severely limits the potential of simple, pure graphene to be used in nanoelectronics. This zero band-gap is responsible for low  $I_{ON}/I_{OFF}$  ratio, and high static power dissipation. For instance, a typical static drain current of roughly  $280 \mu\text{A}/\mu\text{m}$  at  $V_{DD} = 2.5\text{V}$  is observed in graphene inverters[241], against approximately  $100 \text{nA}/\mu\text{m}$  at  $V_{DD} = 0.75\text{V}$  for Si based logic transistors[242]. Band gap opening is therefore heavily investigated, with techniques ranging from quantum confinement in 2D (graphene nanoribbons) and 1D (graphene quantum dot), selective chemical functionalization[198] to applying a transvers electric field to bilayer graphene[243], [244], or even via substrate-induced effects; a band gap of up to  $0.5 \text{eV}$  was reported[245] in graphene on h-BN and h-BN/Ni(111) for instance.

Despite this drawback, the prospect that graphene devices could be scaled to extremely short channel lengths and high-frequencies while managing heat dissipation thanks to its astounding thermal properties[246] ensure an ever-growing number of studies on GFETs (Graphene Field Effect Transistors). The first GFET was reported in 2007 [247], and many have followed since, with increasingly promising characteristics[248]–[251].

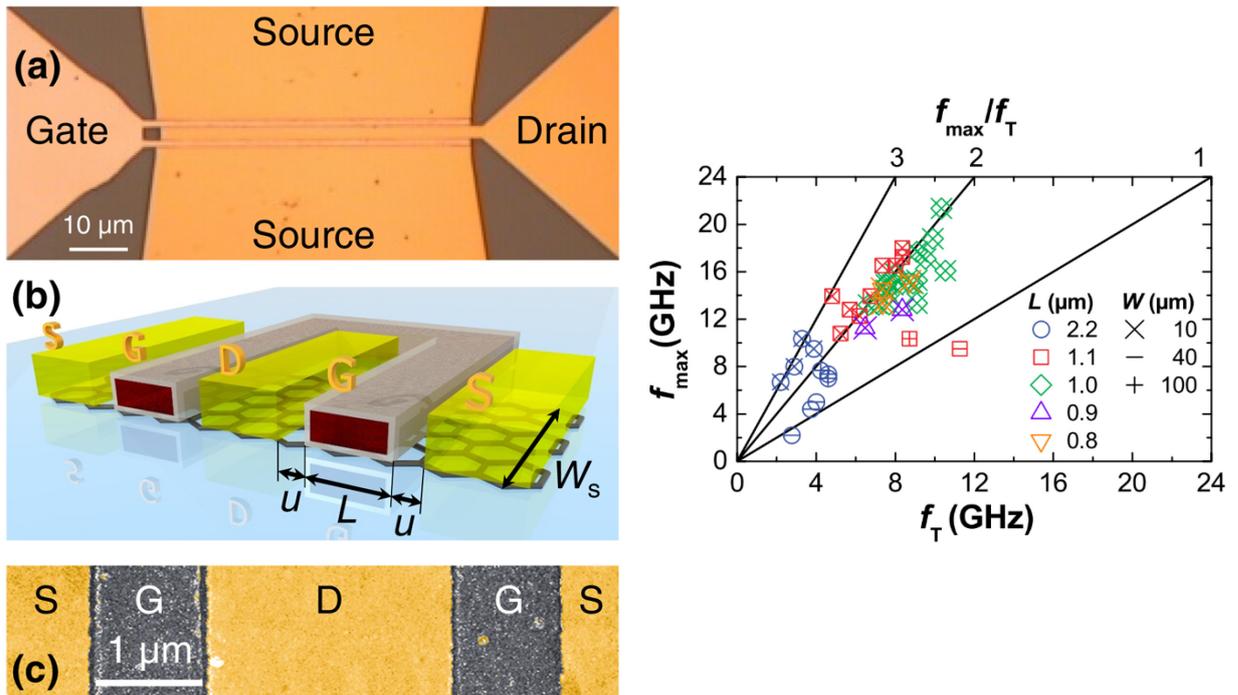


Figure 21. Left: High frequency GFET (a)Optical image of the GFET (b)Schematic of the central part of the GFET (c)SEM image of the central part of the GFET. Right: Maximum oscillation frequency as a function of the cutoff frequency of GFETs with varying gate lengths and channel widths [252].

A recent, encouraging GFET[252] provided high gain, frequency and transconductance, while outlining that several technological challenges such as improving the quality of CVD graphene and lowering both contact and gate resistance remain. While many challenges they face are as of now unresolved, GFETs remain a very promising avenue for post-Si electronics[253]–[255].

TMDs have also been considered and studied for use in FETs. Their semiconducting behavior and direct band-gaps ranging from roughly 1 to 2 eV especially MoS<sub>2</sub> being very attractive for logic uses. One of the first TMD-based FET was reported in 2004[256] and was based on WSe<sub>2</sub>; it showed high p-type mobility, but a low  $I_{ON}/I_{OFF}$  of  $10^4$  and therefore was not suited for the intended logic applications. In 2011 however, a similar WSe<sub>2</sub> p-type device that was top-gated by a high- $\kappa$  dielectric yielded far more promising performances, notably an  $I_{ON}/I_{OFF}$  of  $10^6$ [257]. During the same year, an MoS<sub>2</sub> based device was also reported and showed great promise for n-type operation[258], yielding a an  $I_{ON}/I_{OFF}$  of  $10^8$  and high electron mobilities. Shortly thereafter, bilayer MoS<sub>2</sub> was used to great effect in the creation of several logic building blocks[135]: an inverter, a NAND gate, static RAM and a five-stage ring oscillator, although the ON currents yielded were lower than that of the aforementioned single-layer MoS<sub>2</sub> FET. In contrast, several issues relating to MoS<sub>2</sub> FETs are yet to be addressed: namely, control over material doping and the quality of electrical contacts need to be drastically overhauled, while p-type operation and ambipolar behavior would be desirable[53].

Beyond MOSFETs, 2D materials could also find their use in both vertical and in-plane TFET architectures. In the case of in-plane TFETs for instance, the quality of the interface is paramount and the absence of dangling bonds and drastically reduced concentration of traps found in 2D materials give them a strong advantage compared to bulk materials. As mentioned in the introduction to this manuscript, TFETs are one of the main avenues outlined by the ITRS for power scaling in transistors. They have the benefit of relying on BTBT and therefore not having any theoretical lower limit for  $SS$ , unlike MOSFETs, which physically cannot yield  $SS$  below 60 mV/dec at RT.

Several in-plane TFETs based on TMDs have been simulated[102], [104], and focused on comparing the viability of the different TMDs for TFET operation. Due to its lower band gap and effective mass,  $WTe_2$  was identified in both cases as the most promising material, and yielded ON currents in the hundreds of  $\mu A/\mu m$  and  $SS$  around 20 to 30mV/dec[102]. In one of those reports, the viability of in-plane heterojunction between TMDs bearing the same chalcogen atom ( $WS_2$ - $MoS_2$  for instance) was investigated, and it was concluded that the  $WTe_2$ - $MoS_2$  heterojunction, once again due to the lower band gaps and effective masses, was the most promising; it was however unable to outperform the simulated  $WTe_2$  homojunction device[104].

Vertical TFETs based on TMDs have also been simulated[99], [259]. In this case, device geometry parameters such as the overlap length between the stacked materials and extension of the gate over the contacts severely impact performance and therefore have to be carefully selected.  $MoS_2$ - $WTe_2$  is the most commonly used pair of materials, due to its favorable band alignment for TFET operation. Low  $SS$  figures of 20 to 30 mV/dec and  $I_{ON}$  as high as  $10^3 \mu A/\mu m$  were reported[99], [259], which is very encouraging. It is worth noting, however, that phonon scattering and the effect of defects and impurities were not taken into account in those reports.

The works mentioned here are only a small portion of the active research happening on the integration of 2D materials in nanoelectronic devices, but they highlight the extremely high interest garnered by this class of materials for potential application in this field.

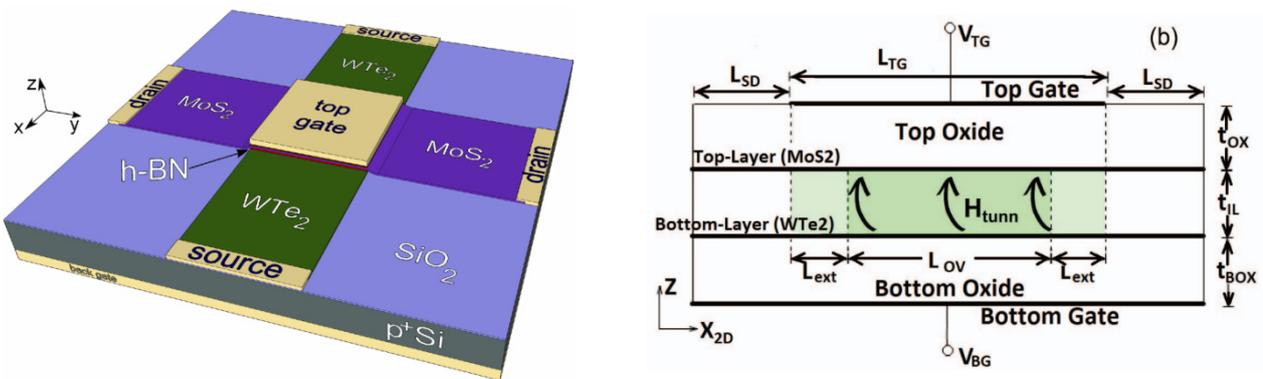


Figure 22. Left:3D sketch of the  $MoS_2$ - $WTe_2$  vertical TFET studied by *Cao et al.*

Right: Sketch of the 2D structure simulated [99].

## 2.4.2 Spintronics

Spintronics is another research field that could benefit greatly from the advent of 2D materials. Unlike traditional electronics, that exploit the transport of electrical charges, spintronics's interest lies with the transport of spin. To this day, spintronics-based logic has been hampered by the need to achieve not only a high degree of control over spin, but also a long spin lifetime. This conflict and duality arises from the fact that a strong spin-orbit coupling character is usually needed to have a high degree of control over spin[260], but that such a strong spin-orbit coupling most often leads to fast spin decoherence[261].

Graphene, in its pristine form, exhibits negligible spin-orbit coupling[262] which leads to long coherence and spin relaxation times; it could therefore be a good candidate for use as a non-magnetic channel through which spin is transported. However, spin relaxation times in the order of nanoseconds (ns) have been reported in graphene[263] and the spin relaxation mechanism is not yet completely clear. Several relaxation mechanisms related to phonon and impurity scattering[260], [264]–[266] as well as the influence of the substrate and contact resistance between graphene and the magnetic electrodes[53] are at play here; further research is therefore needed to quantify and identify the contribution of each mechanism and tune the devices accordingly.

In addition to logic applications, graphene spintronic devices could potentially be used for sensing applications; thanks to its long spin diffusion length (beyond  $30\mu\text{m}$  in single layer graphene[267] and up to  $100\mu\text{m}$  in few layer graphene[268]), it could be used to develop magnetic sensors in the pT to nT range. Such spintronic sensors could find use in medicine, for instance to assist in tumour reduction or onsite drug delivery[53].

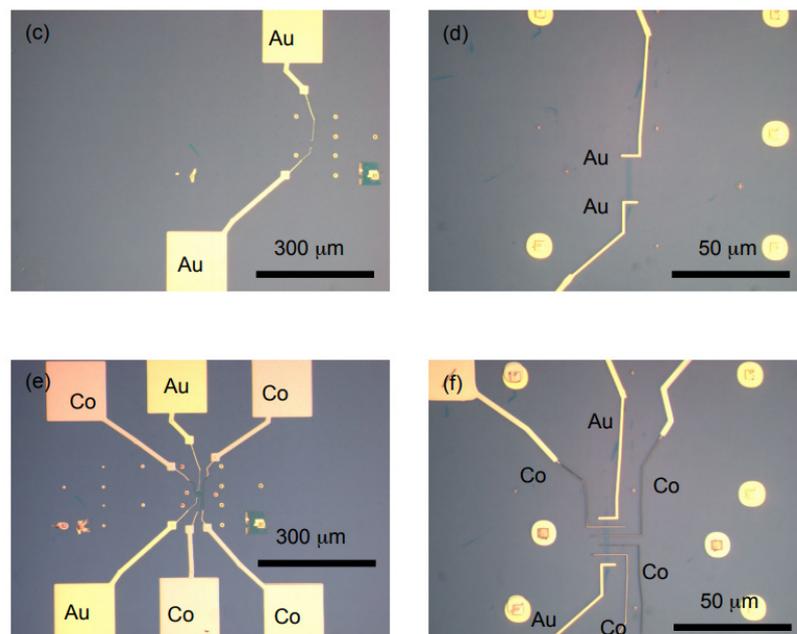


Figure 23. Graphene spin-valves on gold contacts (c,d) and with copper electrodes (e,f) [269]

As is often the case for other applications, graphene is the most prominently studied 2D material in the field of spintronics. However, it is by no means the only 2D material with possible use in this field. It has been theorized[270] and later shown[271], that MoS<sub>2</sub>, non-magnetic in its pristine form, can acquire a magnetic moment by adsorption of other transition metal atoms (Mn, Fe, Co, Ni) on a Mo site, allowing for MoS<sub>2</sub> based spintronics applications[53], [272], [273].

Due to their generated valley in the K and K' point of the Brillouin zone, TMDs also show great promise[274], [275] in the field of valleytronics[276], [277], in which an optical excitation can be used to finely control carrier momentum, therefore using different valleys to store information separately.

### 2.4.3 Optoelectronics and photonics

Photonics and optoelectronics are among the research fields that are heavily impacted by the advent of 2D materials, and only a small sliver of the many possible applications are mentioned here. Graphene, especially, has a slew of advantages compared to usually used materials: it has very large carrier concentrations[278], wavelength-independent absorption[279], low dissipation rates[280] and its optical properties can be tuned by electrostatic doping, just to name a few. For instance, thanks to its high compatibility with CMOS processes, graphene is a promising candidate for optical interconnects operating at high data rates[281]–[283], and its flexibility would allow for integration on a flexible substrate[284]. Another example would be the detection of wavelengths outside the limit set by the band gaps of semiconductors currently used; thanks to its wide absorption spectrum, detection in the far infra-red (THz range), as well as short-wave infra-red would be possible with graphene. This property could also be used[285] to create optical limiters (devices with a low transmittance for high intensity light) across a broad spectrum; such limiters garner great interest for eye protection and sensing applications since, in their current form, no limiter can cover both the visible and the near-infra-red range[285]. Indeed, broad optical limiting capabilities were reported for LPE graphene in the case of ns pulses[286]. Photodetectors can also benefit from the wide range of absorption[287], [288] and ultrafast response found in graphene[289]; many photodetectors with varying designs based on graphene have been realized[290]–[292] and yielded impressive performance, such as in a communications link at 10 Gbit.s<sup>-1</sup>[289] for instance.

Laser technology based on graphene has been studied since the late 2000s, and yielded promising results. An ultrafast LASER, mode-locked by a graphene saturable absorber was first reported in 2009[293] with a low output power of 1 mW, but following reports[294]–[296] have improved upon this work and reached output powers beyond 3 W[294], for discrete pulses ranging from 1 to 2μm depending on the report. The widest range reported yet is found in ref [296] and extends from 1525 to 1559nm, for picosecond (ps) pulses.

TMDs can also find use[297] in optoelectronics thanks to their transparency and flexibility. Among other applications, photodetectors based on MoS<sub>2</sub> have shown stable switching times of 50 ms[298] and high photoresponsivity[299] (880 A.W<sup>-1</sup> at 561 nm), and the ability to tune their gap depending on the number of layers allows for the detection of several wavelengths[300]. Overall, while graphene is suited for ultrafast, broadband technologies, TMDs are geared towards applications where strong light absorption[301] and electroluminescence[302] are required.

Although it is not expanded upon in this thesis for obvious concision purposes, graphene and other 2D materials hold strong potential for applications in plasmonics[303]–[306], antennas[307]–[310], light emitting devices[233], [234], [311] and more, and we refer the reader to the mentioned references for information and insight on these topics.

#### 2.4.4 Sensors

Thanks to their one-atom thickness (or almost, in the case of TMDs) and their high flexibility, 2D materials are perfect for sensing applications. They could revolutionize this field and allow for cheap, reliable and flexible devices to be used in sensor arrays or as individual on-chip sensors. Because of their ultimate surface to body ratio, each atom that composes a 2D material is in direct contact with the environment of the sensor, which leads to an incredible degree of sensitivity[312] that is beneficial for all manner of sensing: mass[313], [314], electrochemical[315], [316], magnetic[312], radiation[317] and many more. For instance, nano-electro-mechanical sensors (NEMs) based on pristine graphene resonators, which measure the shift in resonance frequency depending on particle adsorption on the device, have been developed and an astonishing detection limit at 158 parts-per-quadrillion for gas molecules at room temperature was reported[318].

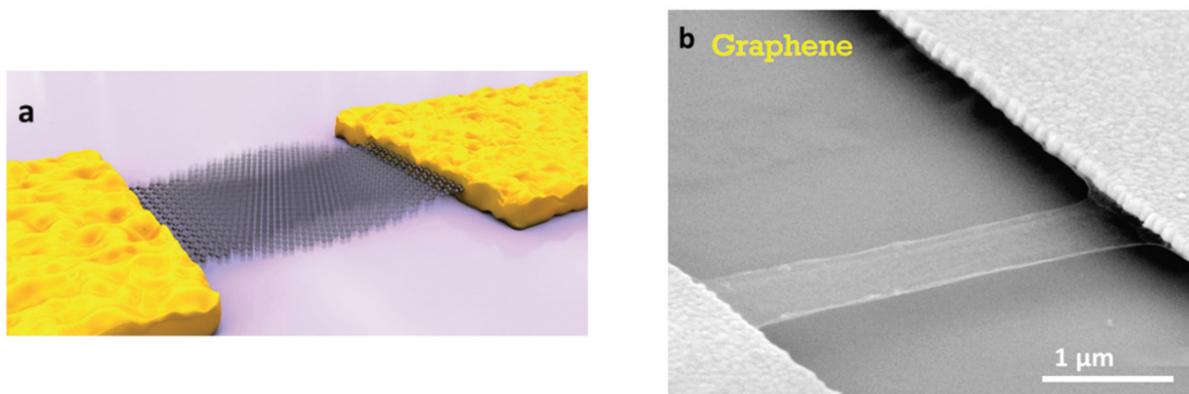


Figure 24. (a) Sketch of a resonating graphene sheet in action. (b) Actual graphene micro-resonator fabricated by SiO<sub>2</sub> etching[319].

Such technology could of course be used to monitor aerosol content in the atmosphere for instance. However, several challenges remain unsolved: while suspended graphene yields the most promising results, it is more difficult and far less stable than graphene on substrate, in which substrate interactions can diminish the sensing capabilities[53]; contamination by hydrocarbons is another issue that can drastically impact performance, and while it can be easily solved by UV light cleaning or annealing in a lab, it is a very real issue in real-world conditions. To remedy this, functionalization or passivation[320] may be required, but such techniques run the risk of undermining the sensing capabilities of the resonator. These types of challenges must therefore be addressed before graphene NEMs can become ubiquitous.

The use of graphene for magnetic sensing is also extremely promising. Current technologies are based on tunneling magnetoresistance and giant magnetoresistance, but are limited by spin-torque instabilities and thermal magnetic noise[321], and their use in the  $\mu\text{T}$  to the nT range is therefore severely limited. Graphene-based Hall sensors yielding a similar sensitivity to that of existing sensors have been reported[322], but sensors based on a combination of extraordinary magnetoresistance and spintronics were able to reach a sensitivity of  $10\text{mV/Oe}$  [321], [323], which is larger than state of the art InAs 2DEG sensors of similar dimensions.

Once again, although graphene spearheads research into 2D materials for sensing applications, other materials, most notably TMDs are promising in this regard. Gas sensors based on  $\text{MoS}_2$  have been reported as early as 1996[324], and, more recently, nitrous oxide sensors based both on single-layer  $\text{MoS}_2$  and multi-layer  $\text{MoS}_2$  have been realized[325]. These showed extremely high sensitivity, detecting nitrous oxide down to 0.8 parts-per-million; it is worth noting that, in this study, sensors based on 2, 3 and 4 layer  $\text{MoS}_2$  were more stable and reliable than their single layer counterpart. Another  $\text{MoS}_2$  based sensor using reduced graphene oxide as contacts was reported[326] to yield a sensitivity as low as 2 parts-per-billion, and its performance could be increased further by platinum functionalization. Even more recently, an  $\text{MoS}_2$  sensor was used to detect DNA particles[327]; in this instance, the sensor has been modified with Au particles, which greatly enhances DNA absorption on  $\text{MoS}_2$ .

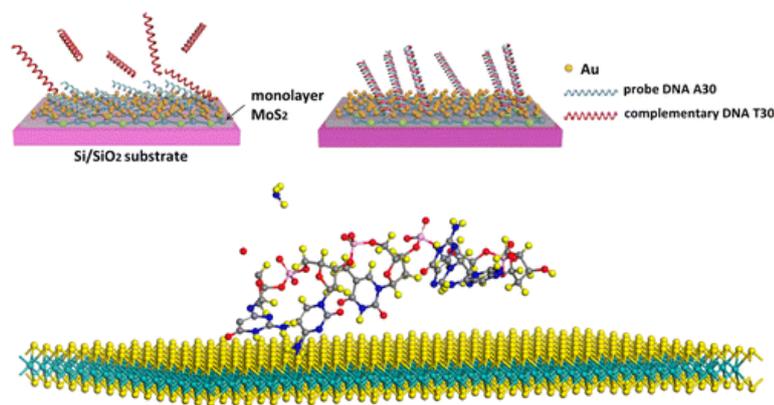


Figure 25. Au modified  $\text{MoS}_2$  monolayer for DNA sensing [327].

### 2.4.5 Energy storage

Energy storage, as well as energy conversion, is yet another technological field in which the potential applications of 2D materials are plentiful. In the specific case of batteries, the biggest challenge is to find the best possible materials to be used as anode and cathode. Li-ion batteries are widely regarded as the most promising technology to be used in future utilities and electric vehicles for instance, and they are made up of an  $\text{LiCoO}_2$  cathode and a graphite anode[328]–[330]. Due to its relatively low specific capacity (ampere-hours available at a given discharge value per unit weight) of  $372 \text{ mAh.g}^{-1}$ [331], graphite does not seem to be the ideal material for this use, but most other materials bearing a higher capacity ( $4200 \text{ mAh.g}^{-1}$  for Si for instance [332]) can only sustain a low number of charge/discharge cycles before their performance starts declining rapidly. Identifying the right materials is therefore a balancing act between several performance indicators, and 2D materials as well as nanostructures such as nanoporous materials[331], [333] could be of extremely high interest. Graphene has shown potential as a conductive additive to nanostructured electrodes[334], [335], while reduced graphene oxide sheets have shown great promise as electrodes, whether in their pristine form[336] or by creating composites with  $\text{SnO}_2$ [337], reaching capacities up to  $780 \text{ mAh.g}^{-1}$  for instance[337]. Once again, TMDs are also very promising in this respect, the weak VdW forces binding the layers allowing for ion diffusion without a significant increase in volume[53]. Exfoliated then restacked  $\text{MoS}_2$  has for example led to a specific capacity of over  $800 \text{ mAh.g}^{-1}$ [338], while layered G/ $\text{MoS}_2$  composites material in which Li ions can be intercalated, leading to a high specific capacity of  $1100 \text{ mAh.g}^{-1}$ [339].

Supercapacitors could also benefit greatly from the advent of 2D materials. Their performance can be improved by increasing the surface area of the electrode while reducing its thickness, and one-atom thick, all-surface materials are a natural fit; strong electrochemical performance in graphene-based supercapacitors has been reported[340]–[343]. Other than pristine graphene, the use of several varieties of graphene oxide in supercapacitors, such as aerosol spray dried graphene oxide[344], microwave expanded graphite oxide[343], [345] and reduced graphene oxide[346] have been investigated and yielded promising results.

Graphene and other 2D materials have also found great interest hydrogen storage and fuel cells, which convert electrochemical energy into electrical energy as long as fuel and oxygen are available, and are used in vehicles, smart phones, and power backup systems for instance. 2D materials have been used to replace the costly noble metal alloys (Pt, Au ...) used in the cathode for the oxygen reduction reaction, and produced promising results [347], [348].  $\text{MoS}_2$  and  $\text{WS}_2$ , thanks to their edges acting as catalytic sites, could also replace those noble metals and have been studied for these purposes[349]. Graphene also holds potential for hydrogen storage thanks to its robustness and flexibility, allowing for the control of hydrogen intake via its curvature[350], [351], but also the production of hydrogen in a more renewable process than the one currently used[352], [353].

## 2.4.6 Flexible electronics

Through their ultimate thinness, their flexibility and incredibly high resistance to strain, 2D materials will enable the advent of flexible electronics, widely considered to be the next ubiquitous platform for the electronics industry[354]; the ultimate goal being to create devices with performance equal to or higher than regular current electronic devices, but in a foldable, transparent and lightweight format by which many new applications would be made possible. Important technological challenges remain however, such as ensuring that all components yield acceptable performance under high deformation and are environmentally sound. A complete revolution of the current low-cost, high output manufacturing processes used will also be necessary before “printable” flexible electronics reach ubiquity, which is a tall order.

As is the case for most applications, graphene is the most promising 2D material for such applications. Its one-atom thickness, high flexibility, transparency and extremely high conductivity[118] make it an ideal candidate to be used in the core components of devices such as antennas, interconnects, RF transistors, and LEDs; many other applications are envisioned, such as flexible displays[355]–[357], flexible chemical sensors[358]–[360], flexible batteries and other energy storage devices[361]–[364].

Before that, however, the properties of graphene will need to be properly tuned depending on the intended application: for instance, a very low resistivity of  $< 5 \Omega/m$  is required for high frequency applications in antennas[365], while a resistivity of a couple hundred  $\Omega/m$  would be sufficient for capacitive touch panels[366]. Graphene resistivity is highly dependent on the deposition technique used though[53], which will be a major challenge to be overcome in order to reach the easily “printable” flexible electronics that would revolutionize the industry.

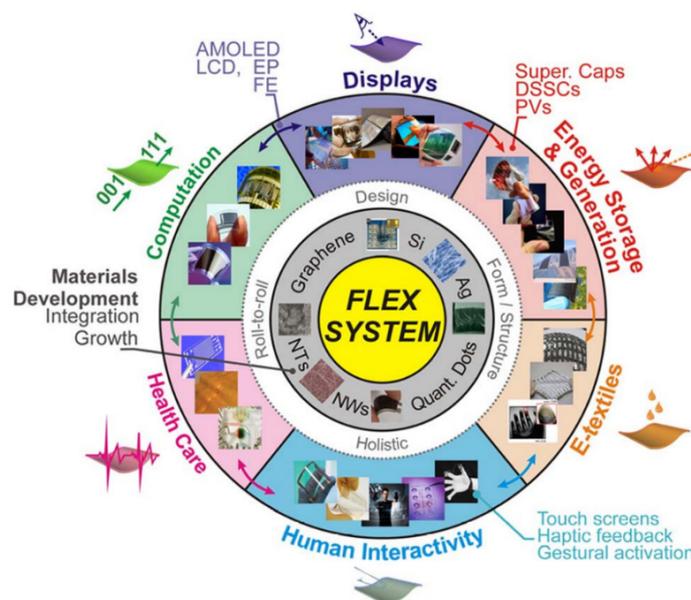


Figure 26. Possible applications of flexible electronics, and the 2D materials and techniques that enable them [354].

However, the prospects offered by graphene are extremely enticing and will without a doubt motivate the industry to develop the necessary techniques and processes to usher society in a world of flexible electronics. Due to its over 90% transmittance in the 200 to 900nm range, graphene has incredible potential as a transparent conductive material; this property could be put to use in solar cells for instance, which exhibit a 10 to 25% power loss originating from the currently used transparent conductive layer[367]. In a similar fashion, graphene has strong potential as anode material in flexible OLED panels[368], solving many issues related to the currently used indium tin oxide (ITO is brittle, indium diffusion impacts performance over time ...). Human-computer interaction is another field that could benefit greatly from 2D materials: experimentally realized transparent and flexible graphene actuators[369] indicate that graphene could enable precise haptic feedback in capacitive touch screens, which are arguably the main way we interact with computers nowadays.

Other 2D materials, such as h-BN or TMDs (namely MoS<sub>2</sub>) hold potential for flexible electronics applications. Graphene/h-BN heterostructures have been shown[370] to enhance GFET performance, and could therefore be used to create flexible GFETs; in a similar way, using h-BN instead of Al<sub>2</sub>O<sub>3</sub> as a top gate oxide in MoS<sub>2</sub> devices could allow for flexible, TMD based FETs. Thanks to their direct band-gap, TMDs such as MoS<sub>2</sub> and WS<sub>2</sub> are very promising for optoelectronics and photovoltaics, and could therefore be used to create novel, flexible optoelectronic devices[53].

While not intended to be all-encompassing, this section provided comprehensive examples of current and future potential applications for various 2D materials. The techniques used to deposit and grow these materials will now be briefly presented, as they are a fundamental part in realizing the full potential of these materials and bringing the aforementioned applications to life.

## 2.5 Brief overview of 2D materials synthesis

Growth and deposition techniques, more specifically at an extremely large scale, are the cornerstone of the previously outlined applications for 2D materials. The development of scalable processes that would allow for the specific tuning of electronic, mechanical and structural properties of those materials would obviously be a huge step towards the realization of those applications. In this section, I will briefly present the main techniques used to synthesize 2D materials, in order to give an overview of this technological side of the field. Once again, the reader is referred to the mentioned references for more precise and detailed information on the mentioned techniques.

Two main classes of synthesis techniques can be distinguished: top-down deposition (via mechanical or liquid-phase exfoliation for instance) and bottom-up growth (via chemical vapor deposition or molecular beam epitaxy).

### 2.5.1 Mechanical and Liquid-Phase Exfoliation

Mechanical exfoliation, also known as the “scotch-tape” method, was the very first technique used to obtain monolayer graphene in 2004 by Geim and Novoselov[93]. Due to the weakness of the van der Waals forces than bind the individual layers of 2D materials in their bulk/3D form, a strong enough force can cleave either a single or several layers of the considered material. Thanks to its simplicity and flexibility, mechanical exfoliation has been used extensively to produce single and multi-layers for a variety of materials ranging from graphene[371]–[375] to TMDs[372], [375]–[377], but also h-BN[375], [378], [379]. As a well-established technique, mechanical exfoliation can provide high quality layers of high purity and of which the size is only limited by that of the starting material[380]. Mechanical exfoliation has for instance been used to produce extremely high quality single layer graphene which was reported to yield a  $10^7 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  carrier mobility at 25 K[381]. However, by its very nature, mechanical exfoliation is not a scalable method and its use is therefore mostly limited to the production of laboratory samples.

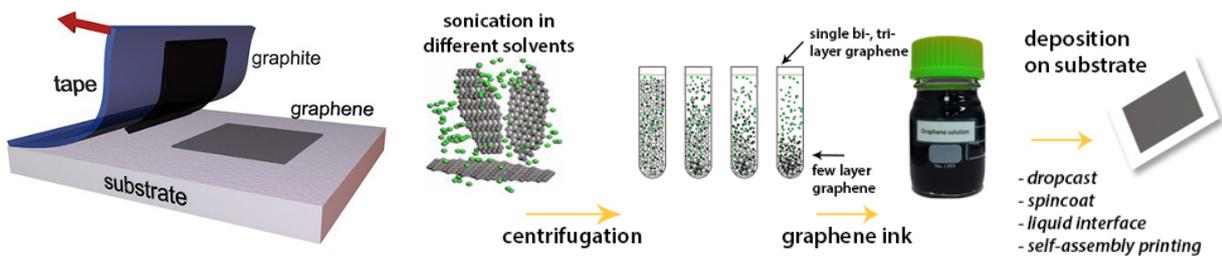


Figure 27. Left: Mechanical Exfoliation. Right: Liquid-Phase Exfoliation [382].

Liquid Phase Exfoliation (LPE) is another widely used method to produce single or multi-layers of 2D materials. First, the bulk material is dispersed in a solvent (N-methyl-2-pyrrolidone is frequently used) using sonication, then the mixture undergoes centrifugation in order to disperse the layers and arrange them in the solvent (single layers at the top, many-layers at the bottom). The concentration of single and few layer compounds depend on the solvent used and can be increased[383], [384] via the use of a surfactant prior to sonication, but chemical treatments are then needed to remove it. From the resulting solution, 2d material “inks” can be produced, and can then be deposited via drop and dip casting[385], [386], spray-coating, ink-jet printing[387] and other techniques. Graphene inks with carrier mobilities up to  $90 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  have for instance been reported[387].

LPE is cheap and relatively scalable, and, contrary to some other techniques, does not rely on growth substrates. However, the size of LPE flakes is limited by the intense exfoliation and purification processes: the area of LPE-produced, single layer graphene flakes rarely exceeds  $1 \mu\text{m}^2$  [383], [384], [387] for instance.

LPE has been used to produce graphene[383], [384], [388], [389], TMDs such as  $\text{MoS}_2$ ,  $\text{WS}_2$ ,  $\text{MoSe}_2$  and  $\text{MoTe}_2$ [390]–[392] as well as h-BN[390]–[392].

## 2.5.2 Molecular Beam Epitaxy

Molecular beam epitaxy (MBE) is an epitaxy technique performed in ultra-high vacuum ( $10^{-8}$  to  $10^{-12}$  Torr). It has been widely used to create epitaxial layers of semiconductors, metals and insulators, and allows for a high degree of control over both doping profile and chemical composition[393], [394]. Due to the high vacuum required and the long deposition times, MBE is more suited for deposition on 2 to 6 inch wafers than on 30-inch ones for instance [395]. This technique allows for precise control over the number of layers deposited, and has been used to deposit graphene on a wide range of substrates including but not limited to h-BN[396], Si(111)[397], SiC[398] or dielectric substrates[399]. MBE-grown TMDs, mainly  $\text{MoSe}_2$ [400]–[402],  $\text{WS}_2$ [220], [403],  $\text{MoTe}_2$ [404] and  $\text{WTe}_2$  [405] have also been reported, as well as MBE grown h-BN[406], [407].

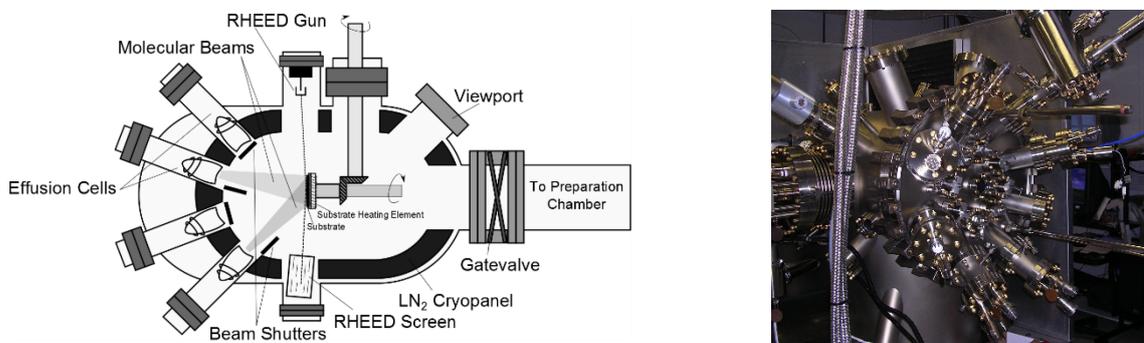


Figure 28. Left: MBE operation sketch. Right: MBE experimental setup[408].

MBE-growth of both silicene[159], [160], [409]–[411] and germanene[168], [412] on specific metallic substrates has been reported, and allows for further investigation of the properties of these relatively new 2D materials.

### 2.5.3 Chemical Vapor Deposition

Chemical Vapor Deposition (CVD) is the most widely used technique to deposit thin films, and has been the cornerstone for semiconductor based devices for decades[413]. It is extremely versatile, as it allows for the deposition of either crystalline or amorphous films from gaseous, solid or liquid precursors. Many specific types of CVD exist, such as plasma-enhanced CVD (PECVD), cold/hot wall CVD and many more, and the selection of the type to be used is dictated by the deposited material.

Graphene CVD is versatile and can be performed by many techniques (thermal-CVD, PECVD ...), and from a variety of precursors (liquid, gaseous or solid), and the first report of the deposition of large area graphene ( $\text{cm}^2$ ) dates back to 2009[414]. Many other reports have followed since[415]–[418], and high quality graphene films were deposited on a wide variety of substrates with carrier mobilities up to  $30\,000\text{ cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1}$ . Another advantage of CVD is that it allows for the deposition of extremely large quantities of high quality material; deposition of  $50\text{ cm}$  graphene films with carrier mobilities around  $10^4\text{ cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1}$  has been reported[395]. CVD has also been used to deposit other 2D materials, namely TMDs: deposition of  $\text{MoS}_2$  [390], [419],  $\text{MoSe}_2$  [218],  $\text{MoTe}_2$ [219], [420],  $\text{WS}_2$ [421],  $\text{WSe}_2$ [421], [422] and  $\text{WTe}_2$ [221], [423] on various substrates has been reported.

Due to its extreme versatility and its ability to deposit large surfaces, CVD is the most prominently used deposition technique for large scale production of thin films and 2D materials.

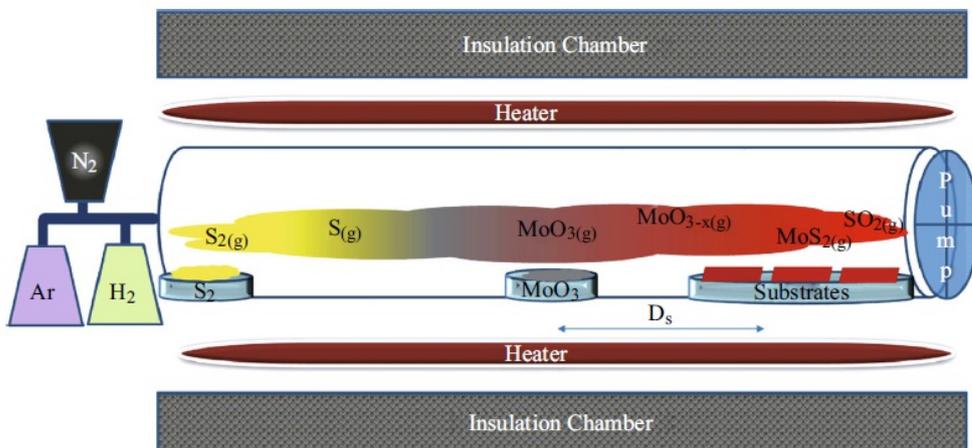


Figure 29. Deposition of MoS<sub>2</sub> flakes via CVD[424].

### 2.5.4 Thermal decomposition of SiC

Graphene growth by thermal decomposition of silicon carbide is another technique that holds potential and attracts a lot of interest. By annealing either the Si-face (0001) or the C face ( $000\bar{1}$ ) of hexagonal SiC the silicon atoms evaporate, leaving behind a reconstructed graphene layer on top of a semiconducting SiC substrate. The resulting graphene is therefore ready for electronic applications and does not need to be transferred onto another substrate, as is the case with several other techniques.

The thermal decomposition of bulk SiC at extremely high temperatures ( $>2000^\circ\text{C}$ ) was originally reported in 1965[425], and was expanded upon and enhanced ( $800^\circ\text{C}$  in UHV) roughly a decade later[426]. Although the graphene produced by this method yielded satisfactory electronic properties[427], it was composed of small grains (from 30 to 200 nm) of varying thickness[428], [429] and was therefore not usable for industrial applications. Since then however, the process has been refined[430]–[432]: by annealing SiC at specific temperatures and in an argon or hydrogen environment, the evaporation rate of silicon is reduced, favoring more precise graphene reconstruction. Graphene samples obtained by similar techniques have shown domains as large as  $50\times 50\ \mu\text{m}$ [433], and in some cases, extremely high electronic mobilities ( $>11\ 000\ \text{cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1}$ )[431].

However, the use of bulk, hexagonal SiC limits wafer sizes and cost and hinders wide machining processes. The use of cubic silicon carbide (3C-SiC) (which can be grown on top or regular silicon via MBE) as a substrate for graphene growth could help overcome these limitations[434]–[436], and has been widely investigated for several years[437]–[439].

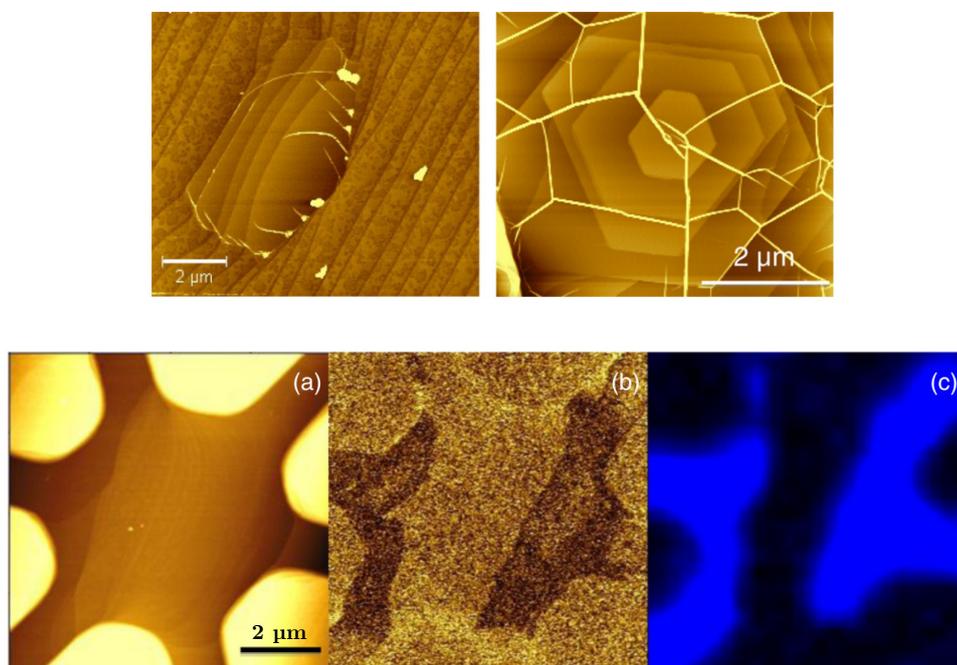


Figure 30. Top: AFM images of graphene on the ( $000\bar{1}$ ) face of SiC. Bottom: (a) AFM topology map, (b) EFM amplitude scan and (c) Raman 2D band intensity map of monolayer graphene growth on a pre-patterned ( $000\bar{1}$ ) face of SiC [440].

Several other graphene production techniques have been developed, such as growth on metals by precipitation[441] for instance, but are not detailed here as this short rundown focused on the main deposition techniques for graphene and other 2D materials.

Now that general nanoelectronics and the scaling issues they face as well as some 2D materials that could potentially bring part of a solution have been introduced, I will present the models and methods used to perform my PhD work.



# Chapter 3

## Physical models used

In this section, I will introduce the theoretical models and approaches I used to investigate the potential TMDs hold for nanoelectronic applications.

First, I will present the Tight-Binding (TB) method, which is the approach used in this work to model the materials themselves as well as their electronic properties. A short introduction on the theory of the TB method will be given, before delving into the actual TB model I used to simulate the considered TMDs, as well as the modifications and adaptations I made upon this model for our quantum transport computation needs.

I will then give some insight on the non-equilibrium Green's function (NEGF) method that was used to model electronic transport through the nanodevices investigated. A short introduction on this method will be presented, followed by information on the implementation of this theoretical framework in our transport code.

### 3.1 Tight-binding formalism

#### 3.1.1 Theoretical overview

Many different approaches can be used to model materials and their electronic properties, and the selection of the correct approach based on the system studied is paramount. Density Function Theory (DFT) for instance, as a true ab-initio method, is well-suited for investigating and predicting features such as the band structure of a small set of atoms; it however cannot be used for larger structures containing thousands of atoms such as transistors and other devices. For such systems, simplified and approximated methods referred to as semi-empirical methods are required. These include the tight-binding approach, empirical pseudo-potential approaches, or the use of k.p Hamiltonians for instance.

Based on the LCAO (linear combination of atomic orbitals) method introduced in 1928 by Finklestein and Horowitz[442], the tight-binding method was introduced by Slater and Koster in 1954[443] as a tool to calculate the band structure of solids.

In this theoretical overview, I will very briefly introduce the theory and the concepts necessary to the understanding of the TB model used and developed over the course of my PhD. Far more in-depth and complete information, as well as examples, can be found in the following references[444]–[449].

As its name suggests, the TB approach considers the electrons to be tightly-bound to their respective atoms. As such, a general set of wave functions can be deduced from the superposition of the wave functions located on each atom, assuming they interact in a limited capacity with surrounding atoms and potentials. The overall Hamiltonian of the structure at position  $\vec{r}$  can therefore be approximated by the sum of all atomic Hamiltonians  $H_{at}$  of the  $n$  atoms located at  $\vec{R}_n$ , along with the interaction potential between the atoms  $\Delta U$ . (In order to improve notation readability, only one orbital per atom is considered in this example)

$$H(\vec{r}) = \sum_n H_{at}(\vec{r} - \vec{R}_n) + \Delta U(\vec{r}) \quad (7)$$

The eigenfunction  $\psi(\vec{r})$  to this Hamiltonian is the solution to the time-independent Schrödinger's equation

$$H(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \quad (8)$$

and can therefore be expressed as a superposition of individual atomic wave functions  $\varphi(\vec{r} - \vec{R}_n)$ , and calculated as a linear combination of the atomic orbitals.

$$\psi(\vec{r}) = \sum_n d(\vec{R}_n)\varphi(\vec{r} - \vec{R}_n) \quad (9)$$

By combining Eqs.(9) and (8) we can obtain Eq.(10) which, when multiplied by  $\varphi^*(\vec{r} - \vec{R}_m)$  and integrated over real space, leads to eqs(11) and (12).

$$H(\vec{r}) \sum_n d(\vec{R}_n)\varphi(\vec{r} - \vec{R}_n) = E \sum_n d(\vec{R}_n)\varphi(\vec{r} - \vec{R}_n) \quad (10)$$

$$\sum_n \left[ \int d\vec{r} \left( \varphi^*(\vec{r} - \vec{R}_m) H(\vec{r}) \varphi(\vec{r} - \vec{R}_n) \right) \right] d(\vec{R}_n) = E \sum_n \left[ \int d\vec{r} \left( \varphi^*(\vec{r} - \vec{R}_m) \varphi(\vec{r} - \vec{R}_n) \right) \right] d(\vec{R}_n) \quad (11)$$

$$\sum_n h_{mn} d(\vec{R}_n) = E \sum_n s_{mn} d(\vec{R}_n) \quad (12)$$

In Eq.(12),  $h_{mn}$  is an element of the Hamiltonian matrix, and  $s_{mn}$  is the overlap between the  $m$  and  $n$  atomic orbitals.

By replacing  $H(\vec{r})$  by Eq.(8) in  $h_{mn}$ , this matrix element can be decomposed as

$$h_{mn} = \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) \left[ \sum_k H_{at}(\vec{r} - \overline{R}_k) + \Delta U(\vec{r}) \right] \varphi(\vec{r} - \overline{R}_n) \quad (13)$$

$$\Leftrightarrow \sum_k \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) H_{at}(\vec{r} - \overline{R}_k) \varphi(\vec{r} - \overline{R}_n) + \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) \Delta U(\vec{r}) \varphi(\vec{r} - \overline{R}_n) \quad (14)$$

$$\Leftrightarrow \sum_k \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) \varepsilon_k \delta_{kn} \varphi(\vec{r} - \overline{R}_n) + \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) \Delta U(\vec{r}) \varphi(\vec{r} - \overline{R}_n) \quad (15)$$

in which  $\delta_{kn}$  is the Kronecker delta, i.e  $\delta_{kn} = 1$  if  $k = n$  and 0 otherwise.

Therefore, the  $h_{mn}$  Hamiltonian matrix element is finally

$$h_{mn} = \varepsilon_n \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) \varphi(\vec{r} - \overline{R}_n) + \int d\vec{r} \varphi^*(\vec{r} - \overline{R}_m) \Delta U(\vec{r}) \varphi(\vec{r} - \overline{R}_n) \quad (16)$$

$$h_{mn} = \varepsilon_n \cdot s_{mn} + t_{mn} \quad (17)$$

In this expression of the matrix element,  $\varepsilon_n$  is called the on-site energy and represents the energy of the atomic orbital of the  $n$ -th atom in vacuum, without taking the neighboring orbitals into account; on the contrary,  $t_{mn}$  represents the coupling between the atomic orbitals found on the  $m$ -th and  $n$ -th atom and is often referred to as the hopping integral. In the case where several orbitals are considered on each atom, each orbital is categorized by an on-site energy as well as couplings to every other orbital, including those located on the same atom.

In practice, a tight-binding Hamiltonian is an  $N \times N$  matrix, where  $N$  is the number of orbitals in the considered system (in the case of a periodic system,  $N$  is the number of orbitals in the unit cell to be repeated). Diagonal elements of this matrix contain the on-site energies, while off-diagonal elements contain the hopping elements between the corresponding orbitals.

As an example, the creation of the TB Hamiltonian for a 2D infinite graphene sheet is shown over the next few pages, and used to calculate the band structure of the system.

### 3.1.2 Building a TB Hamiltonian for graphene

For this example, we will investigate a 2D infinite graphene sheet as shown in Figure 31 a) (periodic along the x and y axes), and apply a very simple tight-binding model in which we consider a single orbital per atom, and only first-neighbor coupling. Many different unit cells can be used to reduce the size of this system, and we chose the one shown in Figure 31 b) that contains 4 atoms, and therefore 4 orbitals.

The resulting tight-binding Hamiltonian is therefore the following  $4 \times 4$  matrix

$$H_0 = \begin{bmatrix} \varepsilon_A & t_{AB} & t_{AC} & t_{AD} \\ t_{BA} & \varepsilon_B & t_{BC} & t_{BD} \\ t_{CA} & t_{CB} & \varepsilon_C & t_{CD} \\ t_{DA} & t_{DB} & t_{DC} & \varepsilon_D \end{bmatrix}$$

Since we only consider first-neighbor coupling, it can be simplified to

$$H_0 = \begin{bmatrix} \varepsilon_A & t_{AB} & 0 & 0 \\ t_{BA} & \varepsilon_B & t_{BC} & 0 \\ 0 & t_{CB} & \varepsilon_C & t_{CD} \\ 0 & 0 & t_{DC} & \varepsilon_D \end{bmatrix}$$

This matrix describes all orbital interactions in the unit cell of the system, but is not sufficient to fully describe the material.

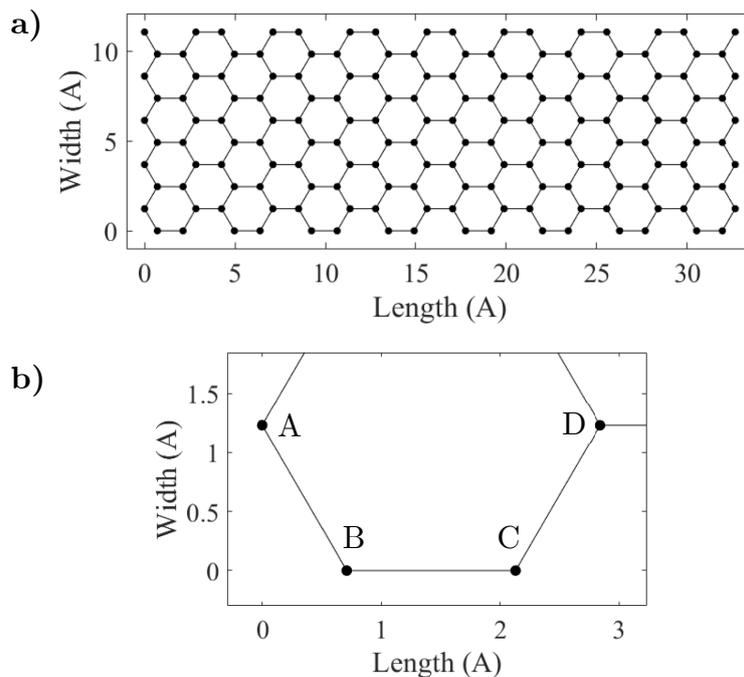


Figure 31. a) 2D infinite graphene sheet (periodic along x and y).  
b) Unit cell used in this example, and naming convention for the atoms.

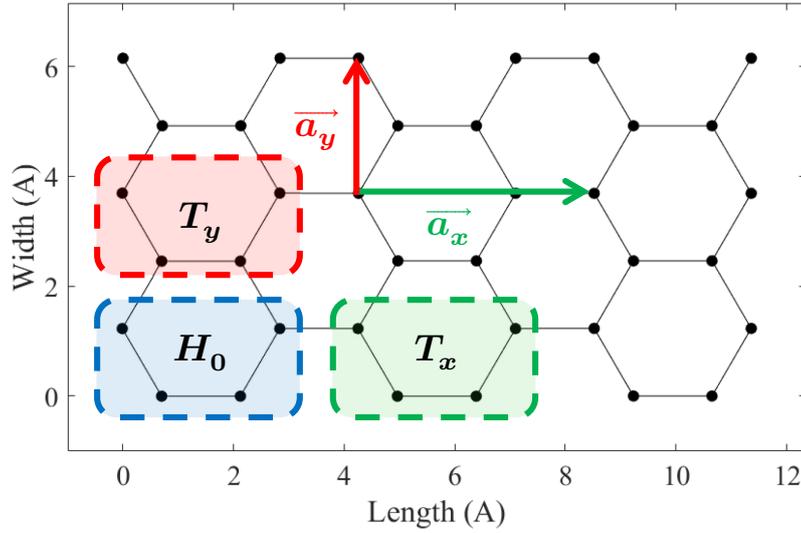


Figure 32. Representation of the unit vectors and neighboring unit cells

In order to compute the bandstructure of a 2D infinite graphene sheet, we have to take periodicity into account. The unit vectors used to reproduce a 2D infinite sheet from the chosen unit cell are  $\vec{a}_x$  and  $\vec{a}_y$  as shown in Figure 32 ( $a_c = 2.46 \text{ \AA}$  is the graphene lattice constant)

$$\vec{a}_x = \begin{pmatrix} \sqrt{3}a_c \\ 0 \end{pmatrix} \quad \vec{a}_y = \begin{pmatrix} 0 \\ a_c \end{pmatrix}$$

We must now create Hamiltonians describing the coupling of the unit cell with the neighboring cells, as shown in Figure 32:

- $T_x$  describes the coupling between the blue unit cell and the green one, which are connected by  $\vec{a}_x$
- $T_y$  describes the coupling between the blue unit cell and the red one, which are connected by  $\vec{a}_y$

These coupling Hamiltonians will therefore be the following  $4 \times 4$  matrices

$$T_x = \begin{bmatrix} t_{A_0A_x} & t_{A_0B_x} & t_{A_0C_x} & t_{A_0D_x} \\ t_{B_0A_x} & t_{B_0B_x} & t_{B_0C_x} & t_{B_0D_x} \\ t_{C_0A_x} & t_{C_0B_x} & t_{C_0C_x} & t_{C_0D_x} \\ t_{D_0A_x} & t_{D_0B_x} & t_{D_0C_x} & t_{D_0D_x} \end{bmatrix} \quad T_y = \begin{bmatrix} t_{A_0A_y} & t_{A_0B_y} & t_{A_0C_y} & t_{A_0D_y} \\ t_{B_0A_y} & t_{B_0B_y} & t_{B_0C_y} & t_{B_0D_y} \\ t_{C_0A_y} & t_{C_0B_y} & t_{C_0C_y} & t_{C_0D_y} \\ t_{D_0A_y} & t_{D_0B_y} & t_{D_0C_y} & t_{D_0D_y} \end{bmatrix}$$

in which  $t_{M_0N_x}$  ( $t_{M_0N_y}$ ) is the coupling between the M atom of the blue unit cell and the N atom of the green (red) unit cell.

By looking at the atomic arrangement of the structure (Figure 32), we can easily eliminate all couplings beyond the first neighbor

$$T_x = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ t_{D_0A_x} & 0 & 0 & 0 \end{bmatrix} \quad T_y = \begin{bmatrix} 0 & t_{A_0B_y} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & t_{D_0C_y} & 0 \end{bmatrix}$$

In the end, we therefore have 3 tight-binding Hamiltonians that describe the whole system. In most simple graphene TB models, the on-site energies are set to 0 eV and the first neighbor hopping parameters  $t_G$  to -2.7 eV.

$$H_0 = \begin{bmatrix} 0 & t_G & 0 & 0 \\ t_G & 0 & t_G & 0 \\ 0 & t_G & 0 & t_G \\ 0 & 0 & t_G & 0 \end{bmatrix} \quad T_x = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ t_G & 0 & 0 & 0 \end{bmatrix} \quad T_y = \begin{bmatrix} 0 & t_G & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & t_G & 0 \end{bmatrix}$$

The bandstructure at a given wave vector  $(k_x, k_y)$  can now be calculated as the eigenvalues of the following  $H_{tot}$  matrix

$$H_{tot} = H_0 + T_x \cdot e^{ik_x \cdot |\vec{a}_x|} + T_x^\dagger \cdot e^{-ik_x \cdot |\vec{a}_x|} + T_y \cdot e^{ik_y \cdot |\vec{a}_y|} + T_y^\dagger \cdot e^{-ik_y \cdot |\vec{a}_y|}$$

$$H_{tot} = t_G \begin{bmatrix} 0 & 1 + e^{ik_y \cdot |\vec{a}_y|} & 0 & e^{-ik_x \cdot |\vec{a}_x|} \\ 1 + e^{-ik_y \cdot |\vec{a}_y|} & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 + e^{-ik_y \cdot |\vec{a}_y|} \\ e^{ik_x \cdot |\vec{a}_x|} & 0 & 1 + e^{ik_y \cdot |\vec{a}_y|} & 0 \end{bmatrix}$$

Because the unit cell chosen contains 4 atoms, the basis contains 4 orbitals and therefore 4 eigenvalues will be obtained for each given wave vector  $(k_x, k_y)$ .

The resulting bandstructure projected along  $k_x$ ,  $k_y$  as well as in 3D is shown in Figure 33.

As this simple example has shown, building a TB Hamiltonian is a matter of carefully selecting the unit cell and therefore the unit vectors that come with it. Then, we simply need to fill out the Hamiltonian matrices depending on the position of the considered orbitals, and calculate the total Hamiltonian for sets of wave vectors  $(k_x, k_y)$ .

Evidently, as the investigated system gets more complicated and the basis gets bigger (considering several orbitals per atom for instance, as well as second or even third neighbor coupling), the creation of the matrices gets more complicated and requires careful consideration and observation.

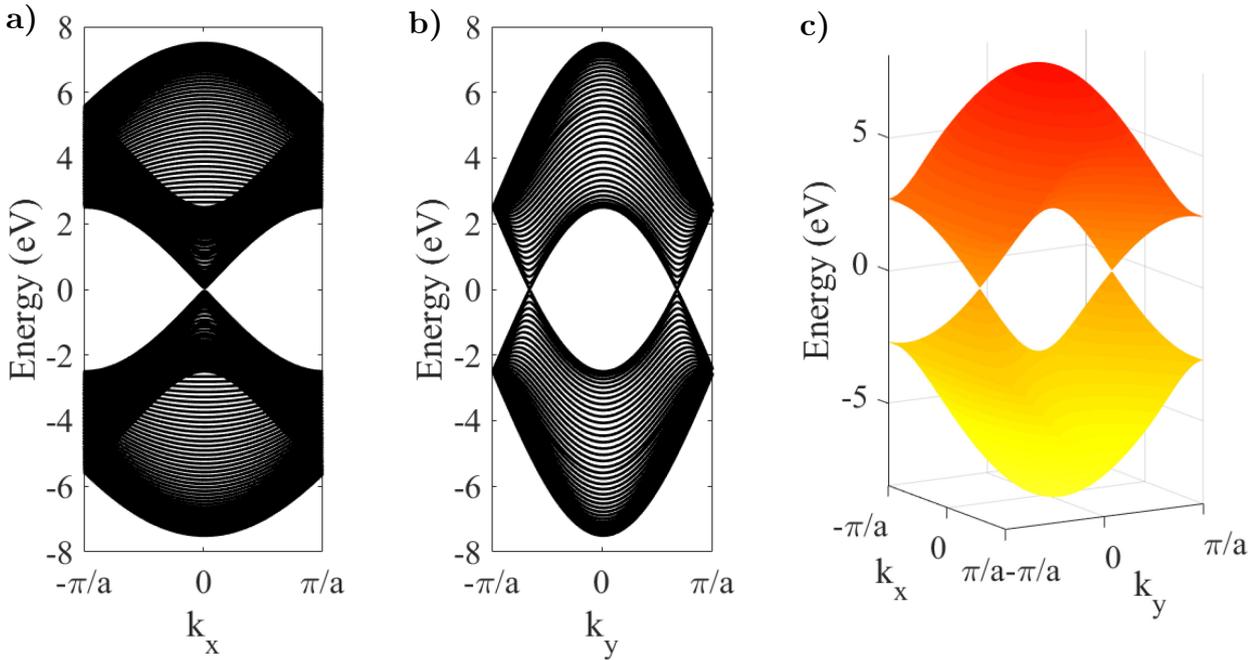


Figure 33. Bandstructure of a 2D infinite graphene sheet projected along  $k_x$  (a),  $k_y$  (b) and in 3D (c).

Finding and selecting a TB model in the literature with information on the on-site energies and coupling parameters in the desired material is of course required. Most TB models are fitted onto DFT bandstructures and aim for accuracy around the band gap.

Now that I have quickly introduced the underlying theory of the tight-binding formalism and shown how to build tight-binding Hamiltonians, I will present the TB model I used for TMDs.

Although I had to modify it in order to use it in our transport calculations, it is important to introduce the model in its original form to present a clear picture of the theoretical approach to material modelling used in this work.

### 3.1.3 Base TB model used for TMDs

The TB model used was developed by Fang et al. and is detailed in [1]. I will briefly introduce its features and parameters here, but I refer the reader to the original paper for much more in-depth information and insight about this model. Some paragraphs are cited directly from the original paper, and will be clearly marked as quotations.

This tight-binding model is based on the Wannier transformation of ab-initio DFT calculations, and takes into account the effect of strain in the limit of a slowly varying in-plane strain field. Although the model is applicable to graphene and hBN as well as TMDs, our interest lies solely with the latter.

Before we get to the TMD model itself, I will cite the article to convey some general information about the construction of the model and the way strain is handled.

As a summary of the work presented, the original paper states:

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*Here we generalize the Wannier method to monolayers with in-plane strain and derive the relevant models, compatible with the underlying crystal symmetry. In increasing order of complexity with the underlying orbital content, we construct such tight-binding models for graphene, hexagonal boron nitride (hBN) and four TMDCs. These models are valid in the presence of slowly-varying in-plane strain field, providing the electronic coupling to long-wavelength in-plane acoustic phonon modes. We also derive the corresponding effective low-energy theories coupled with the strain field, consistent with the effective models derived from the principles of symmetry group representations, which by itself can identify all symmetry-allowed terms but is insufficient to provide estimates for the values of the coupling constants involved. Our ab initio Wannier tight binding approach thus complements the powerful symmetry group analysis, gives accurate values of the parameters in the model, and empowers calculations of large-scale structures of strained materials.*

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Detailing the way strain is modelled, Fang et. al state

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*The slowly varying in-plane strain field can be described by the displacement deformation vector field  $u = (u_x(x, y), u_y(x, y))$ . The coordinates  $x$  and  $y$  denote the undistorted crystal coordinate, which is mapped to the new position  $(x + u_x(x, y), y + u_y(x, y))$  in space. Since a constant displacement field introduces no physical changes to the layers, the strain field is characterized by the derivative of  $u$ , defined in tensor form*

$$u_{ij} = (\partial_i u_j + \partial_j u_i)/2$$

*where  $i, j = x, y$ . This second rank tensor can be decomposed in the trace scalar part  $(u_{xx} + u_{yy})$ , and the doublet  $(u_{xx} - u_{yy}, -2u_{xy})$  which forms a two-dimensional irreducible representation of the  $C_{3v}$  symmetry group of the crystal. There is also a rotational piece,  $\omega_{xy} = \partial_x u_y - \partial_y u_x$  which we take  $\omega_{xy} = 0$  by choosing the proper set of coordinates.*

*We can further simplify the modeling by applying the local density approximation to the strain effects, that is, by assuming locally the tight-binding parameters are approximated by the strained periodic crystal with constant  $u_{ij}$ . In the following, these strain model parameters are extracted from the Wannier transformation of DFT calculations with periodic unit cells for the uniformly strained crystals. A structure with non-uniform strain can be modeled by combining these local-strain tight-binding parameters which have only long-wavelength variations compared to the lattice constants. The key steps in constructing these microscopic Hamiltonians are:*

*(i) In linear elastic theory, the deformed microscopic displacement vector  $v' = (v'_x, v'_y, v'_z)$  between atomic sites is*

$$\begin{aligned} v'_x &= v_x + v_x \partial_x u_x + v_y \partial_y u_x \\ v'_y &= v_y + v_x \partial_x u_y + v_y \partial_y u_y \\ v'_z &= v_z \end{aligned} \tag{A1}$$

*with  $v = (v_x, v_y, v_z)$  the unstrained vector.*

Though these relations hold for the primitive lattice vectors, strictly speaking this approximation, the Cauchy-Born rule, is only valid for a Bravais lattice with a single atom basis. For a strained primitive unit cell with multiple basis atoms, the relative position or orientation of these atoms varies, in addition to the relations prescribed by Eq.(A1). For example, in layered materials such as phosphorene, TMDCs and puckered graphene-like materials, there is a height variation in the position of individual atoms under strain.[...]We include the height corrections for the chalcogen atoms in TMDCs by generalizing the above Cauchy-Born approximation.

(ii) To incorporate the strain effects in the tight-binding Hamiltonians, the hopping integral between orbitals on different sites is assumed to scale with the pair distance, known as the central force approximation. Up to leading order linear response, the strained hopping integral can be approximated as

$$t'_{\alpha\beta} = t_{\alpha\beta}^0 + \mu \delta_{\alpha\beta} \cdot (\delta_{\alpha\beta} \cdot \Delta) \cdot u \quad \mu = \frac{1}{|\delta_{\alpha\beta}|} \frac{dt_{\alpha\beta}}{d|\delta_{\alpha\beta}|} \quad (A2)$$

Some empirical models go beyond the linear order by proposing a functional form which depends on the pair distance, such as exponential functions or algebraic functions of  $|r|$ . For the orbitals that are not  $s$ -like, the hopping integrals within the two-center Slater-Koster approximation can be decomposed into various channels related to the angular momentum projection, such as the  $\sigma$  and  $\pi$  bonds in  $p$ - $p$  orbital coupling. The scaling can be applied to each channel as a function of pair distance. In general, the scaling of the hopping integral reflects the shapes of the orbitals and the changes in the crystal field potential. These translate into more involved forms of scaling beyond merely the pair distance dependence. For example, if the crystal is stretched along a direction that is perpendicular to the bond, the central force approximation would dictate no change for the hopping, which is not accurate. Here, we derive the models up to linear order in the strain and beyond the central force approximation. All the terms that couple  $(u_{xx} + u_{yy})$ ,  $(u_{xx} - u_{yy})$  and  $u_{xy}$  are retained in the Hamiltonian, and their forms are constrained by the underlying crystal symmetry. Thus, the hoppings along a bond acquire corrections when the crystal is stretched along the perpendicular direction to the bond, which captures the local environment change. Many layered materials involve orbitals beyond  $s$ -like ones, and have a more complicated geometry for atomic configurations and relative orientations.

(iii) Treatments of strain effects on tight-binding Hamiltonians typically involve only the scaling of hopping terms and neglect the variations for on-site energy terms. The on-site energy variations will be relevant for a layer with non-uniform strain field, also called the deformation potential. We extract the relevant potential information and work function from DFT calculations and define the energy reference point to be zero at the vacuum level outside the layer. In experiments, the presence of a substrate or encapsulating layers, and the charge redistribution in the layer with non-uniform strain result in further modification of the electrostatic environment, the screening for interactions and hence of the onsite terms.

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In practice, the displacements  $(u_{xx} + u_{yy})$ ,  $(u_{xx} - u_{yy})$  and  $(-2u_{xy})$  act as modifiers when properly building the tight-binding Hamiltonian matrices.

The TMD model takes into account the five  $d$  orbitals of the metal atoms and the three  $p$  orbitals of the chalcogen atoms. Since the TMD unit cell is  $MX_2$ , this results in a  $5 + 3 \times 2 = 11$  orbital basis, which in turn results in seven valence bands and four conduction bands in the obtained band structure.

In this 11 orbital basis, the orbitals are grouped in four sectors ( $A, B, C, D$ ) and classified as odd (o) or even (e) with respect to an  $xy$  mirror plane symmetry as follows

$$\Psi_A^{(o)} = \begin{pmatrix} \phi_x = d_{xz} \\ \phi_y = d_{yz} \end{pmatrix} \quad \Psi_B^{(o)} = \begin{pmatrix} \phi_x = p_x \\ \phi_y = p_y \\ \phi_z = p_z \end{pmatrix}$$

$$\Psi_C^{(e)} = \begin{pmatrix} \phi_x = d_{xy} \\ \phi_y = d_{x^2-y^2} \\ \phi_z = d_{z^2} \end{pmatrix} \quad \Psi_D^{(e)} = \begin{pmatrix} \phi_x = p_x \\ \phi_y = p_y \\ \phi_z = p_z \end{pmatrix}$$

The coupling matrices that will be used to create the total Hamiltonian couple these sectors, and are therefore  $3 \times 3$ ,  $2 \times 3$ ,  $3 \times 2$  or  $2 \times 2$  matrices (depending on whether the  $A$  sector is involved) and are

$$\langle \Psi_i | H | \Psi_j \rangle = \begin{bmatrix} H_{xx} & H_{xy} & H_{xz} \\ H_{yx} & H_{yy} & H_{yz} \\ H_{zx} & H_{zy} & H_{zz} \end{bmatrix}$$

where  $H_{mn} = \langle \phi_m^i | H | \phi_n^j \rangle$ .

Thanks to the three-fold symmetry of the hexagonal lattice of TMDs (see Figure 34), the number of necessary parameters is greatly reduced and only a third of the matrices are given here (from which the rest can be derived through a rotation operation).

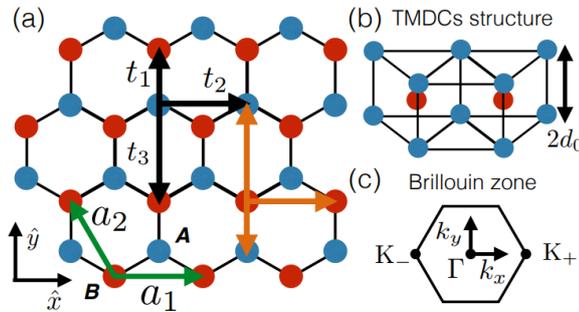


Figure 34. a) Top view of the TMD lattice in which the orange arrows represent the couplings for which matrices are given here (black arrows relate to hBN and graphene). b) Side view of a TMD. c) First Brillouin zone in the momentum space [1]

The model takes into account first (M-X), second (M-M or X-X) and third (M-X) neighbor coupling, and the corresponding coupling Hamiltonians matrices contain parameters given in Appendix A. These matrices are of the type  $H_{IJ}^{(n)}$  where  $I, J = [A, B, C, D]$  and  $n$  indicates the order of coupling (same atom, first/second/third neighbor).

The on-site couplings  $H_{JJ}^{(0)}$  include the on-site energy as well as the hybridization between orbitals located on the same atom.  $H_{AA}^{(0)}$ ,  $H_{BB}^{(0)}$ ,  $H_{CC}^{(0)}$  and  $H_{DD}^{(0)}$  are calculated as

$$H_{JJ}^{(0)} = \begin{bmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_1 & 0 \\ 0 & 0 & \epsilon_0 \end{bmatrix} + (u_{xx} + u_{yy}) \begin{bmatrix} \alpha_1^{(0)} & \alpha_1^{(0)} & 0 \\ 0 & \alpha_1^{(0)} & 0 \\ 0 & 0 & \alpha_1^{(0)} \end{bmatrix} \\ + (u_{xx} - u_{yy}) \begin{bmatrix} \beta_0^{(0)} & 0 & 0 \\ 0 & -\beta_0^{(0)} & \beta_1^{(0)} \\ 0 & \beta_1^{(0)} & 0 \end{bmatrix} + 2u_{xy} \begin{bmatrix} 0 & \beta_0^{(0)} & \beta_1^{(0)} \\ \beta_0^{(0)} & 0 & 0 \\ \beta_1^{(0)} & 0 & 0 \end{bmatrix}$$

The first and third neighbor couplings both follow the same pattern and occur between the A/B and C/D sectors. Third neighbor coupling between the A/B sectors is neglected. Therefore,  $H_{BA}^{(1)}$ ,  $H_{DC}^{(1)}$  and  $H_{DC}^{(3)}$  are calculated as

$$H_{IJ}^{(n)} = \begin{bmatrix} t_0^{(n)} & 0 & 0 \\ 0 & t_1^{(n)} & t_2^{(n)} \\ 0 & t_3^{(n)} & t_4^{(n)} \end{bmatrix} + (u_{xx} + u_{yy}) \begin{bmatrix} \alpha_0^{(n)} & 0 & 0 \\ 0 & \alpha_1^{(n)} & \alpha_2^{(n)} \\ 0 & \alpha_3^{(n)} & \alpha_4^{(n)} \end{bmatrix} \\ + (u_{xx} - u_{yy}) \begin{bmatrix} \beta_0^{(n)} & 0 & 0 \\ 0 & \beta_1^{(n)} & \beta_2^{(n)} \\ 0 & \beta_3^{(n)} & \beta_4^{(n)} \end{bmatrix} + 2u_{xy} \begin{bmatrix} 0 & \beta_5^{(n)} & \beta_6^{(n)} \\ \beta_7^{(n)} & 0 & 0 \\ \beta_8^{(n)} & 0 & 0 \end{bmatrix}$$

The second neighbor couplings  $H_{AA}^{(2)}$ ,  $H_{BB}^{(2)}$ ,  $H_{CC}^{(2)}$  and  $H_{DD}^{(2)}$  are calculated as

$$H_{JJ}^{(2)} = \begin{bmatrix} t_0^{(2)} & t_3^{(2)} & t_4^{(2)} \\ -t_3^{(2)} & t_1^{(2)} & t_5^{(2)} \\ -t_4^{(2)} & t_5^{(2)} & t_2^{(2)} \end{bmatrix} + (u_{xx} + u_{yy}) \begin{bmatrix} \alpha_0^{(2)} & \alpha_3^{(2)} & \alpha_4^{(2)} \\ -\alpha_3^{(2)} & \alpha_1^{(2)} & \alpha_5^{(2)} \\ -\alpha_4^{(2)} & \alpha_5^{(2)} & \alpha_2^{(2)} \end{bmatrix} \\ + (u_{xx} - u_{yy}) \begin{bmatrix} \beta_0^{(2)} & \beta_3^{(2)} & \beta_4^{(2)} \\ -\beta_3^{(2)} & \beta_1^{(2)} & \beta_5^{(2)} \\ -\beta_4^{(2)} & \beta_5^{(2)} & \beta_2^{(2)} \end{bmatrix} + 2u_{xy} \begin{bmatrix} 0 & \beta_6^{(2)} & \beta_7^{(2)} \\ \beta_6^{(2)} & 0 & \beta_8^{(2)} \\ \beta_7^{(2)} & -\beta_8^{(2)} & 0 \end{bmatrix}$$

As mentioned above, these are only a third of the coupling matrices (those referring to atoms connected by the  $\delta$  bonds shown in orange in Figure 34). The other couplings can be obtained by a three-fold rotation of these  $\delta$  bonds, so the corresponding Hamiltonians can be determined as such

$$H_{\delta'}(u_{xx}, u_{yy}, 2u_{xy}) = \mathcal{U}_R^\dagger \cdot H_\delta(u_{xx}', u_{yy}', 2u_{xy}') \mathcal{U}_R$$

where  $\delta'$  is a  $\frac{2\pi}{3}$  counter-clockwise rotation of the original  $\delta$  bond, in which the updated displacements  $u_{xx}'$ ,  $u_{yy}'$  and  $2u_{xy}'$  are calculated as

$$u_{xx}' = \frac{u_{xx}}{4} + \frac{3u_{yy}}{4} - \frac{\sqrt{3}u_{xy}}{2} \quad u_{yy}' = \frac{3u_{xx}}{4} + \frac{u_{yy}}{4} + \frac{\sqrt{3}u_{xy}}{2}$$

$$2u_{xy}' = \frac{\sqrt{3}u_{xx}}{2} - \frac{\sqrt{3}u_{yy}}{2} - u_{xy}$$

and  $\mathcal{U}_R$ , the  $3 \times 3$  matrix describing the rotation operation, is as follows

$$\mathcal{U}_R = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

By applying this rotation operation twice (to obtain  $\delta'$  and  $\delta''$ ), all couplings in the material will be taken into account. The bandstructure of the considered TMDs can therefore be calculated.

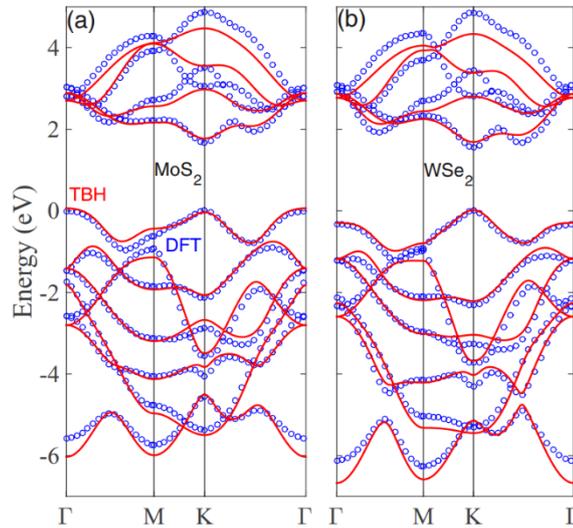


Figure 35. Comparison of the TB bandstructure against DFT results for MoS<sub>2</sub> and WSe<sub>2</sub> [450]

Figure 35, which is pulled from the original article[450] about the TB model that did not yet include the effect of strain, compares the bandstructures obtained with this TB Hamiltonian for  $\text{MoS}_2$  and  $\text{WSe}_2$  against DFT calculations in which the interaction between ionic cores and valence electrons is described by pseudopotentials of the projector augmented wave (PAW) type, and the exchange-correlation energy of electrons is treated within the generalized gradient approximation (GGA) as parametrized by Perdew, Burke, and Ernzerhof (PBE). As we can see, the TB model yields very good results close to the band gap. As we get further away from the gap however, the accuracy of the model falters because it was calibrated to accurately reproduce the highest VB and lowest CB, which is where our interests lie. The model is therefore well suited for our needs.

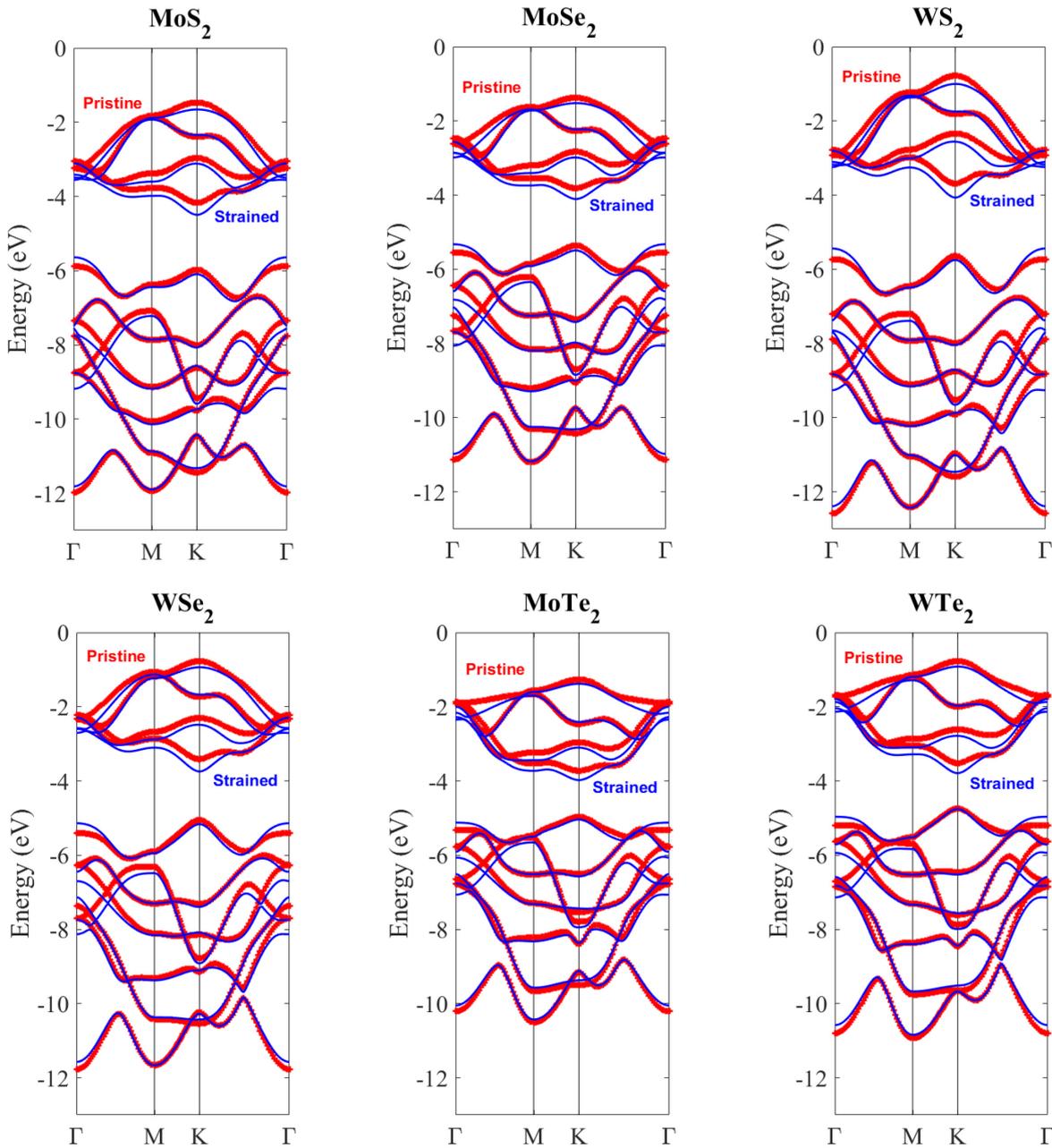


Figure 36. Bandstructures for the six considered TMD in their pristine form (red crosses) and under a 2.5% tensile strain (blue lines)

Figure 36 shows the impact of a 2.5% tensile strain on the bandstructures of all six considered TMDs along high symmetry points in the first Brillouin zone. The bandstructure is modified mainly around the K and  $\Gamma$  high symmetry points, namely the bottom of the CB is pulled towards lower energies at the K point, while the VB is pulled towards higher energies at the  $\Gamma$  point. The band gap is therefore reduced.

This tendency is highlighted in Figure 37, which shows the impact of compressive and tensile strains on the band alignment and band gap in all six considered TMDs. Compressive strains tend to pull both VB and CB towards higher energies, although at different rates, only slightly impacting the band gap. Tensile strains however, as evidenced above, pull the VB up and the CB down, resulting in a dramatic decrease in band gap. Note that while these band gaps are direct in pristine TMDs, these become indirect under any strain roughly  $< -1\%$  or  $> 2\%$ .

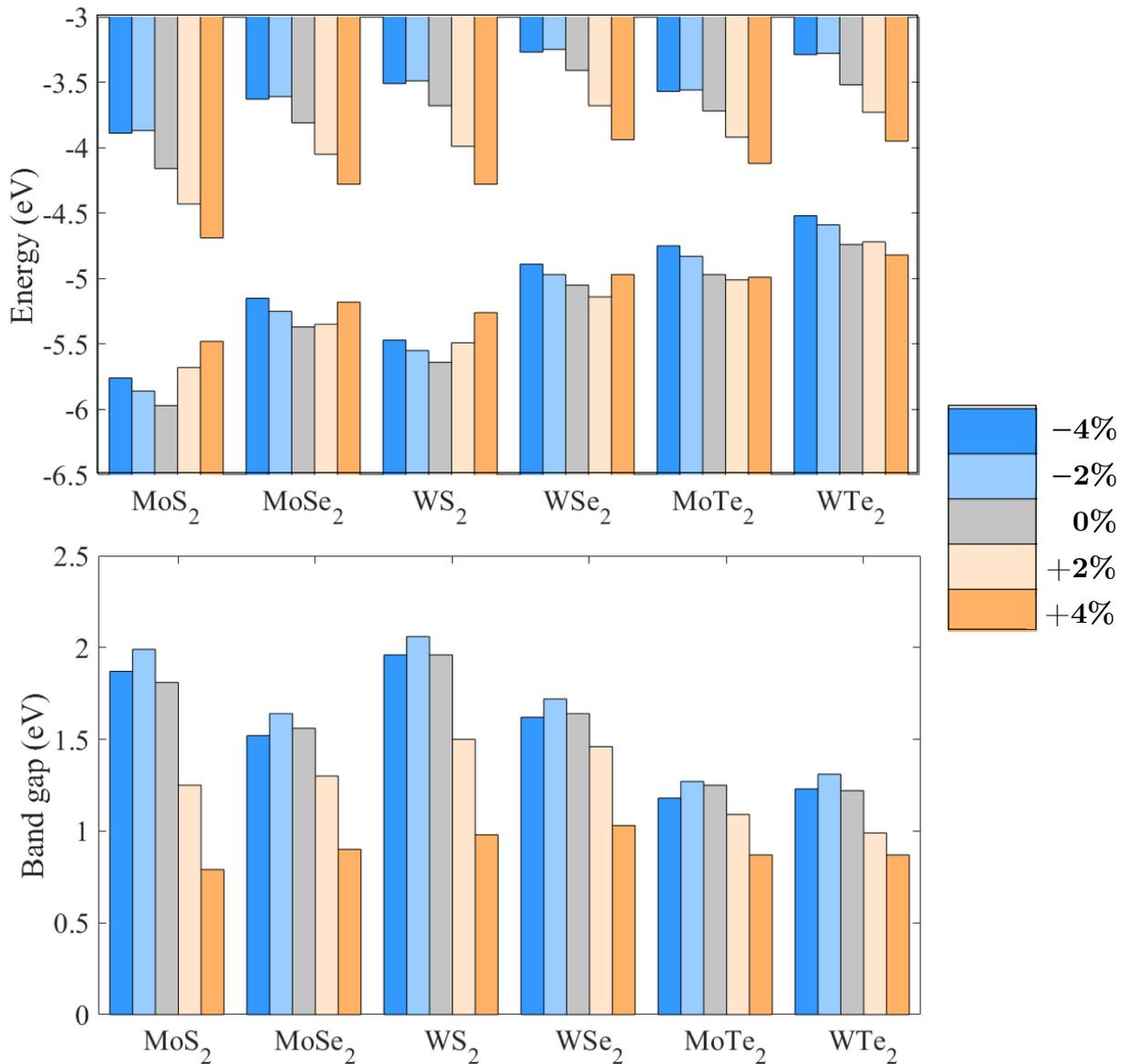


Figure 37. Influence of compressive ( $<0$ ) and tensile ( $>0$ ) strains of the highest VB and lowest CB (a) and on the band gap (b) of all six considered TMDs. In a), the vacuum level is set to 0 eV

The goal of this section was solely to properly describe the TB model used and to show the examples of materials modelled with it, therefore I will get further into the detail of band alignment and the possibilities strain offers in this regard in later sections.

Tables containing the TB parameters are given in Appendix A. Please note that in the original article, only 4 TMDs are modelled ( $\text{MoS}_2$ ,  $\text{WS}_2$ ,  $\text{MoSe}_2$  and  $\text{WSe}_2$ ). Due to the interest  $\text{WTe}_2$  and  $\text{MoTe}_2$  had for use in TFETs (mainly low band gap and interesting band alignment with other TMDs), I contacted Shiang Fang, the author of the original article, to inquire about the availability of such parameters for  $\text{WTe}_2$  and  $\text{MoTe}_2$ . Although the work needed to derive those TB parameters had not yet been undertaken, he accepted due to my request, which was the starting point of a fruitful collaboration.

The tables presented in Appendix A contain the TB parameters for all six TMDs.

### 3.1.4 Basis modification

Now that the base TB model and its features have been introduced, I will present the modifications I made upon this model so that it would suit our computing needs.

As will be shown later, due to the NEGF formalism we use for transport calculations, the unit cell we use must be reproducible along the transport direction; this is not the case of the base, 11-orbital  $\text{MX}_2$  unit cell (yellow area in Figure 38). A change in the basis was therefore necessary.

We elected to use a  $(\text{MX}_2)_2$  unit cell (red area in Figure 38) that can be easily reproduced along the transport direction, resulting in a 22-orbital basis. However, the original TB model was not built for this change in unit cell, mainly due to the way it describes coupling between sectors in discrete matrices.

In order to facilitate this basis modification and the creation of the  $22 \times 22$  Hamiltonians that will follow, a reworking of the model was necessary.

My goal was to create  $11 \times 11$  matrices that describe the coupling of orbitals based solely on the positions of the atoms on which they are located; this way, building the final  $22 \times 22$  Hamiltonians would only be a matter of adding up the correct matrices based on the atomic bonds considered.

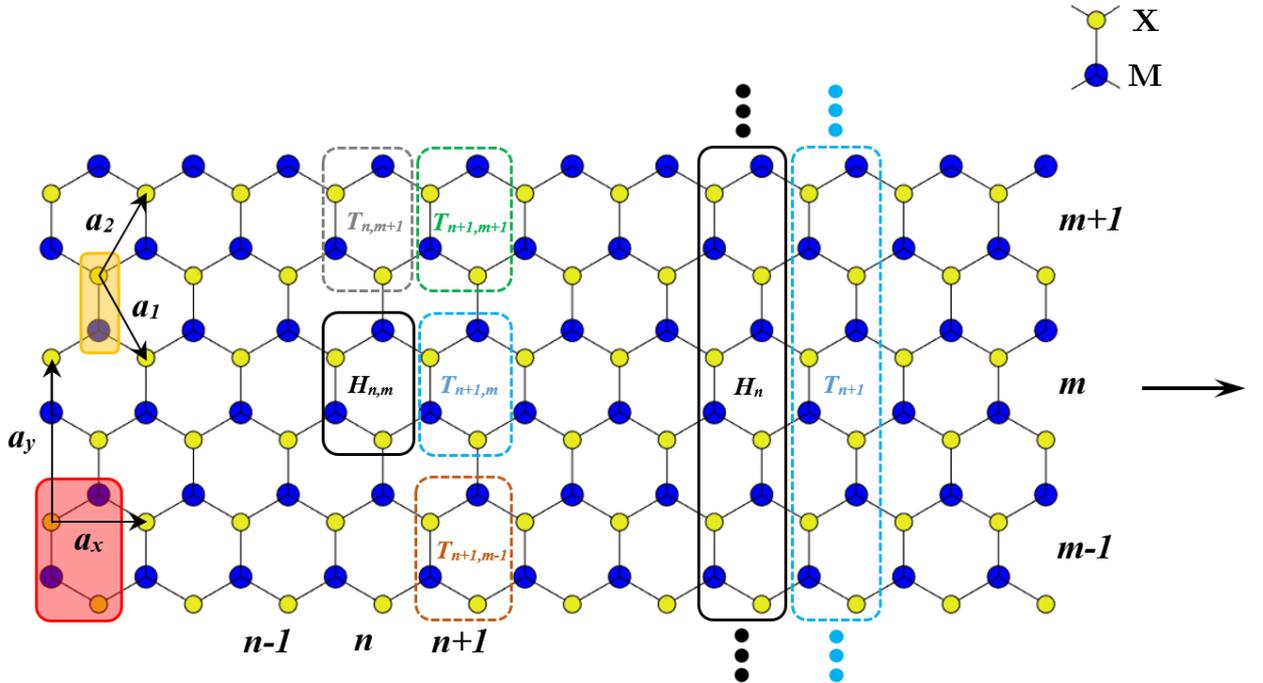


Figure 38. Atomic arrangement of TMDs. The yellow area represents the base, 11-orbital unit cell with the corresponding unit vectors  $a_1$  and  $a_2$ , while the red area represents the 22-orbital unit cell used in our work, with its unit vectors  $a_x$  and  $a_y$ .  $H_{n,m}$  and  $H_n$  are the Hamiltonians of a single unit cell and a single material “layer”, respectively. Finally,  $T_{i,j}$  and  $T_i$  represent the coupling of the  $(i,j)$  unit cell, and the coupling of the  $(i)$  layer with the  $(n)$  layer, respectively. Transport direction is indicated by the arrow.

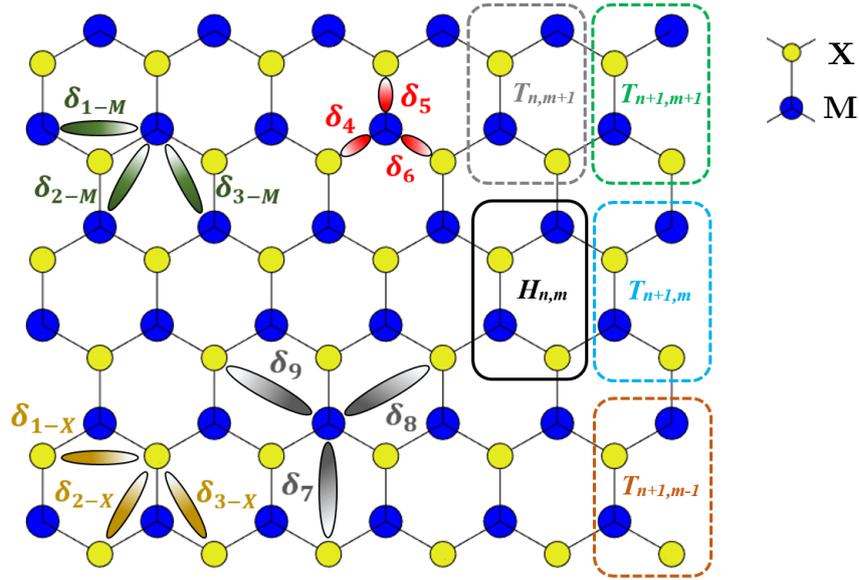


Figure 39. Lattice arrangement of a TMD. The highlighted  $\delta_1$  through  $\delta_9$  areas represent the coupling matrices between various orbitals on the considered atoms.

There are nine “position pairs” that lead to coupling in this TMD arrangement, referred to as  $\delta_1$  to  $\delta_9$  in Figure 39. In this figure, coupling direction follows the color gradient (for instance,  $\delta_4$  to  $\delta_9$  represent the coupling from X to the M atom)

- $\delta_1$ ,  $\delta_2$  and  $\delta_3$  represent the coupling between orbitals located on atoms of the same type (either M-M or X-X coupling); they are split into separate  $\delta_{i-X}$  and  $\delta_{i-M}$  matrices to simplify Hamiltonian construction later on.
- $\delta_4$ ,  $\delta_5$  and  $\delta_6$  represent the first-neighbor coupling between orbitals located on atoms of a different type (X-M coupling).
- $\delta_7$ ,  $\delta_8$  and  $\delta_9$  represent the third-neighbor coupling between orbitals located on atoms of a different type (X-M coupling).

In the original model, only a third of the coupling Hamiltonians are given, from which the rest can be calculated due to the rotational symmetry of the structure. The same approach is used here: only  $\delta_1$ ,  $\delta_5$  and  $\delta_7$  are given, and the rest can be determined from those thanks to  $\mathcal{A}_R$ , an  $11 \times 11$  version of the  $\mathcal{U}_R$  matrix which describes the rotation operation.

The full,  $11 \times 11$  matrices for  $\delta_1$ ,  $\delta_5$ ,  $\delta_7$  and  $\mathcal{U}_R$  are given on the next page, where  $H_{XY_{ij}}^{(n)}$  is the  $(i,j)$  element of the  $H_{XY}^{(n)}$  matrix.





Thanks to this matrix,  $\delta_3$  can be determined from  $\delta_1$ ,  $\delta_4$  from  $\delta_5$ , and  $\delta_8$  from  $\delta_7$  as follows:

$$\delta_3 = \mathcal{A}_R^\dagger \delta_1 \mathcal{A}_R \quad \delta_4 = \mathcal{A}_R^\dagger \delta_5 \mathcal{A}_R \quad \delta_8 = \mathcal{A}_R^\dagger \delta_7 \mathcal{A}_R$$

From these newly calculated matrices,  $\delta_2$ ,  $\delta_6$  and  $\delta_9$  can be calculated by applying the same rotation operation

$$\delta_2^\dagger = \mathcal{A}_R^\dagger \delta_3 \mathcal{A}_R \quad \delta_6 = \mathcal{A}_R^\dagger \delta_4 \mathcal{A}_R \quad \delta_9 = \mathcal{A}_R^\dagger \delta_8 \mathcal{A}_R$$

It is worth noting that by applying  $\mathcal{A}_R$  on  $\delta_3$ , we obtain  $\delta_2^\dagger$  and not  $\delta_2$  because, due to the way the vectors were defined (see Figure 39),  $\vec{\delta}_3$  becomes  $-\vec{\delta}_2$  via this  $\frac{2\pi}{3}$  counter-clockwise rotation.

Finally, an  $11 \times 11$  matrix containing the on-site energies has to be created before we can construct the  $22 \times 22$  Hamiltonians based on the new, expanded unit cell

$$E_i = \begin{bmatrix} H_{AA11}^{(0)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & H_{AA22}^{(0)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & H_{BB11}^{(0)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & H_{BB22}^{(0)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & H_{BB33}^{(0)} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & H_{CC11}^{(0)} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & H_{CC22}^{(0)} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & H_{CC33}^{(0)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & H_{DD11}^{(0)} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & H_{DD22}^{(0)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & H_{DD33}^{(0)} \end{bmatrix}$$

Now that we have all  $11 \times 11$  matrices describing the on-site energies and all possible couplings in the material, they can be used to create the  $22 \times 22$  Hamiltonians that will describe the material in the new basis.

As is shown in Figure 40, five unique  $22 \times 22$  Hamiltonians are necessary to fully describe the material

- $H_{n,m}$ : the Hamiltonian of the new unit cell
- $T_{n+1,m}, T_{n,m+1}, T_{n+1,m-1}$  and  $T_{n+1,m+1}$ : the coupling Hamiltonian of the  $(n, m)$  unit cell with the  $(i, j)$  cell.

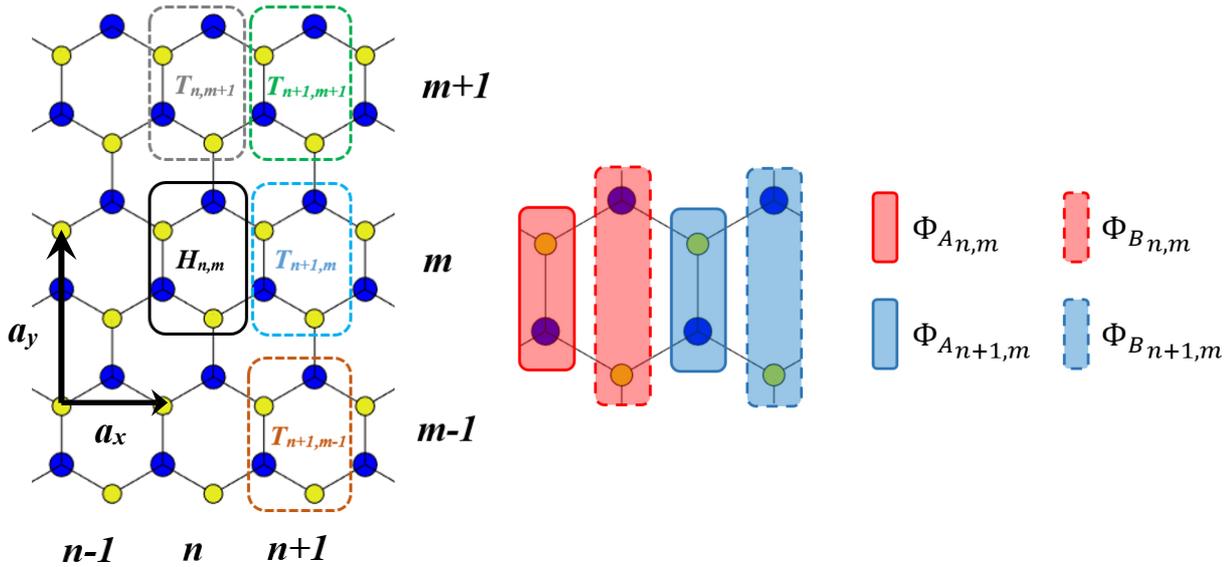


Figure 40. Left:  $22 \times 22$  Hamiltonians that will have to be created to take all couplings (up to third neighbor) into account:  $H_{n,m}$  is the Hamiltonian of a single unit cell, and  $T_{i,j}$  represents the coupling of the  $(n,m)$  cell with the  $(i,j)$  unit cell. Right: Visualisation of the A and B sublattices in two adjacent unit cells. Full (dashed) lines represent the A (B) sublattice, and their color indicates the unit cell to which they belong (red for the  $(n,m)$  unit cell, blue for the  $(n+1,m)$  unit cell).

The new  $(MX_2)_2$  unit cell is twice the size of the original one, and can be decomposed into 2 sublattices A and B as shown in Figure 40. Each of them is associated with the original  $11 \times 11$  basis

$$\Phi_A = |d_{xz}\rangle, |d_{yz}\rangle, |p_x\rangle, |p_y\rangle, |p_z\rangle, |d_{xy}\rangle, |d_{x^2-y^2}\rangle, |d_{z^2}\rangle, |p_x\rangle, |p_y\rangle, |p_z\rangle$$

$$\Phi_B = |d_{xz}\rangle, |d_{yz}\rangle, |p_x\rangle, |p_y\rangle, |p_z\rangle, |d_{xy}\rangle, |d_{x^2-y^2}\rangle, |d_{z^2}\rangle, |p_x\rangle, |p_y\rangle, |p_z\rangle$$

Each  $22 \times 22$  Hamiltonian is therefore composed of four  $11 \times 11$  matrices  $\Psi_{X_{i,j} \cdot Y_{k,l}}$ . Those matrices are linear combinations of the  $\delta_i$  and  $E_i$  matrices, and describe the coupling between the X sub-lattice of the  $(i,j)$  unit cell and the Y sublattice of the  $(k,l)$  unit cell. They can be constructed by carefully observing Figure 39 and selecting the couplings that apply to the case considered, just as we did in the example TB for graphene.

$H_{n,m}$  (the Hamiltonian of the unit cell) and  $T_{i,j}$  (the Hamiltonians describing the coupling between the unit cell and adjacent cells), can be constructed as

$$H_{n,m} = \begin{pmatrix} \Psi_{A_{n,m} \cdot A_{n,m}} & \Psi_{B_{n,m} \cdot A_{n,m}} \\ \Psi_{A_{n,m} \cdot B_{n,m}} & \Psi_{B_{n,m} \cdot B_{n,m}} \end{pmatrix} \quad T_{i,j} = \begin{pmatrix} \Psi_{A_{n,m} \cdot A_{i,j}} & \Psi_{B_{n,m} \cdot A_{i,j}} \\ \Psi_{A_{n,m} \cdot B_{i,j}} & \Psi_{B_{n,m} \cdot B_{i,j}} \end{pmatrix}$$

with  $i = [n-1, n, n+1]$  and  $j = [m-1, m, m+1]$ .

Finally, we obtain

$$\begin{aligned}
H_{n,m} &= \begin{pmatrix} E_i + \delta_5 + \delta_5^\dagger & \delta_6^\dagger + \delta_4 + \delta_{3-X} + \delta_{2-M}^\dagger \\ \delta_6 + \delta_4^\dagger + \delta_{3-X}^\dagger + \delta_{2-M} & E_i + \delta_7 + \delta_7^\dagger \end{pmatrix} \\
T_{n+1,m} &= \begin{pmatrix} \delta_{1-X}^\dagger + \delta_{1-M}^\dagger + \delta_8^\dagger + \delta_9 & 0 \\ \delta_{3-M} + \delta_{2-X}^\dagger + \delta_6^\dagger + \delta_4 & \delta_{1-X}^\dagger + \delta_{1-M}^\dagger \end{pmatrix} & T_{n,m+1} &= \begin{pmatrix} \delta_7 & \delta_{2-X}^\dagger \\ \delta_{3-M}^\dagger & \delta_5^\dagger \end{pmatrix} \\
T_{n+1,m-1} &= \begin{pmatrix} 0 & 0 \\ \delta_{3-X} & \delta_9 \end{pmatrix} & T_{n+1,m+1} &= \begin{pmatrix} 0 & 0 \\ \delta_{2-M}^\dagger & \delta_8^\dagger \end{pmatrix}
\end{aligned}$$

as the five unique Hamiltonians needed to fully describe the material.

Those couplings are symmetrical with respect to the original  $(n, m)$  unit cell, so that

$$T_{n-k,m-l} = T_{n+k,m+l}^\dagger$$

From these Hamiltonian, the bandstructure at a given wave vector  $\vec{k}$  can be calculated as we did in the example about graphene. As they are  $22 \times 22$  matrices, we obtain twice as many bands as with the original  $\text{MX}_2$  unit cell and its 11-orbital basis

$$\begin{aligned}
H_{tot} &= H_{n,m} + T_{n+1,m} \cdot e^{i\vec{k} \cdot \overrightarrow{a_{n+1,m}}} + T_{n+1,m}^\dagger \cdot e^{-i\vec{k} \cdot \overrightarrow{a_{n+1,m}}} \\
&\quad + T_{n,m+1} \cdot e^{i\vec{k} \cdot \overrightarrow{a_{n,m+1}}} + T_{n,m+1}^\dagger \cdot e^{-i\vec{k} \cdot \overrightarrow{a_{n,m+1}}} \\
&\quad + T_{n+1,m+1} \cdot e^{i\vec{k} \cdot \overrightarrow{a_{n+1,m+1}}} + T_{n+1,m+1}^\dagger \cdot e^{-i\vec{k} \cdot \overrightarrow{a_{n+1,m+1}}} \\
&\quad + T_{n+1,m-1} \cdot e^{i\vec{k} \cdot \overrightarrow{a_{n+1,m-1}}} + T_{n+1,m-1}^\dagger \cdot e^{-i\vec{k} \cdot \overrightarrow{a_{n+1,m-1}}}
\end{aligned}$$

in which

$$\begin{aligned}
\overrightarrow{a_{n+1,m}} = \overrightarrow{a_x} &= \begin{pmatrix} a_{MX_2} \\ 0 \end{pmatrix} & \overrightarrow{a_{n,m+1}} = \overrightarrow{a_y} &= \begin{pmatrix} 0 \\ \sqrt{3}a_{MX_2} \end{pmatrix} \\
\overrightarrow{a_{n+1,m+1}} = \overrightarrow{a_x} + \overrightarrow{a_y} &= \begin{pmatrix} a_{MX_2} \\ \sqrt{3}a_{MX_2} \end{pmatrix} & \overrightarrow{a_{n+1,m-1}} = \overrightarrow{a_x} - \overrightarrow{a_y} &= \begin{pmatrix} a_{MX_2} \\ -\sqrt{3}a_{MX_2} \end{pmatrix}
\end{aligned}$$

where  $a_{MX_2} = 3.18 \text{ \AA}$  for  $\text{MoS}_2$  and  $\text{WS}_2$ .

3.31  $\text{ \AA}$  for  $\text{MoSe}_2$  and  $\text{WSe}_2$ .

3.55  $\text{ \AA}$  for  $\text{MoTe}_2$  and  $\text{WTe}_2$ .

The bandstructure of all 6 TMDs along high symmetry points in the first Brillouin zone is shown in Figure 41. Due to the basis modification resulting in the  $22 \times 22$  Hamiltonians, 22 bands are obtained. As expected for all six materials, this bandstructure is in agreement with the one obtained in the original basis: the additional bands originate from the band folding that occurs due to the doubling of the unit cell along the  $k_x$  direction, and is highlighted in Appendix B.

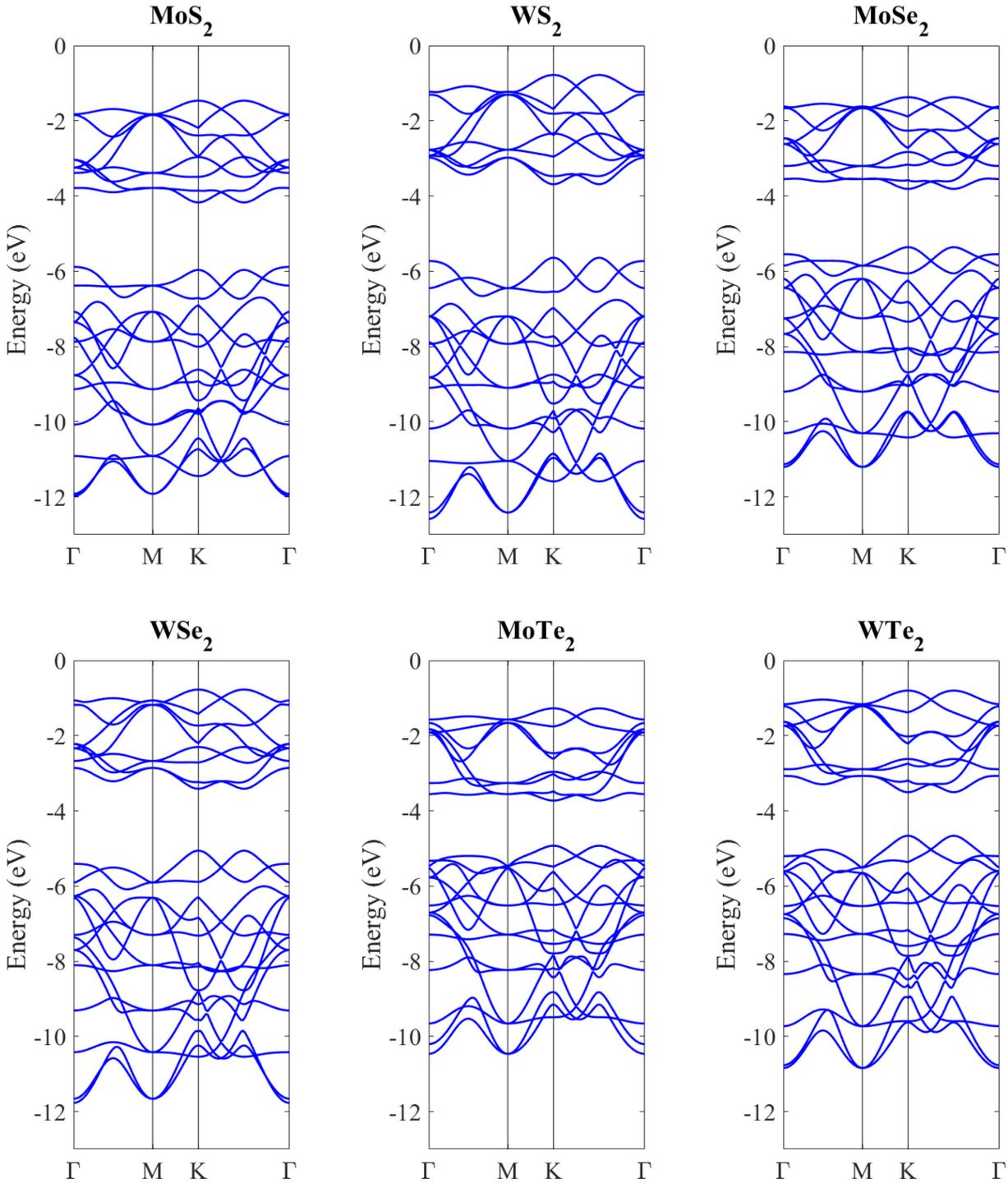


Figure 41. Bandstructure for all six TMDs as obtained with the  $22 \times 22$  Hamiltonians resulting from the expanded unit cell.

### 3.1.5 Band alignment in TMDs

As mentioned in Section 1.4, band alignment is paramount in TFETs due to their reliance on band-to-band-tunneling.

The band alignment obtained between the TMDs considered in this TB model will therefore strongly dictate TFET performance and impact the heterostructures we choose to investigate. As a reminder, carriers tunnel from the source VB to the channel CB in an n-type TFET, therefore in the case of heterostructure-based TFETs, optimal operation requires a high VB and a low CB.

Pristine TMDs obtained with this TB model yield the band alignment shown in Figure 42 (the vacuum level is set to 0 eV). MoS<sub>2</sub> has by far the lowest CB at  $-4.17$  eV, and is therefore a great candidate for use as the channel/drain material. As for the source material, we can see that WTe<sub>2</sub> yields the highest VB at  $-4.74$  eV, followed by MoTe<sub>2</sub> and WSe<sub>2</sub> around  $-5.0$  eV. These TMDs could therefore be used as a source material in the heterojunction TFETs envisioned.

However, this band alignment is only valid for TMDs in their pristine form, therefore when no strain is applied. As mentioned in Section 2.2.2, the lattice parameter in TMDs is dictated by the chalcogen atom and ranges from  $3.18$  Å for MoS<sub>2</sub> and WS<sub>2</sub> to  $3.55$  Å for MoTe<sub>2</sub> and WTe<sub>2</sub>, and  $3.31$  Å for MoSe<sub>2</sub> and WSe<sub>2</sub>.

In the case of a heterojunction between two TMDs with different chalcogen atoms, the lattice parameter will not be the same on either side of the interface, and the material will experience strain so that lattice matching can be reached.

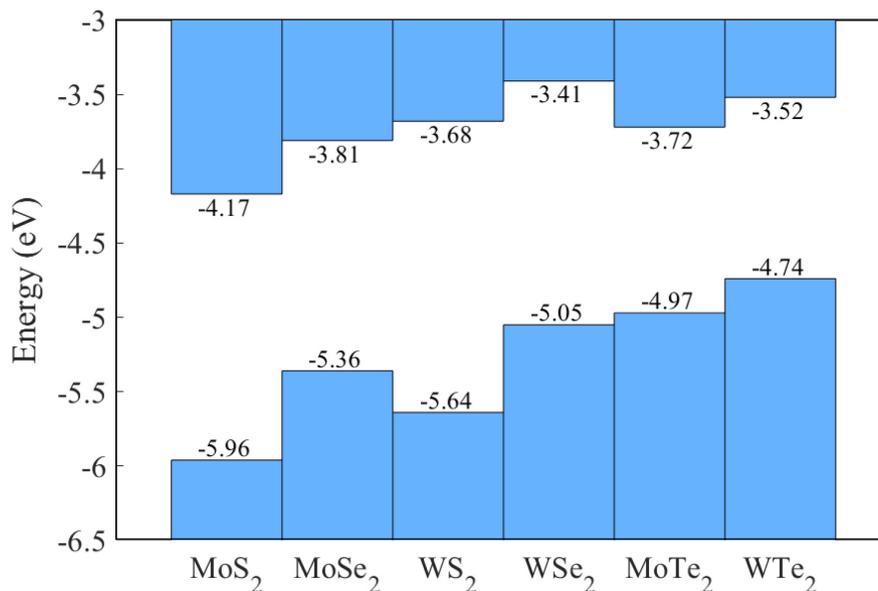


Figure 42. Band alignment in pristine TMDs obtained by using this TB model. The vacuum level is set to 0 eV.

In the case of the MoSe<sub>2</sub>/MoS<sub>2</sub> and WSe<sub>2</sub>/MoS<sub>2</sub> heterojunctions, we approximate that only MoS<sub>2</sub> will experience strain. Therefore, a tensile strain of roughly 4.3% will be applied onto MoS<sub>2</sub> to reach  $a_{ASe_2} = 3.31 \text{ \AA}$  (as mentioned in Chapter 2., TMDs can withstand strains of up to 20% before breaking). Under this strain, the bandstructure of MoS<sub>2</sub> is heavily modified, as shown in Figure 43 (left): the CB is substantially lowered, but its minimum remains at the *K* point, while the VB is also modified, its maximum shifting to the  $\Gamma$  point.

Figure 43 (right) shows the lowest CB and highest VB of both pristine and strained MoS<sub>2</sub>, and of MoSe<sub>2</sub> (top) and WSe<sub>2</sub> (bottom). It highlights the impact of strain on the band alignment of these materials, and on the benefits this strain has for TFET operation. Band offset is reduced by 680 meV in both cases, resulting in a 510 meV band offset for MoSe<sub>2</sub>/MoS<sub>2</sub> and 200 meV for WSe<sub>2</sub>/MoS<sub>2</sub>.

In this case, the strain caused by the lattice mismatch will probably benefit TFET performance of the MoSe<sub>2</sub>/MoS<sub>2</sub> and WSe<sub>2</sub>/MoS<sub>2</sub> heterojunctions.

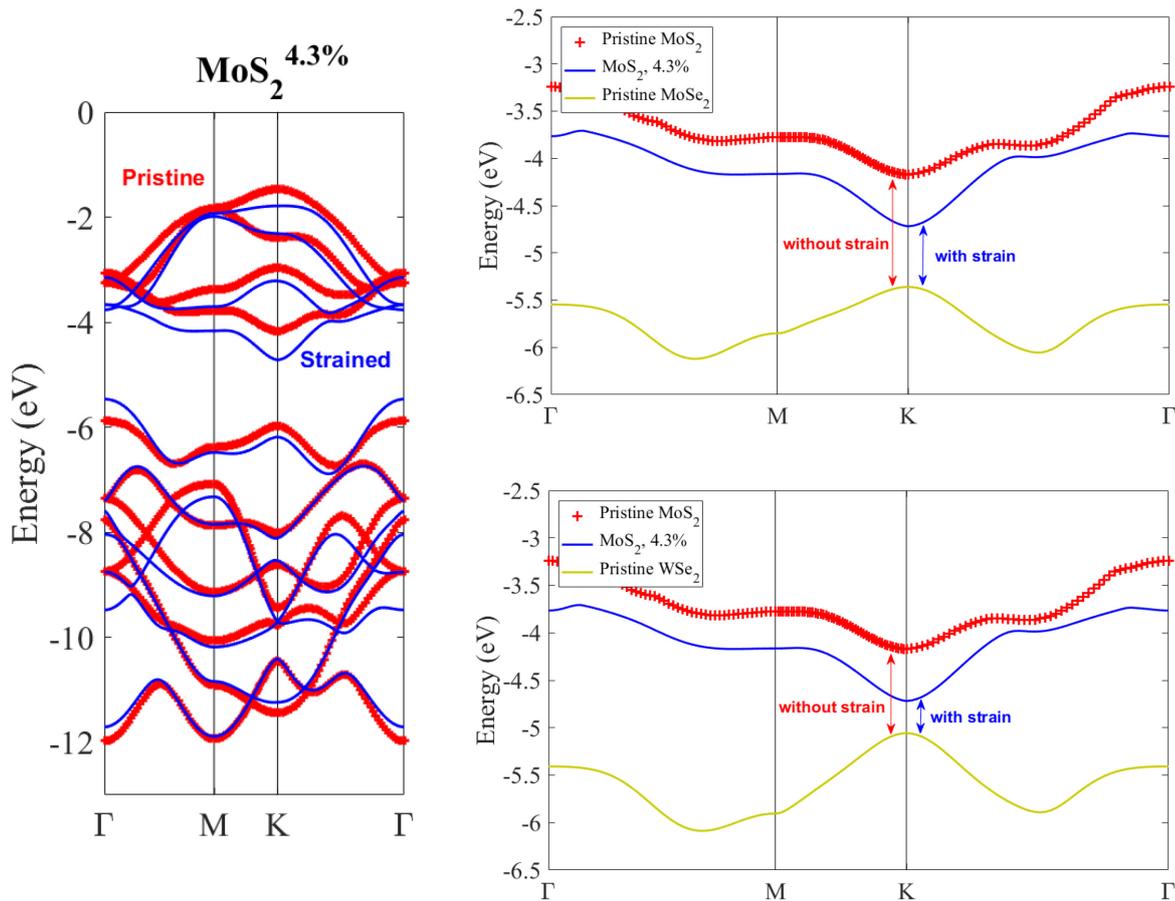


Figure 43. Left: Bandstructure of MoS<sub>2</sub> in pristine form (red crosses) and under a 4.3% tensile strain (blue curves). Right: Highest VB of MoSe<sub>2</sub> (top), WSe<sub>2</sub> (bottom) (gold curve) and lowest CB of both pristine and strained MoS<sub>2</sub> (resp. red crosses and blue curve)

In the case of the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  heterojunctions, the lattice mismatch is much greater ( $0.37 \text{ \AA}$ ). Therefore, we approximate that both materials will experience strain so that a common lattice parameter of  $a = 3.35 \text{ \AA}$  is reached. Therefore, a tensile strain of roughly 5.3% will be applied onto  $\text{MoS}_2$ , while a compressive strain of roughly 5.6% will be applied onto  $\text{MoTe}_2$  and  $\text{WTe}_2$ . Under this strain, the bandstructure of all three materials are heavily modified, as shown in Figure 44: in  $\text{MoS}_2$  the changes are the same as those mentioned before, while in  $\text{MoTe}_2$  and  $\text{WTe}_2$  the minimum of the CB shifts outside of the  $K$  point, while the VB is heavily pulled towards higher energies, its maximum remaining in the  $K$  point.

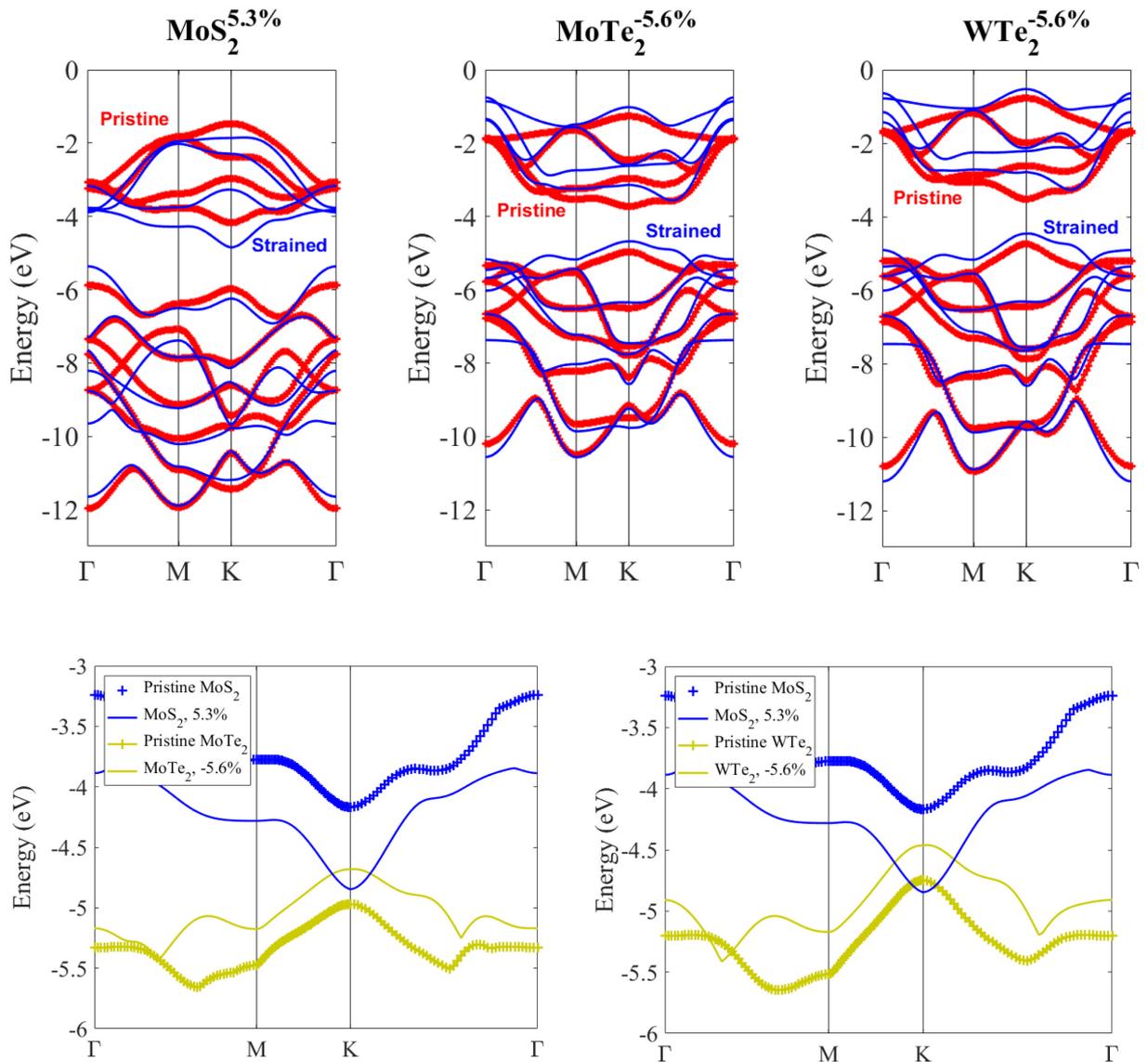


Figure 44. Top: Bandstructures of  $\text{MoS}_2$ ,  $\text{MoTe}_2$  and  $\text{WTe}_2$  both in their pristine form (red crosses) and under the necessary strains to reach lattice matching (blue curves). Bottom: Highest VB of  $\text{MoTe}_2$  and  $\text{WTe}_2$  in their pristine form and under strain (resp. gold crosses and gold curve), and lowest CB of  $\text{MoS}_2$  both in its pristine form and under strain (resp. blue crosses and blue curve)

Figure 44 (bottom) once again highlights the benefits of this strain on the band alignment. In the case of the  $\text{MoTe}_2/\text{MoS}_2$  heterojunction, the band offset goes from roughly 800 meV without strain to  $-170$  meV under strain: the  $\text{MoTe}_2$  VB maximum is actually higher than the bottom of the  $\text{MoS}_2$  CB. This configuration is known as a “broken gap”, and is expected to be extremely beneficial to TFET performance.

The  $\text{WTe}_2/\text{MoS}_2$  heterojunction yields similar results: the band offset goes from roughly 570 meV without strain to  $-390$  meV under strain.

Figure 45 shows the band alignment that occurs in all heterojunction TFETs when the proper strain is applied, and highlights the broken gap configuration of the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  heterojunctions.

As will be shown in Chapter 6, this strain-induced “broken gap” allows the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  heterojunction TFETs to yield extremely promising results

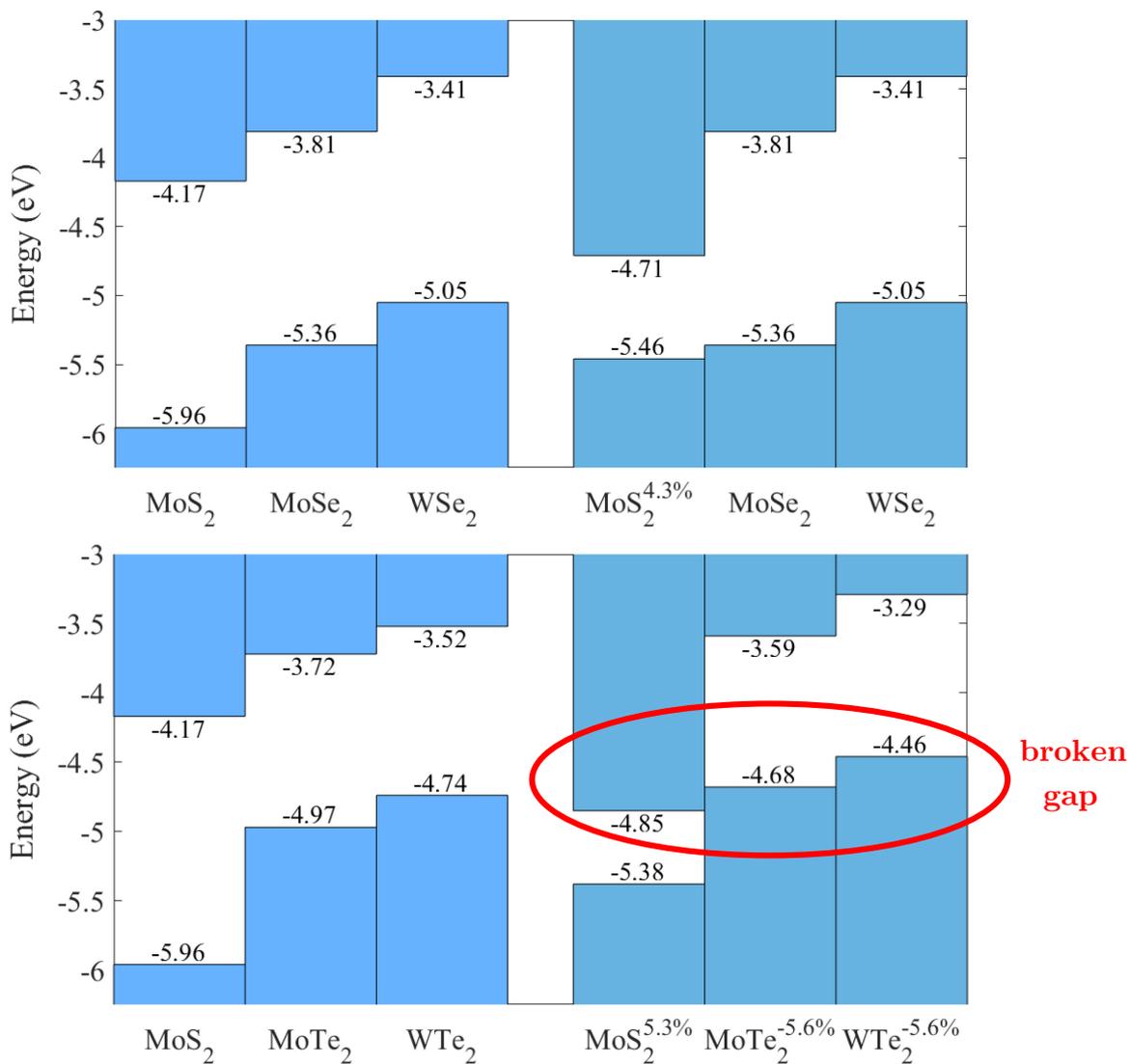


Figure 45. Top: CB and VB of  $\text{MoS}_2$ ,  $\text{MoSe}_2$  and  $\text{WSe}_2$  in their pristine form and under the strain applied in the  $\text{ASe}_2/\text{MoS}_2$  heterojunctions. Bottom: CB and VB of  $\text{MoS}_2$ ,  $\text{MoTe}_2$  and  $\text{WTe}_2$  in their pristine form and under the strain applied in the  $\text{ATe}_2/\text{MoS}_2$  heterojunctions.

This section introduced the most important aspect of the tight-binding approach and model used in this thesis. The TB theory was briefly explained, before highlighting and showing in detail the creation of the fully atomistic tight-binding Hamiltonians that will be used in the electronic transport simulation.

The next section will briefly introduce the NEGF formalism, before focusing on its implementation in the transport code.

## 3.2 Non-Equilibrium Green's Function (NEGF) formalism

In this section, I will very briefly describe the main aspects of the NEGF formalism, and its use in transport calculations.

For much more detailed information about this technique, the reader is referred to dedicated handbooks [451]–[454].

### 3.2.1 Definition of Green's function

The Green's function method is a technique that can strongly simplify the solving of linear differential equations.

For instance, consider

$$Dy(x) = f(x) \quad (18)$$

where  $D$  is an operator.

The Green's function associated to  $D$  is defined as

$$DG(x, x') = \delta(x - x') \quad (19)$$

in which  $\delta$  is the delta function.

The solution  $y(x)$  can therefore be calculated as

$$y(x) = \int G(x, x')f(x')dx' \quad (20)$$

Solving Eq.(19) is easier than Eq.(18) because it does not include  $f(x)$  and  $y(x)$  and only depends on the operator  $D$ . Plus, this technique is extremely versatile as  $G(x, x')$  can be used to solve all equations of the type Eq.(18), no matter  $y(x)$ .

Thanks to this versatility, the Green's function method is often used to solve linear differential equations in a wide range of applications.

Obviously, its use in the computation of electronic transport is the aspect we are focused on, and I will introduce it in further detail.

### 3.2.2 Use in quantum transport calculations

Green's functions are commonly used to solve Schrödinger's or Poisson's equation in the case of quantum transport.

From Schrödinger's equation

$$H|\varphi\rangle = E|\varphi\rangle \quad (21)$$

which can be rewritten as a function of the  $(E - H)$  operator as follows

$$(E - H)|\varphi\rangle = 0 \quad (22)$$

we can define Green's function as

$$(E - H)G(r, r'; E) = \delta(r - r') \quad (23)$$

Once a specific basis has been defined, the previous operators can be written in matrix form

$$(EI - H)G(E) = I \quad G(E) = (EI - H)^{-1} \quad (24)$$

However, this simple approach would only work for isolated systems with no coupling to their surroundings, which is obviously not the case in transport problems.

In most transport problems, the considered system can be divided into three distinct regions (see Figure 46): the left and right semi-infinite contacts, and the device region, connecting the two.

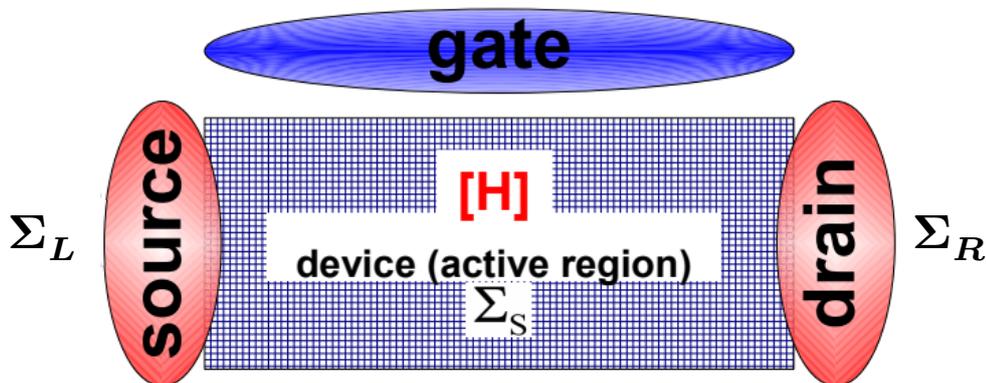


Figure 46. Schematic representation of a transistor highlighting the three regions (source, device and drain) [455]



The matrices describing the self-energies are therefore  $N \times N$  matrices as well

$$\Sigma_L = \begin{bmatrix} \Sigma_L^S & 0 & & & & \\ 0 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & 0 & \\ & & & 0 & 0 & \end{bmatrix} \quad \Sigma_R = \begin{bmatrix} 0 & 0 & & & & \\ 0 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & 0 & \\ & & & 0 & \Sigma_R^S & \end{bmatrix}$$

$\Sigma_L^S$  and  $\Sigma_R^S$  can be obtained [457] by solving

$$\Sigma_L^S = H_{DL} \cdot g_0^L \cdot H_{LD} \quad \Sigma_R^S = H_{DR} \cdot g_0^R \cdot H_{RD} \quad (26)$$

where  $H_{DL}$  is the coupling between the first layer of the device region and the first layer of the source region ( $H_{LD} = H_{DL}^\dagger$ ),  $H_{DR}$  is the coupling between the  $N$ -th layer of the device region and the first layer of the drain region ( $H_{RD} = H_{DR}^\dagger$ ), and  $g_0^{L(R)}$  is the surface Green's function at the left (right) contact.

These surface Green's functions are defined[457] by the recursive relation

$$g_n^{L(R)} = \left( E + i0^+ - H_n^{L(R)} - H_{n,n+1}^{L(R)} \cdot g_{n+1}^{L(R)} \cdot H_{n+1,n}^{L(R)} \right)^{-1} \quad (27)$$

While this equation can technically be solved, it proves extremely challenging from a convergence standpoint. I will not detail it here since it is widely available elsewhere[456], [456], [457], but a so-called ‘‘quick-iterative scheme’’ was introduced by Sancho et al. in 1984[458]. It uses an enhanced solving method that allows for the consideration of  $2^n$  layers after  $n$  iterations, compared to simply solving Eq.(27), which solves one layer per iteration.

### 3.2.2.2 Recursive Green's function algorithm

Transmission and Density of States (DOS) are the most important characteristics for transport and device analysis, mainly because most other characteristics such as electrical ones can be derived from them.

Due to the often very large size of the device Hamiltonian  $H_D$ , it can be computationally impossible to obtain the device's Green's function matrix by direct inversion. It has been shown[457], [459] that to reduce the computational burden of this method, one can compute only specific elements of the Green's function matrix which are those needed to calculate DOS and ballistic transmission.

These elements are  $G_{11}$  or  $G_{NN}$  for the transmission, and  $G_{i1}$ ,  $G_{1i}^\dagger$ ,  $G_{iN}$  and  $G_{Ni}^\dagger$  for the calculation of DOS at the  $i$ -th layer.

$G_{11}$  and  $G_{NN}$  can be calculated using a recursive algorithm based on the Dyson's equations ( $G_{11}$  is shown here but  $G_{NN}$  can be calculated in a similar manner; more detail available in [457], [459])

$$\text{Calculate } G_{NN}^S = (E + i0^+ - H_N - \Sigma_R)^{-1}$$

$$\text{for } j = N, N-1, \dots, 3, 2 \rightarrow G_{jj}^S = (E + i0^+ - H_j - H_{j,j+1} \cdot G_{j+1,j+1}^S \cdot H_{j+1,j})^{-1}$$

$$G_{11} = G_{11}^S = (E + i0^+ - H_1 - \Sigma_L - H_{12} \cdot G_{22}^S \cdot H_{21})^{-1} \quad (28)$$

As for  $G_{i1}$ ,  $G_{1i}^\dagger$ ,  $G_{iN}$  and  $G_{Ni}^\dagger$ , they can be calculated as follows (in which  $A = E + i0^+ - H - \Sigma_L - \Sigma_R$ )

for  $G_{i1}$ :

$$A_{11}G_{11} + A_{12}G_{21} = 1$$

$$A_{21}G_{11} + A_{22}G_{21} + A_{23}G_{31} = 0$$

$$\vdots$$

$$A_{i,i-1}G_{i-1,1} + A_{i,i}G_{i,1} + A_{i,i+1}G_{i+1,1} = 0 \quad (29)$$

for  $G_{iN}$ :

$$A_{NN}G_{NN} + A_{N,N-1}G_{N-1,N} = 1$$

$$A_{N-1,N}G_{NN} + A_{N-1,N-1}G_{N-1,N} + A_{N-1,N-2}G_{N-2,N} = 0$$

$$\vdots$$

$$A_{i,i-1}G_{i-1,N} + A_{i,i}G_{i,N} + A_{i,i+1}G_{i+1,N} = 0 \quad (30)$$

Using these techniques allows for a drastic reduction of the computing resources required compared to the traditional, "brute-force" inversion of the large device Hamiltonian.

### 3.2.3 Calculation of transport properties from NEGF

Now that the matrix form (or at least the necessary elements) of the Green's function of the device has been calculated, it can be used to access electrical and transport characteristics in the device such as transmission, DOS, LDOS and current.

#### 3.2.3.1 Transmission

When considering ballistic transport, the transmission through the system can be calculated as [451], [457], [460]

$$T = \text{trace}[\Gamma_L G \Gamma_D G^\dagger] \quad (31)$$

where  $\Gamma_{L(R)} = i[\Sigma_{L(R)} - \Sigma_{L(R)}^\dagger]$  corresponds to the energy level broadening due to the coupling with the source (drain).

However, if we used the recursive approach to calculate only specific elements of the Green's matrix as detailed in the previous section, the transmission can be obtained in two distinct ways

$$T(E) = \text{trace}[\hat{\Gamma}_L (i(\mathbf{G}_{11} - \mathbf{G}_{11}^\dagger) - \mathbf{G}_{11} \hat{\Gamma}_L \mathbf{G}_{11}^\dagger)] \quad (32)$$

$$T(E) = \text{trace}[\hat{\Gamma}_R (i(\mathbf{G}_{NN} - \mathbf{G}_{NN}^\dagger) - \mathbf{G}_{NN} \hat{\Gamma}_L \mathbf{G}_{NN}^\dagger)] \quad (33)$$

where  $\hat{\Gamma}_{L(R)} = i[\hat{\Sigma}_{L(R)} - \hat{\Sigma}_{L(R)}^\dagger]$  (as a reminder,  $\hat{\Sigma}_{L(R)} = H_{DL(R)} \cdot g_0^{L(R)} \cdot H_{L(R)D}$ )

#### 3.2.3.2 DOS and LDOS

The density of states corresponds to the number of states per unit volume within a given energy interval  $[E, E + dE]$  and is therefore given as

$$D(E) = \frac{dN(E)}{dE} \quad (34)$$

which can be rewritten using the delta function

$$D(E) = \sum_n \delta(E - E_n) \quad (35)$$

It has been shown[451], [457], [460] that the Lorentz form of the delta function

$$\sum_n \delta(E - E_n) = \lim_{\eta \rightarrow 0} \sum_n \frac{\eta}{\pi(E - E_n)^2 + \eta^2} \quad (36)$$

where  $\eta = 0^+$  can be used to obtain the DOS when using the Green's function method. By defining the spectral function  $A = i[G - G^\dagger]$ , the DOS can be calculated as

$$D(E) = \frac{\text{trace}(A)}{2\pi} = \frac{i \times \text{trace}(G - G^\dagger)}{2\pi} \quad (37)$$

The local density of states corresponds to the density of states at a specific point in real-space. Therefore, it can simply be calculated for the  $i$ -th layer from the  $G_{ii}$  element of the Green's matrix as

$$D_{ii}(E) = \frac{\text{trace}(A_{ii})}{2\pi} = \frac{i \times \text{trace}(G_{ii} - G_{ii}^\dagger)}{2\pi} \quad (38)$$

Because  $A_{ii} = i[G_{ii} - G_{ii}^\dagger] = -2\text{Im}(G_{ii})$ , it can also be obtained as follows

$$D_{ii}(E) = -\text{trace} \left[ \frac{\text{Im}(G_{ii})}{\pi} \right] \quad (39)$$

LDOS is an important analysis tool in nanoelectronic transport because it can reveal quantum effects such as resonances that arise due to confinement.

### 3.2.3.3 Electrical current and conductance

The ballistic electrical current flowing through the device when a voltage bias is applied can be calculated from the transmission via the standard Landauer's formula[451], [457], [460]

$$I = \frac{2e}{h} \int [f_L(E - \mu_L) - f_R(E - \mu_R)] T(E) dE \quad (40)$$

where  $f_{L(R)}(E - \mu_{L(R)})$  is the Fermi function (see Chapter 1.2.1) of the left (right) contact, in which  $\mu_{L(R)} = E_{F_{L(R)}} + U_{L(R)}$ ,  $E_{F_{L(R)}}$  being the Fermi energy in the left (right) contact and  $U_L - U_R = eV_{DS}$

In a similar manner, ballistic conductance can be calculated as

$$G_e(\mu, T_0) = \lim_{V_{DS} \rightarrow 0} \frac{I}{V_{DS}} = \frac{2e^2}{h} \int \frac{\partial f(E, \mu, T_0)}{\partial E} T(E) dE \quad (41)$$

In this section, the basic theory of the NEGF method and its use in the computation of nanoelectronic transport have been detailed.

I will now focus on its implementation with the TB model, and their implementation in the transport code.

### 3.3 Implementation of TB and NEGF models

Now that the TB theory and model used as well as the NEGF method have been introduced, this section aims to present their interaction with one another as well as their implementation in the electronic transport code.

#### 3.3.1 Creation of the layer Hamiltonians

As shown in the previous section, in NEGF theory the device region has to be divided into repeating layers along the transport direction, which results in the change in basis of the TB model detailed in Section 3.1.4.

The  $22 \times 22$  Hamiltonians  $H_{n,m}, T_{n+1,m}, T_{n,m+1}, T_{n+1,m-1}$  must therefore be used to create the layer Hamiltonians  $H_n$  and  $T_{n+1}$  shown in Figure 48.

Since they regroup the influence of a whole layer into a single Hamiltonian,  $H_n$  will be calculated solely from  $H_{n,m}$  and  $T_{n,m+1}$ , while  $T_{n+1}$  will be calculated using  $T_{n+1,m}, T_{n+1,m-1}$  and  $T_{n+1,m+1}$ .

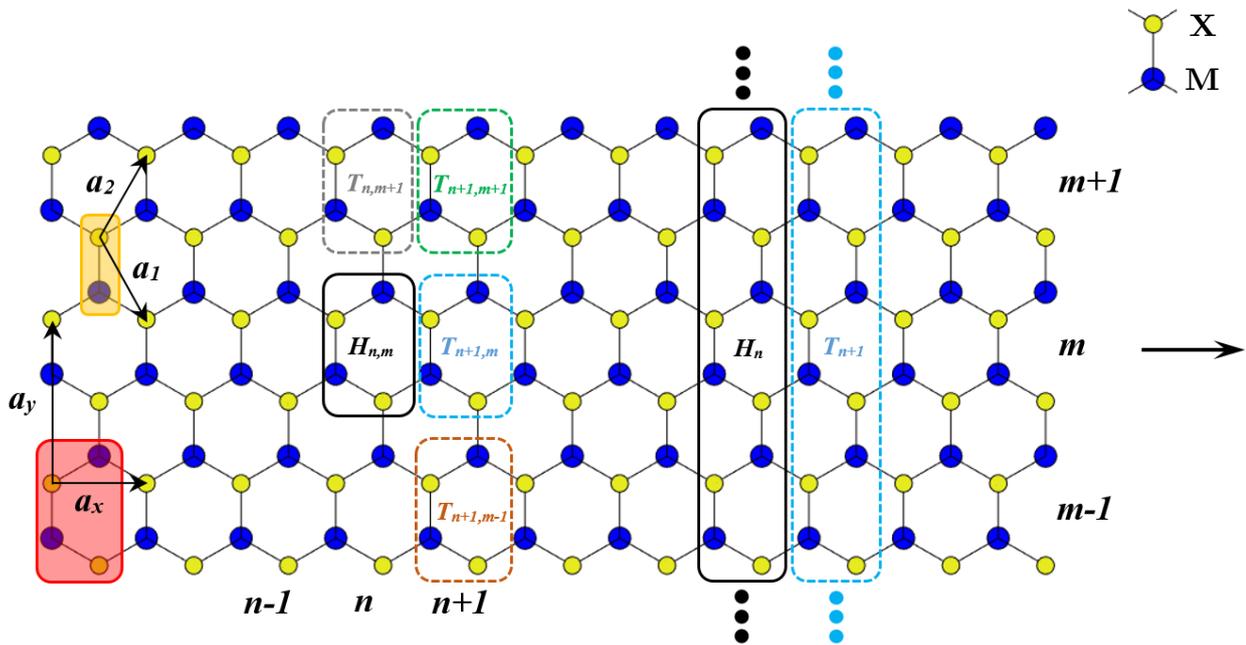


Figure 48. Atomic arrangement of TMDs. The yellow area represents the base, 11-orbital unit cell with the corresponding unit vectors  $a_1$  and  $a_2$ , while the red area represents the 22-orbital unit cell used in our work, with its unit vectors  $a_x$  and  $a_y$ .  $H_{n,m}$  and  $H_n$  are the Hamiltonians of a single unit cell and a single material “layer”, respectively. Finally,  $T_{i,j}$  and  $T_i$  represent the coupling of the  $(n,m)$  cell with the  $(i,j)$  unit cell, and the coupling of the  $(i)$  layer with the  $(n)$  layer, respectively. Transport direction is indicated by the arrow

At a given  $y$  component of the wave vector  $k_y$ , these matrices can be calculated as follows

$$H_n(k_y) = H_{n,m} + T_{n,m+1} \cdot e^{i.k_y.a_y} + T_{n,m-1} \cdot e^{-i.k_y.a_y} \quad (42)$$

$$T_{n+1}(k_y) = T_{n+1,m} + T_{n+1,m-1} \cdot e^{-i.k_y.a_y} + T_{n+1,m+1} \cdot e^{i.k_y.a_y} \quad (43)$$

$$T_{n-1}(k_y) = T_{n+1}(k_y)^\dagger = T_{n+1,m}^\dagger + T_{n+1,m-1}^\dagger \cdot e^{i.k_y.a_y} + T_{n+1,m+1}^\dagger \cdot e^{-i.k_y.a_y} \quad (44)$$

They are therefore  $22 \times 22$  matrices as well.

With those layer Hamiltonians now calculated, the total Hamiltonian at a given wave vector  $(k_x, k_y)$  can be calculated as

$$H_{tot}(k_x, k_y) = H_n(k_y) + T_{n+1}(k_y) \cdot e^{i.k_x.a_x} + T_{n-1}(k_y) \cdot e^{-i.k_x.a_x} \quad (45)$$

This Hamiltonian fully describes a single layer of the 2D infinite TMD and its coupling to the surrounding layers at a given wave vector.

In the case of an in-plane heterojunction as shown in Figure 49, the appropriate orbital couplings are used in each material, and the coupling at the interface is calculated as the average of the coupling parameters of the materials on either side of the interface.

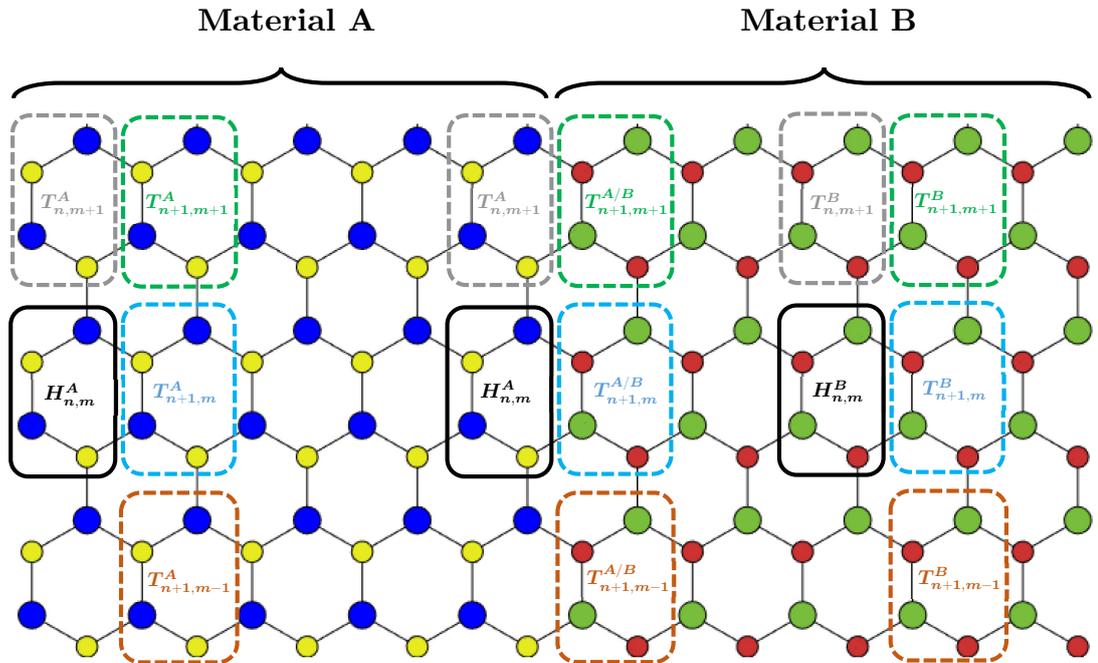


Figure 49. Heterojunction between TMDs A (left) and B (right), and the couplings considered





However, rather than performing a brute-force inversion of the huge resulting matrix, we use the recursive algorithm presented in Section 3.2.2.2 to compute only the elements of the matrix necessary to obtain the transmission and DOS which helps to drastically reduce computation times.

In order to resolve spatial information such as LDOS, charge, potential etc, a simple 2D mesh adapted to each simulated device is created using the Gmsh software. The lattice parameter of the considered material is used as mesh size, so that each unit cell corresponds to a single mesh element.

### 3.3.3 Validity of the approximations used

Several approximations are made in this work, mainly that transport is fully ballistic (no phonon scattering is considered), and that the strain is applied uniformly across the device and the contact regions.

This section will provide insight into why these approximations were made, and present supporting material.

- **Ballistic approximation:** Mean free paths around 20 nm have been reported [461] in MoS<sub>2</sub> so, in the case of short devices, this ballistic approximation is expected to provide reliable results.

While the deformation potentials reported for TMDs are rather small [462]–[464], phonon scattering would undoubtedly impact performance, namely by reducing ON current and increasing *SS*, depending on the device channel length.

- **Uniform strain:** in the case of the heterojunctions that give rise in a lattice mismatch, the appropriate strain is applied uniformly to each material, including the contacts, to recover lattice matching across the full device. A more realistic approach to strain modelling would have been to gradually relax the strain away from the interface and consider pristine contacts. However, from a computational standpoint, we would have needed as many different layer Hamiltonians and coupling Hamiltonians as there are layers in the considered system which is extremely taxing, not to mention scaling the mesh size accordingly.

What's more, in similar heterostructures (WSe<sub>2</sub>-MoS<sub>2</sub>) strain has been shown to relax over several tens of nanometers[465] (see Figure 50). Considering the length of most of the devices investigated is < 40 nm, the uniformly applied strain approximation is not outlandish.

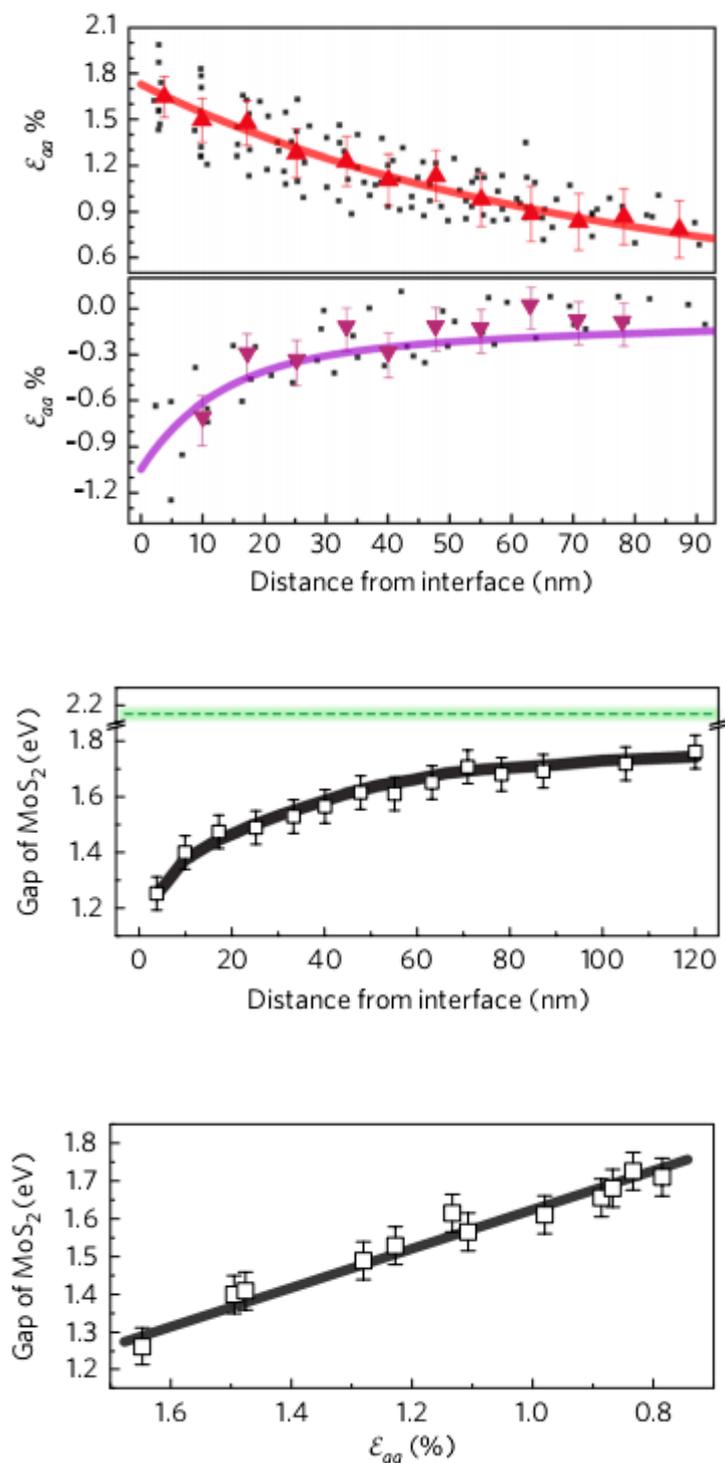


Figure 50. (top) Evolution of tensile and compressive uniaxial strains observed in an experimental MoS<sub>2</sub>/WSe<sub>2</sub> in-plane heterojunction as distance to the interface increases. (middle) Evolution of the MoS<sub>2</sub> band gap observed in the same heterojunction as distance to the interface increases (bottom) Evolution of the MoS<sub>2</sub> band gap observed in the same heterojunction as the tensile strain decreases.

### 3.3.4 Self-consistent transport simulation flowchart

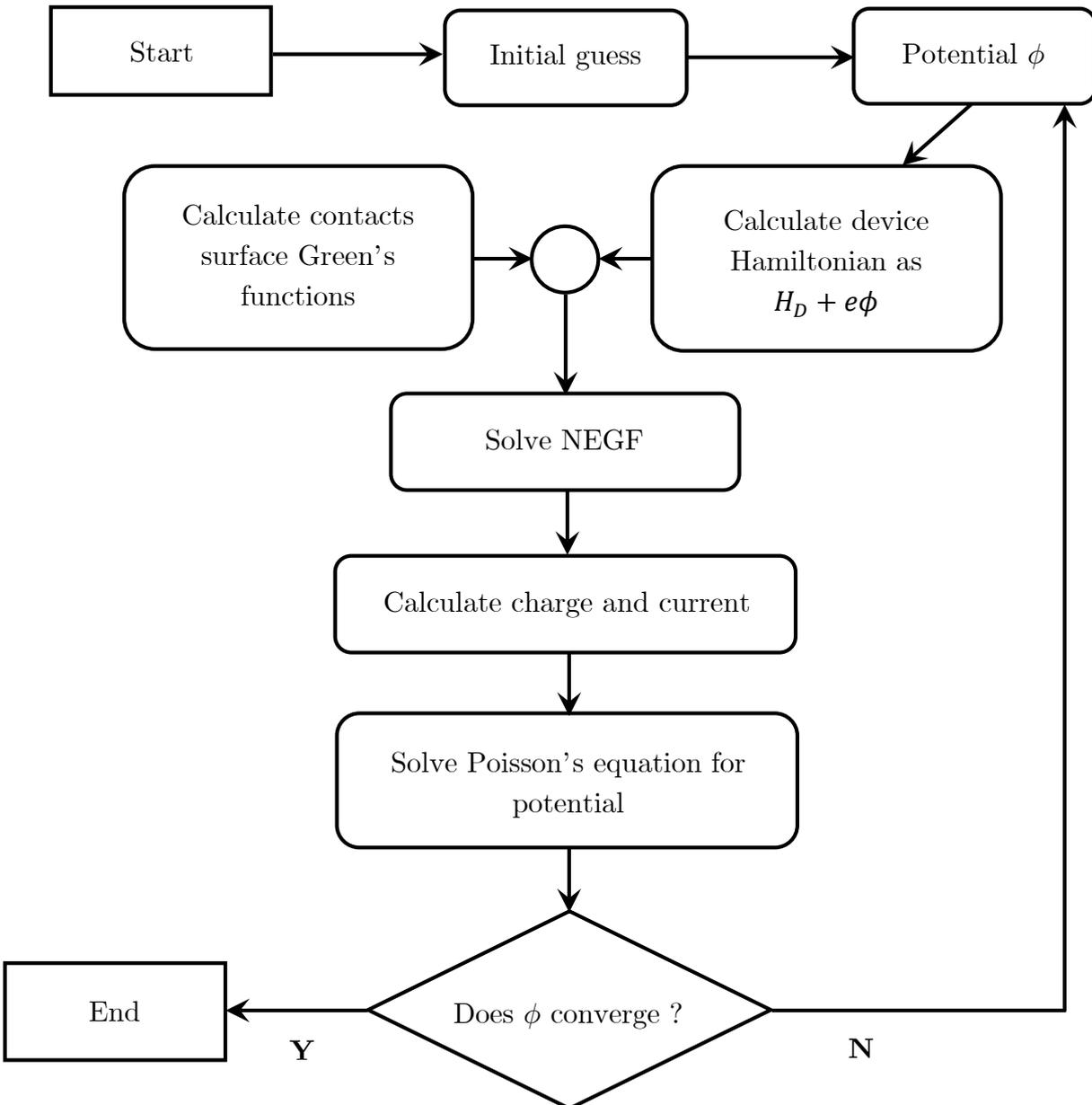
The flowchart for the transport simulation is presented here.

In simplified terms, an initial guess based on the bias voltage is used to compute the initial Green's function of the device, from which the charge and current are extracted.

This charge distribution is then used to calculate the potential via Poisson's equation

$$\nabla \cdot (\epsilon \nabla \cdot \phi) = -\frac{\rho}{\epsilon_0} \quad (52)$$

where  $\phi$  is the electrostatic potential and  $\rho$  is the charge density. This updated potential profile is used to calculate an updated Green's function for the device, from which a new potential profile is obtained. This loop is repeated until convergence is reached.



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Now that the theory behind the TB model and the NEGF method used for transport has been detailed, I will present and analyze the first devices I investigated over the course of my PhD work: homojunction TMD transistors.

# Chapter 4

## Homojunction TMD transistors

In this chapter, I will quickly present simulation results pertaining to homojunction TMD based transistors (both MOSFET and TFET).

The unremarkable performance of the devices considered in this chapter will be used to highlight and contrast with the outstanding performance of heterojunction-based TFETs. As such, these devices and their performance will not be analyzed in as much detail as those presented in later chapters.

However, this chapter will also be used to introduce important concepts that will also apply to heterojunction TFETs, such as the effect and significance of backgate voltages for instance.

### 4.1 Homojunction TMD MOSFETs

The first type of devices I investigated were basic, n-type inversion MOSFETs based on a single TMD monolayer. Those devices will give us insight about the limited capabilities of TMDs in traditional MOSFETs.

#### 4.1.1 Device architecture

The MOSFETs presented here all share the same architecture, shown in Figure 51:

- SiO<sub>2</sub> buried oxide with thickness  $t_{BOX} = 10 \times a_{MX_2}$  (3.18 nm for MoS<sub>2</sub>/WS<sub>2</sub>, 3.31 nm for MoSe<sub>2</sub>/WSe<sub>2</sub> and 3.55 nm for MoTe<sub>2</sub>/WTe<sub>2</sub>).
- High- $\kappa$  top gate oxide with equivalent oxide thickness  $EOT = 4 \times a_{MX_2}$  (1.272 nm for MoS<sub>2</sub>/WS<sub>2</sub>, 1.324 nm for MoSe<sub>2</sub>/WSe<sub>2</sub> and 1.42 nm for MoTe<sub>2</sub>/WTe<sub>2</sub>).
- TMD source, channel and drain of lengths  $L_S$ ,  $L_{ch}$  and  $L_D$  with  $L_S = L_D = 30 \times a_{MX_2}$  (roughly 10 nm) and  $L_{ch}$  ranging from  $30 \times a_{MX_2}$  to  $80 \times a_{MX_2}$  (roughly 26 nm).

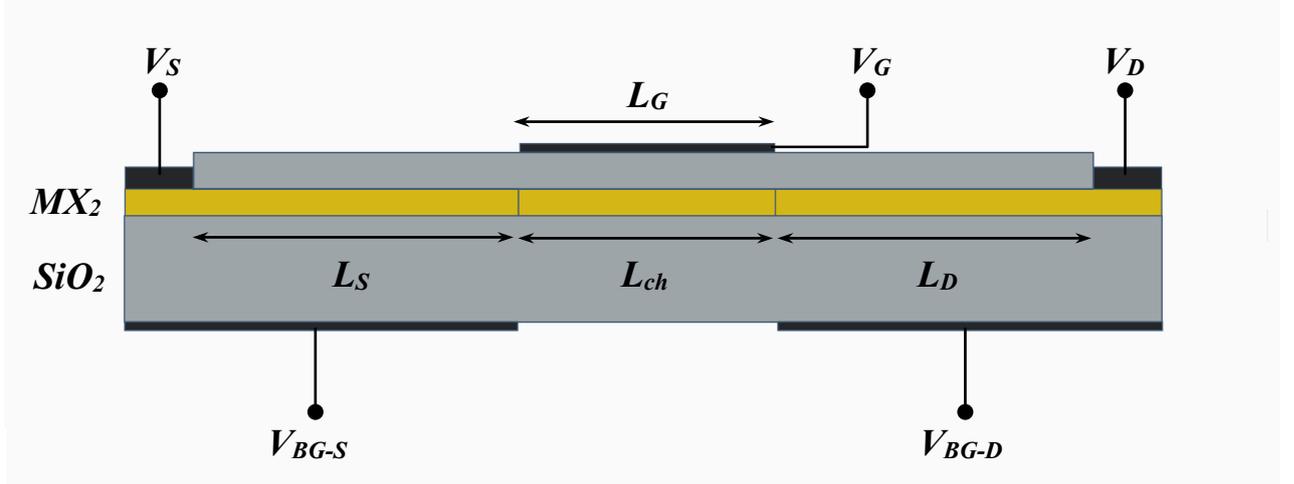


Figure 51. Device architecture for the considered MOSFETs. A single TMD acts as the source, channel and drain, while  $\text{SiO}_2$  is used as a buried oxide, and a high- $\kappa$  dielectric as the top gate oxide.

- Source and drain contacts to which voltages  $V_S = 0$  and  $V_D = V_{DS}$  are applied which will control the Fermi energies in the contacts.
- A top gate of length  $L_G = L_{ch}$ , to which a voltage  $V_G$  is applied. This gate will control current flow through the device.
- Source and drain backgates to which voltages  $V_{BG-S}$  and  $V_{BG-D}$  are applied. Since the active layer is purely 2D, we can use backgates rather than chemical doping to control charge densities in the contacts.
- The workfunction of the top gate as well as the source and drain backgates in each device is the following: 5.07 eV for  $\text{MoS}_2$ , 4.71 eV for  $\text{MoSe}_2$ , 4.58 eV for  $\text{WS}_2$ , 4.31 eV for  $\text{WSe}_2$ , 4.62 eV for  $\text{MoTe}_2$  and 4.42 eV for  $\text{WTe}_2$ .

### 4.1.2 Electronic transport simulations

Electronic transport simulations across MOSFETs based on  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ,  $\text{WS}_2$ ,  $\text{WSe}_2$ ,  $\text{MoTe}_2$  and  $\text{WTe}_2$  were carried out using the self-consistent transport code outlined in Section 3.3.4.

The response of these transistors was studied for gate voltages ranging from 0 to 1.5 V, at a supply voltage  $V_{DD} = 0.3$  V, and at backgate voltages  $V_{BG-D} = V_{BG-S} = 1.9$  V. The gate length  $L_{ch}$  is  $40 \times a_{MX_2}$  so it ranges from 12.72 nm to 14.2 nm depending on the TMD considered. The resulting  $I_D$ - $V_G$  characteristics are shown both in log scale and in linear scale in Figure 52.

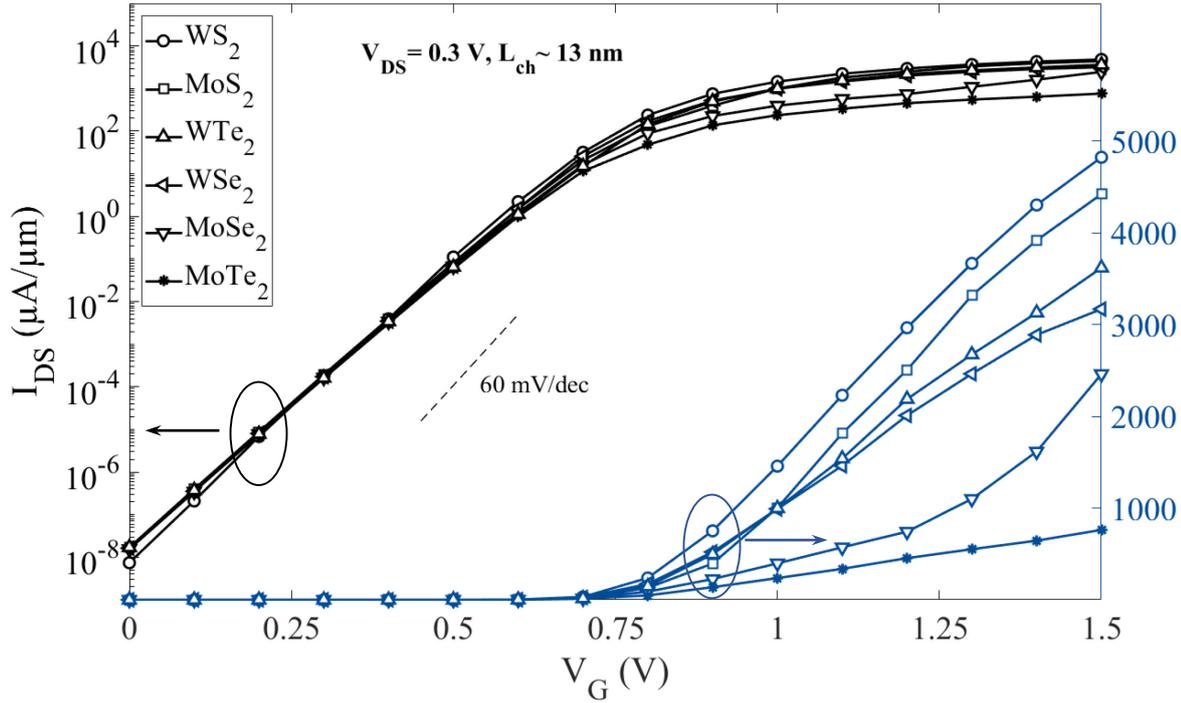


Figure 52.  $I_D$ - $V_G$  characteristics of all six TMD-based n-type inversion MOSFETs at  $V_{DS} = 0.3$  V,  $V_{BG-D} = V_{BG-S} = 1.9$  V and  $L_{ch} = 40 \times a_{MX_2} \sim 13$  nm. The dotted line indicates a 60 mV/dec sub-threshold swing, the theoretical lower limit for MOSFETs.

The workfunction of the top gate as well as the source and drain backgates in each device is the following: 5.07 eV for MoS<sub>2</sub>, 4.71 eV for MoSe<sub>2</sub>, 4.58 eV for WS<sub>2</sub>, 4.31 eV for WSe<sub>2</sub>, 4.62 eV for MoTe<sub>2</sub> and 4.42 eV for WTe<sub>2</sub>.

The simulated MOSFETs behave as expected, which is to say they are in the OFF state (no current flow) when no gate voltage is applied, and slowly switch to the ON state (current flows from the source to the drain) as  $V_G$  increases.

The six transistors share a common threshold voltage  $V_T \sim 0.75$  V, and a sub-threshold swing of roughly 75 mV/dec. As a reminder,  $SS$  is evaluated as shown in Eq.(3), between  $I_{DS} = 10^{-5}$  and  $10^{-2}$   $\mu\text{A}/\mu\text{m}$  in this case.

Out of all six transistors, the WS<sub>2</sub> and MoS<sub>2</sub> MOSFETs yield the highest ON currents, beyond 4000  $\mu\text{A}/\mu\text{m}$  at  $V_G = 1.5$  V. The WTe<sub>2</sub> and WSe<sub>2</sub> follow closely, yielding ON currents  $> 3000$   $\mu\text{A}/\mu\text{m}$ , while MoSe<sub>2</sub> and MoTe<sub>2</sub> yield far lower currents.

Figure 53. shows the lowest CB in the MoS<sub>2</sub> MOSFET during the transition from the OFF ( $V_G = 0$  V) to the ON state ( $V_G = 0.8$  V) and highlights the working mechanism of MOSFETs: as  $V_G$  increases, the electric field generated by the gate lowers the energy barrier between the source and channel until carriers are able to flow freely across the device.

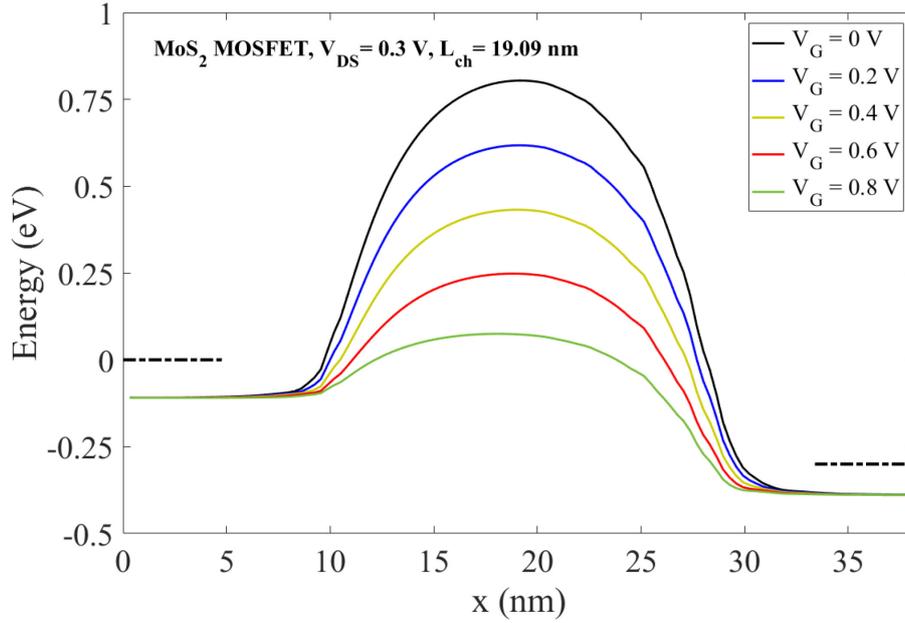


Figure 53. Lowest CB in the MoS<sub>2</sub> MOSFET highlighting the OFF/ON transition at  $V_{DS} = 0.3$  V,  $L_{ch} = 19$  nm and  $V_G$  ranging from 0 to 0.8 V. The black dotted lines indicate the Fermi energies in the source and drain (resp. 0 eV and  $-0.3$  eV).

The influence of design parameters such as channel length and backgate voltages will now be highlighted and briefly investigated.

#### 4.1.2.1 Influence of backgate voltages

As mentioned earlier, we use backgates rather than chemical doping to control charge densities in the contacts because the active layer of the devices is fully 2D. Chemical doping consists of introducing atoms bearing either more or fewer electrons than the base material atoms, therefore increasing the number of electrons or holes available for transport. However, the appearance of defects and atomic reconstruction are a common side-effect of chemical doping, which degrades the transport properties. The use of electrostatic doping via backgates as shown here is therefore preferable whenever possible.

Physically, the backgates are used to force the potential to a certain value ( $V_{BG-S/D}$ ) and therefore to control the energy level of the bands in the contacts, as well as their relationship with the Fermi energy.

The voltages applied to the backgates must therefore be carefully selected to obtain a functioning device. For instance, by applying an excessively low  $V_{BG-S}$ , the lowest CB in the source would be forced at higher energies than  $\mu_S$  and be partially (or completely) devoid of carriers (see the Fermi-Dirac distribution in Section 1.2.1), which would result in the absence of current. Similarly, applying backgate voltages resulting in the CB being at higher energies in the drain than in the source would prevent current flow.

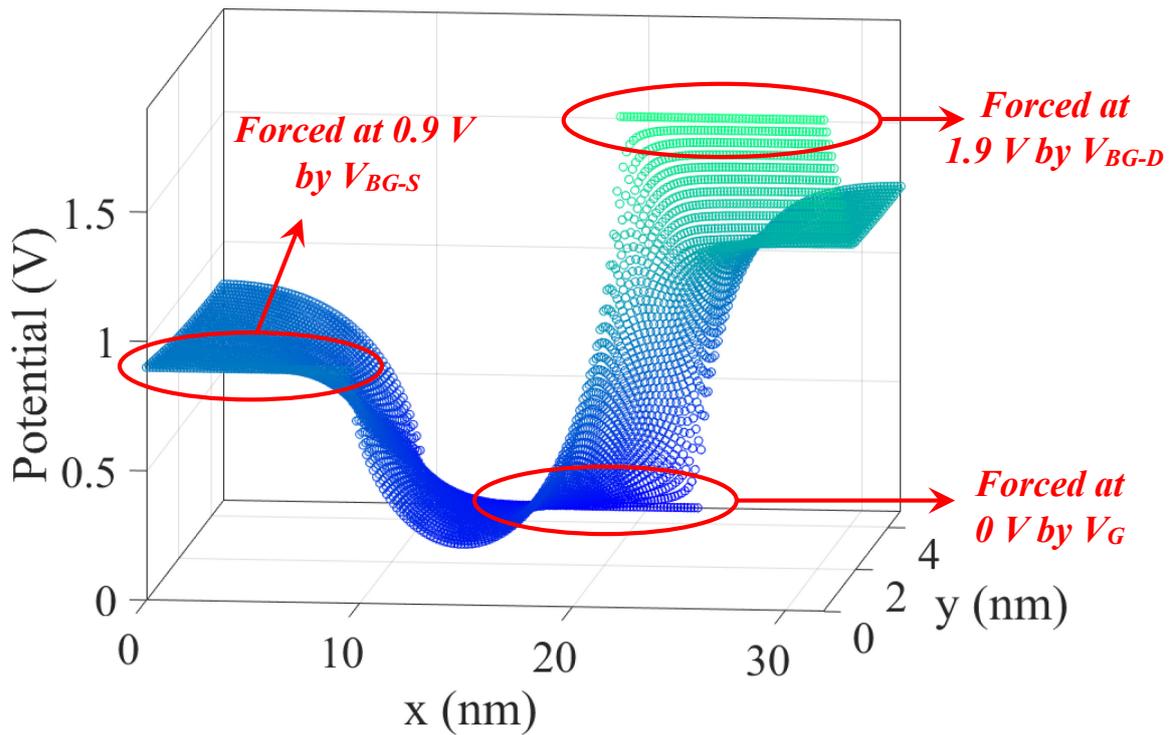


Figure 54. Potential profile in the WS<sub>2</sub> MOSFET at  $V_G = 0$  V,  $V_{BG-S} = 0.9$  V and  $V_{BG-D} = 1.9$  V. The active layer (TMD) is located at  $y = 3.2$  nm.

Figure 54 shows the potential profile in the WS<sub>2</sub> MOSFET for  $L_{ch} = 12.72$  nm,  $V_G = 0$  V,  $V_{BG-S} = 0.9$  V and  $V_{BG-D} = 1.9$  V. The red ellipses highlight the areas where the potential is forced by the gates (left: source backgate, right: drain backgate, bottom: top-gate). The potential profile in the active layer (located at  $y = 3.2$  nm) is therefore highly impacted by all three voltages and will dictate whether current flows or not.

The current characteristics of the WS<sub>2</sub> device were investigated for several backgate voltages ranging from 1.15 V to 2.9 V, and are shown in Figure 55.

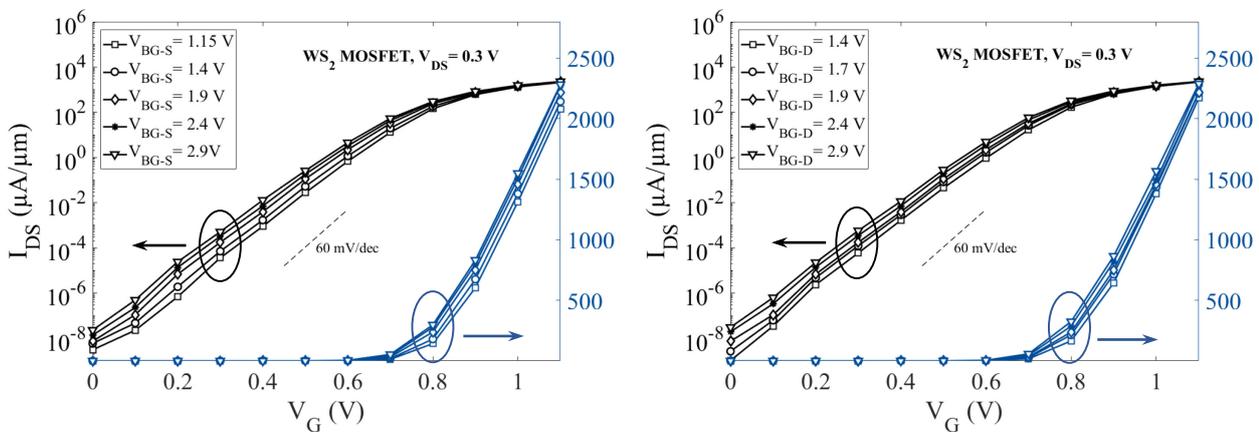


Figure 55.  $I_D$ - $V_G$  characteristics for the WS<sub>2</sub> device at  $L_{ch} = 12.72$  nm and  $V_{DS} = 0.3$  V.

Left:  $V_{BG-D} = 1.9$  V and  $V_{BG-S}$  ranges from 1.15 V to 2.9 V.

Right:  $V_{BG-S} = 1.9$  V and  $V_{BG-D}$  ranges from 1.4 V to 2.9 V.

The  $I_D$ - $V_G$  characteristics show the mild impact of such changes to both  $V_{BG-S}$  and  $V_{BG-D}$  to device operation. The overall behavior remains the same, but the OFF state is more impacted than the ON state: by applying low backgate voltages, the OFF current can be reduced ten-fold (compared to  $V_{BG-S/D} = 2.9$  V) while only marginally impacting ON current.

While only the  $\text{WS}_2$  device is investigated here, the influence of  $V_{BG-S/D}$  is observed to be the same across all six devices.

In the case of these MOSFETs, the backgate voltages act as a fine-tuning tool to slightly enhance performance as long as they are kept in the appropriate range.

#### 4.1.2.2 Influence of channel length

Channel length is another important design parameter in FETs. As channel length decreases, short-channel effects (SCE) such as carrier velocity saturation, high DIBL, source-to-drain tunneling and more can arise and degrade device performance.

The performance of the TMD-based MOSFETs was therefore investigated for gate lengths ranging from  $30 \times a_{\text{MX}_2}$  (roughly 12 nm) to  $80 \times a_{\text{MX}_2}$  (roughly 26 nm).

The lowest CB of these two  $\text{MoS}_2$  MOSFETs for  $V_G$  ranging from 0 V to 0.8 V is shown in Figure 56 and gives strong indications on the behavior of these devices.

At  $V_G = 0$  V, the top of the CB barely reaches 0.45 eV in the short-channel device while it exceeds 0.75 eV in the long-channel device; we can therefore expect an increase in OFF current (both by thermionic injection and by tunneling through the shorter energy barrier) as channel length is reduced.

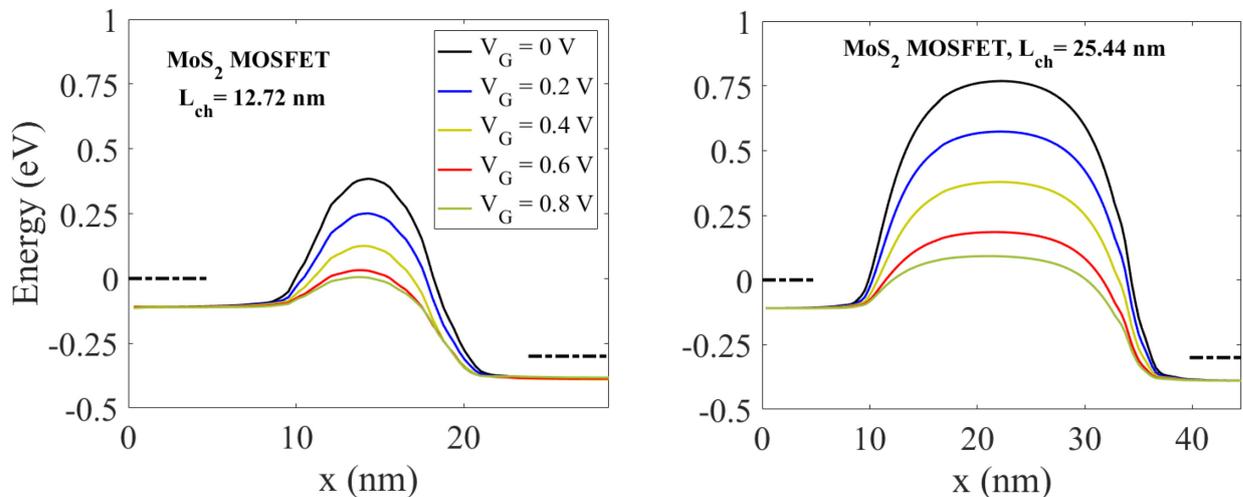


Figure 56. Lowest CB in the  $\text{MoS}_2$  MOSFET for  $V_G$  ranging from 0 V to 0.8 V,  $V_{DS} = 0.3$  V,  $V_{BG-S} = V_{BG-D} = 1.9$  V, and (left)  $L_{ch} = 12.72$  nm (right) 25.44 nm.

This lower energy barrier is due to the fact that the drain backgate (which forces the potential and the level of the CB in the drain) is much closer to the source when the channel is short, and therefore prevents the CB from reaching high energies in the channel.

The  $I_D$ - $V_G$  characteristics of all six MOSFETs are shown at  $L_{ch} = 30 \times a_{MX_2}$ ,  $40 \times a_{MX_2}$ ,  $60 \times a_{MX_2}$  and  $80 \times a_{MX_2}$ ,  $V_{DS} = 0.3$  V and  $V_{BG-S/D} = 1.9$  V are shown in Figure 57.

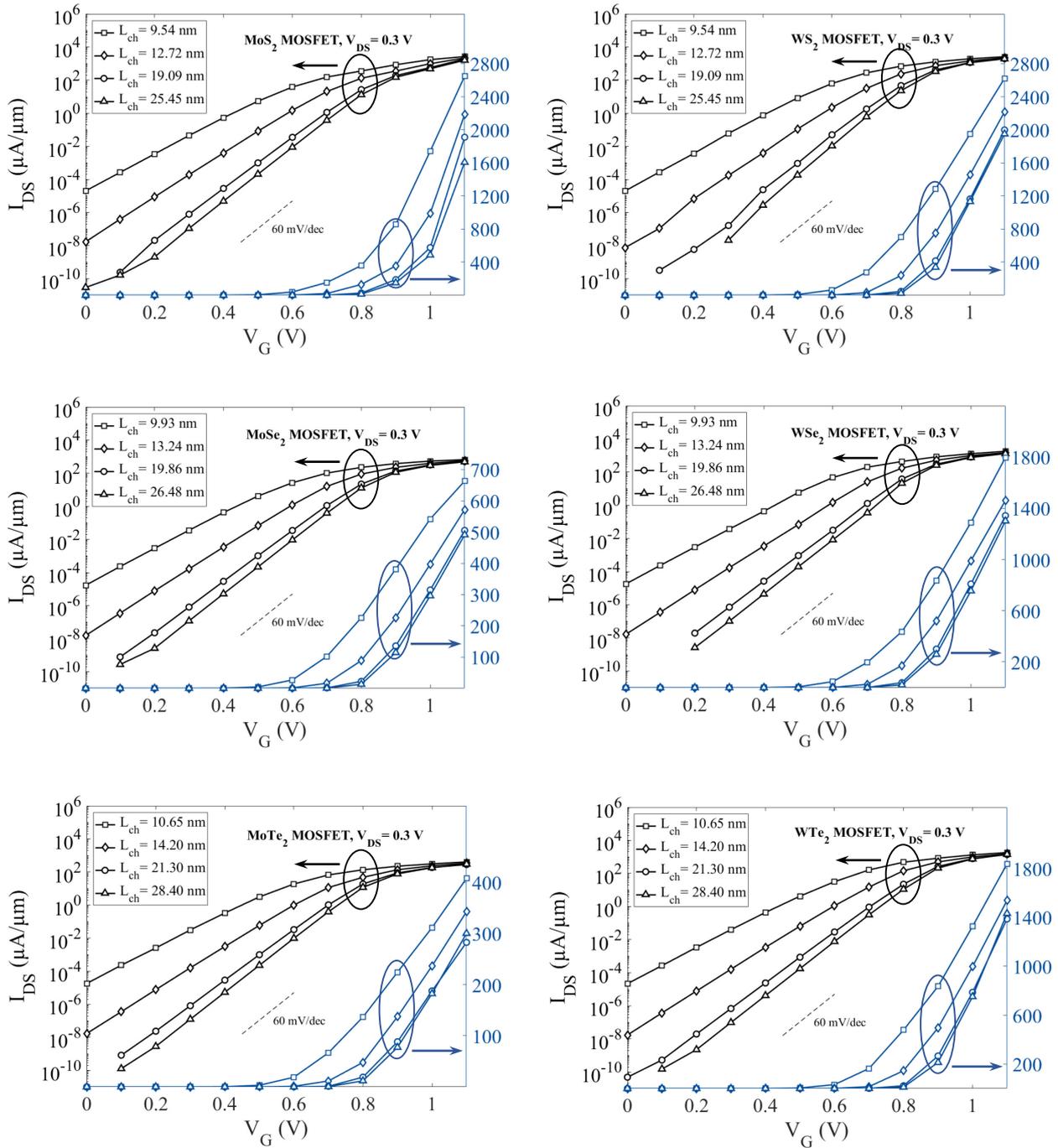


Figure 57.  $I_D$ - $V_G$  characteristics for all six devices, with  $L_{ch}$  ranging from 10 to 28 nm,  $V_{DS} = 0.3$  V and  $V_{BG-S/D} = 1.9$  V.

The same behavior is observed in all devices and is the one expected from investigating the CB profiles in Figure 56.

In the case of the shortest channel, the device can hardly be fully turned OFF, yielding currents around  $I_{DS} = 2.10^{-5}$   $\mu\text{A}/\mu\text{m}$  at  $V_G = 0$  V due to the low energy barrier and carrier tunneling straight from source to drain as evidenced by the LDOS and current density shown in Figure 58.

However, as channel length increases, the OFF current strongly decreases, and can even be reduced by a factor of up to  $10^6$  at low  $V_G$  due to the increased barrier height and electrostatic integrity of the channel.

Sub-threshold swing is also impacted by  $L_{ch}$ : a high 85 mV/dec  $SS$  is observed in the case of the shortest channel, while the theoretical lower limit of 60 mV/dec is reached by the devices bearing the 28 nm channel; this highlights the fact that in the case of the longest channel, current in the OFF state is purely due to the thermionic injection of carriers above the barrier, while tunneling strongly contributes to the OFF current observed in the short-channel devices (see the current densities shown in Figure 58).

Finally,  $L_{ch}$  also influences the threshold voltage  $V_T$  of these devices, which can once again be explained by the increased proximity of the drain backgate voltage and its influence on the CB in the channel. As a result,  $V_T \sim 0.65$  V in the short-channel devices compared to  $\sim 0.85$  V in the case of the longer-channels. Even though  $V_T$  increases with channel length, the ON current at a given  $V_G = V_T + V_I$  remains unchanged.

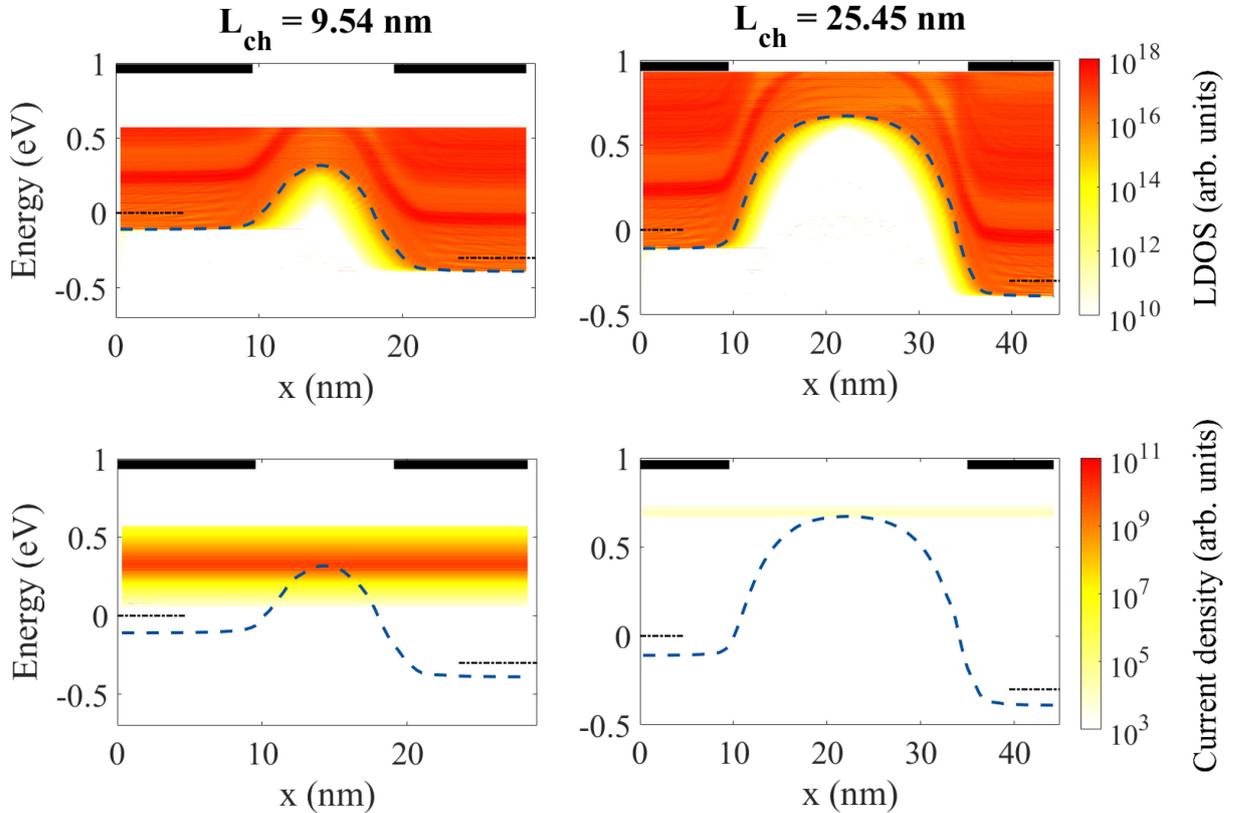


Figure 58. LDOS (top) and current density (bottom) in the MoS<sub>2</sub> MOSFET in the OFF state ( $V_G = 0.2$  V), at  $V_{DS} = 0.3$  V and  $V_{BG-S/D} = 1.9$  V for (left)  $L_{ch} = 9.54$  nm and (right)  $L_{ch} = 25.45$  nm.

Channel length is therefore identified as an important parameter in the case of these MOSFETs. A short channel ( $<15$  nm) will strongly impact device performance, increasing both the OFF state current and  $SS$ . However, if the channel length is beyond approximately 20 nm, the device can yield its peak performance both in the OFF and the ON state without any significant drawbacks, in the ballistic approximation.

In the end, these MOSFETs yield somewhat unremarkable performances: their ON currents are respectable, ranging from a couple hundred to several thousand  $\mu\text{A}/\mu\text{m}$  (in the ballistic regime), but are no match for today's top of the line Si-based technology. These results are in-line with recent experimental work on such devices: due to their relatively low mobility, TMDs have been all but abandoned in the quest to find a successor to silicon in MOSFET technology.

## 4.2 Homojunction TMD TFETs

The second type of device investigated in this work is the n-type homojunction TFET. These devices will be presented and investigated even more briefly than the MOSFETs previously mentioned, for reasons that will quickly become obvious.

They will however be useful as they will present the working mechanism of a TFET and, by being used as comparison, highlight the importance of material selection and band alignment in heterojunction-based TFETs.

### 4.2.1 Device architecture

The device architecture for homojunction TFETs is the same as that of the MOSFETs presented previously (see Figure 51), except that  $L_S = 50 \times a_{MX_2}$  (roughly 16.5 nm).

The main difference when it comes to operating the device will be the voltages applied to the source and drain backgates. In an n-type TFET, carriers tunnel from the source VB to the channel CB. The backgates, which control the profile of the electronic bands, must therefore be set to appropriate voltages (allowing for an energy interval to be both below the top of the source VB and above the bottom of the channel/drain CB). Therefore, the source backgate voltage will be strongly negative, so that the source VB will be pushed upwards towards  $\mu_F$ , while the drain backgate voltage will remain positive, as was the case in the studied MOSFETs.

### 4.2.2 Considered TMDs

As TFETs rely on BTBT as a working mechanism, the band gap of the material used will be directly related to the length of the depletion region (the region through which carriers will tunnel from the source VB to the channel CB).

If the band gap is too wide, no amount of gate voltage will allow carriers to tunnel through the resulting depletion region.

In the TB model used, MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub> all have band gaps wider than 1.6 eV. These wide band gaps induce a long depletion region (>10 nm), no matter the gate and source/drain backgate voltages applied, which prevents the tunneling of carriers and therefore current flow through the device. As such, these materials cannot be used for homojunction TFET operation.

MoTe<sub>2</sub> and WTe<sub>2</sub>, however, have narrower band gaps at around 1.2 eV and therefore seem more suited for use in homojunction TFETs. The only devices presented in this section are therefore MoTe<sub>2</sub> and WTe<sub>2</sub> homojunction TFETs.

### 4.2.3 Electronic transport simulations

The same transport code was used to simulate electronic transport simulations in the MoTe<sub>2</sub> and WTe<sub>2</sub> homojunction TFETs.

Their behavior was studied for gate voltages ranging from  $V_G = 0$  V to 1.5 V, at  $V_{DS} = 0.3$  V,  $L_{ch} = 28.4$  nm and backgate voltages of  $V_{BG-S} = -1.75$  V and  $V_{BG-D} = 0.75$  V.

The corresponding current characteristics are shown in Figure 59.

A few things are immediately obvious from looking at these current characteristics:

- Both transistors yield very low currents: while both homojunction TFETs present “transistor-like” characteristics (clear transition from an OFF to an ON state followed by a current saturation), the resulting ON-state currents are in the nA/ $\mu$ m range for WTe<sub>2</sub> and in the tens of pA/ $\mu$ m for MoTe<sub>2</sub>. While small, the ON-state current in the WTe<sub>2</sub> device is larger than that of the MoTe<sub>2</sub> device by a factor of approximately  $10^2$ , which can be attributed to its slightly narrower band gap.
- In both devices, the sub-threshold swing exceeds 60 mV/dec even though, contrary to MOSFETs, TFETs can in principle yield  $SS$  below this theoretical limit as detailed in Chapter 1.

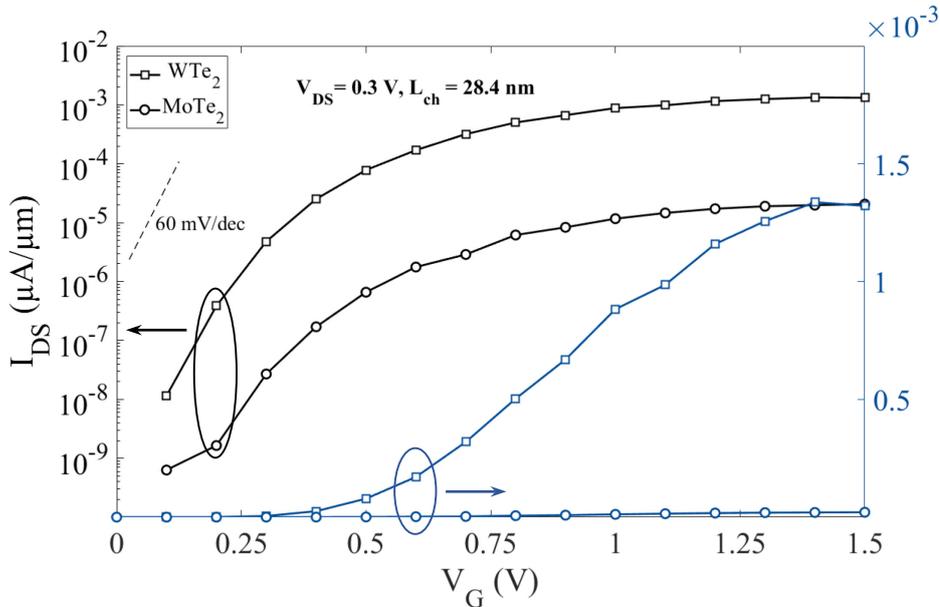


Figure 59.  $I_D$ - $V_G$  characteristics of the MoTe<sub>2</sub> and WTe<sub>2</sub> homojunction TFETs at  $V_{DS} = 0.3$  V,  $L_{ch} = 28.4$  nm and backgate voltages of  $V_{BG-S} = -1.75$  V and  $V_{BG-D} = 0.75$  V. The dotted line indicates a 60 mV/dec sub-threshold swing, the theoretical lower limit for MOSFETs.

The overall performance of these devices is therefore extremely poor, and they cannot be used as transistors for CMOS circuits due to their extremely low ON-state currents.

However, they provide a good example and valuable insight into the workings of a TFET as is evidenced by Figure 60 and Figure 61.

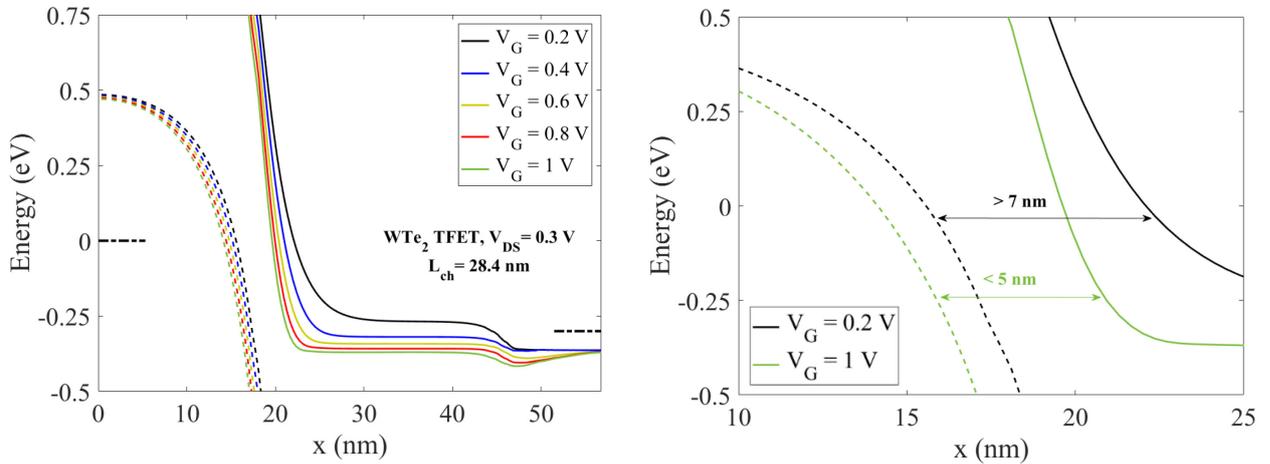


Figure 60. Left: Highest VB (dotted lines) and lowest CB (full lines) in the  $\text{WTe}_2$  device at  $V_{DS} = 0.3$  V,  $L_{ch} = 28.4$  nm and for  $V_G$  ranging from 0 V to 0.8 V. Right: Highest VB (dotted lines) and lowest CB (full lines) in the same device, highlighting the length of the depletion region through which carriers must tunnel in the OFF ( $V_G = 0$  V) and ON state ( $V_G = 0.8$  V).

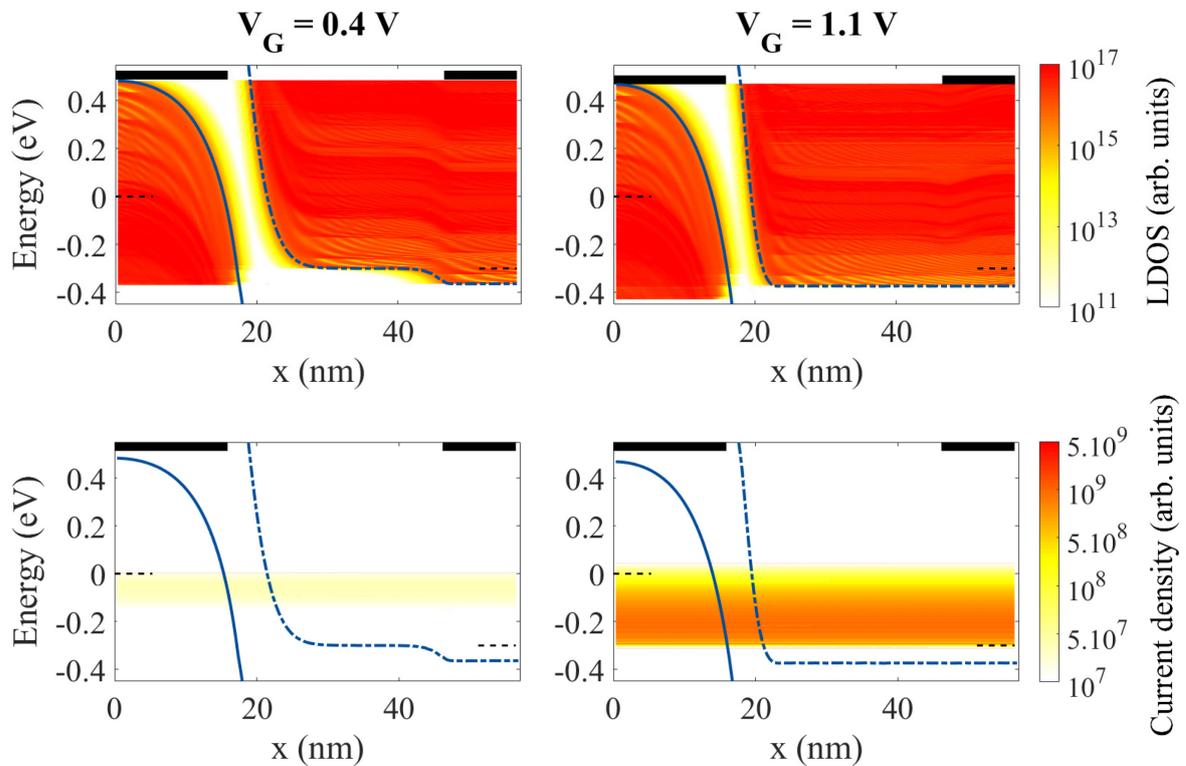


Figure 61. (top) LDOS and (bottom) current density figures in the same  $\text{WTe}_2$  device in the (left) OFF and (right) ON state, as well as highest VB (full line) and lowest CB (dashed line). The black bars represent the backgates. The effect of the gate voltage is obvious: as it increases, the length of the depletion region between the source VB and channel CB is reduced and carriers can tunnel through.

Figure 60 shows the highest VB and lowest CB of the  $\text{WTe}_2$  device when transitioning from the OFF state ( $V_G = 0$  V) to the ON state ( $V_G = 0.8$  V), and Figure 61 shows LDOS and current density figures for the same device.

Both figures highlight the effect of the gate voltage on the bands: as  $V_G$  is increased, the CB in the channel is pushed towards lower energies, and gets closer to the source VB. As such, the length of the depletion region (the region through which the carriers will have to tunnel) is reduced from over 7 nm in the OFF state, to less than 5 nm in the ON state. This seemingly small change is enough to allow carriers to tunnel from one band to the other, and therefore establish current.

Even though these devices do not yield satisfactory results, the influence of channel length and backgate voltages will now be briefly discussed.

#### 4.2.3.1 Influence of backgate voltages

As explained in Section 4.1.2.1, backgate voltages force the potential to a given value, and therefore control the profile of the bands in the contacts.

In the case of an n-type TFET, the source backgate voltage must be strongly negative, so that the source VB is pushed upwards towards  $\mu_S$  ( $\mu_S = 0$ ) and in the same energy range as the channel CB.

Figure 62 shows the influence of the source and drain backgate voltages on the current characteristics of the  $\text{WTe}_2$  device.  $V_{BG-S}$ , which controls the level of the VB in the source, has a strong impact on the behavior of the transistor: as expected, if it is not negative enough only the very top of the VB will be available for tunneling and current will drop significantly.  $V_{BG-D}$ , however, has little to no impact on device performance, only slightly impacting ON-state current.

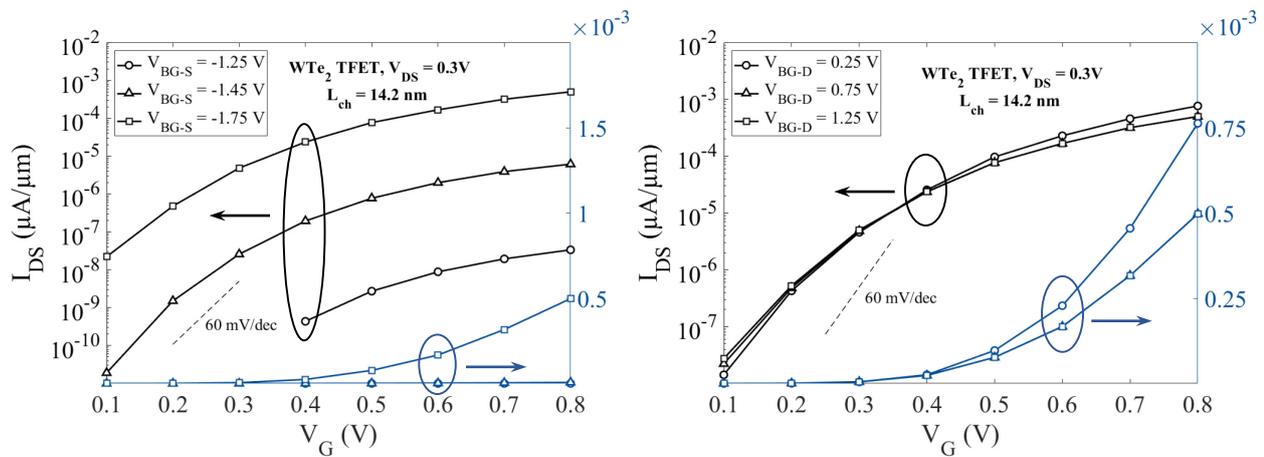


Figure 62.  $I_D$ - $V_G$  characteristics for the  $\text{WTe}_2$  TFET at  $L_{ch} = 14.2$  nm and  $V_{DS} = 0.3$  V.

Left:  $V_{BG-D} = 0.75$  V and  $V_{BG-S}$  ranges from  $-1.25$  V to  $-1.75$  V.

Right:  $V_{BG-S} = -1.75$  V and  $V_{BG-D}$  ranges from  $0.25$  V to  $1.25$  V.

### 4.2.3.2 Influence of channel length

As was the case for the MOSFETs presented in Section 4.1, the impact of channel length on the performance of the MoTe<sub>2</sub> and WTe<sub>2</sub> homojunction TFETs is briefly investigated here.

$I_D$ - $V_G$  characteristics for both devices with  $L_{ch}$  ranging from 5.4 nm to 28 nm are shown in Figure 63.

It is clear that, for channel lengths exceeding roughly 14 nm, the behavior of the transistor is unchanged by  $L_{ch}$ , whether in the OFF state or in the ON state.

However, as the channel length approaches 10 nm, the current at extremely low gate voltages increases by a factor of  $\sim 10$ .

Finally, as channel length decreases further (down to 5.3 nm as shown in Figure 63), the OFF state current keeps increasing until the device cannot be properly turned off. This behavior is expected and is due to uncontrolled source-to-drain tunneling, a common short-channel effect which was already observed in the case of MOSFETs (see Figure 57).

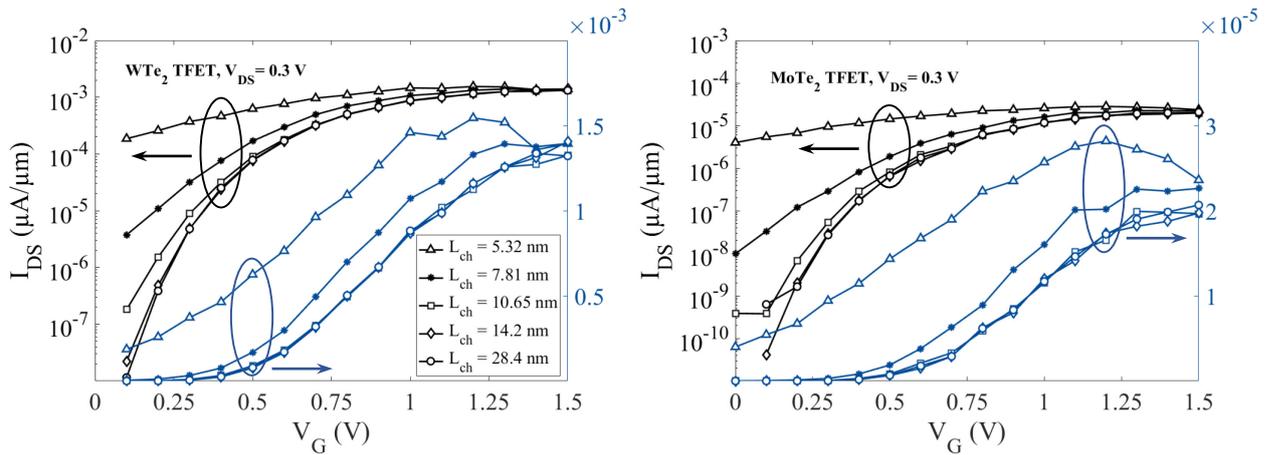


Figure 63.  $I_D$ - $V_G$  characteristics of the WTe<sub>2</sub> and MoTe<sub>2</sub> devices for  $L_{ch}$  ranging from 5 nm to 28 nm at  $V_{DS} = 0.3$  V,  $V_{BG-S} = -1.75$  V and  $V_{BG-D} = 0.75$  V; the legend applies to both figures. Source-to-drain tunneling is observed and strongly degrades OFF-state current for channel lengths below.

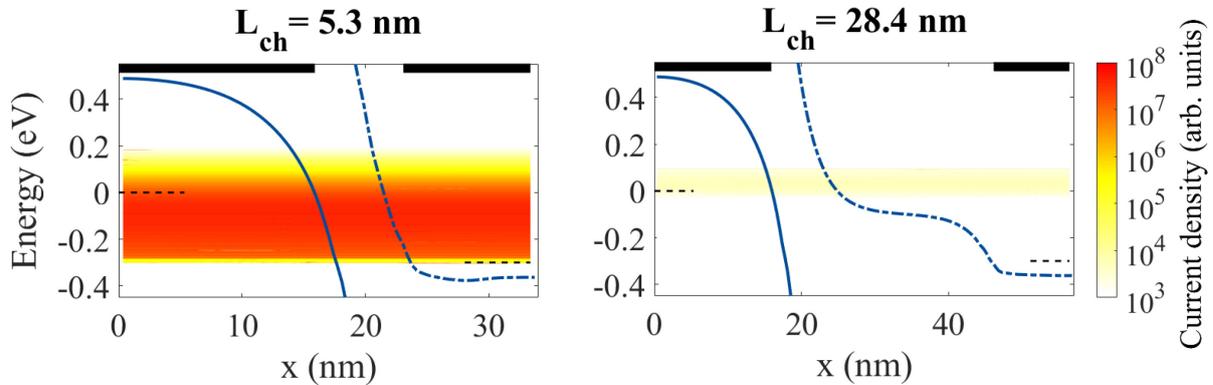


Figure 64. Current density, highest VB (full line) and lowest CB (dashed line) in the WTe<sub>2</sub> device at  $V_G = 0.1$  V for  $L_{ch} = 5.3$  nm (left) and  $L_{ch} = 28.4$  nm. The black bars at the top represent the backgates. In the case of the short channel, the proximity of the drain backgate pulls the CB down in the channel despite the low gate voltage, leading to the tunneling of carriers from the source VB to the channel CB.

The origin of this tunneling at very low gate voltage in the case of extremely short channels is highlighted by Figure 64, which shows current densities for the  $\text{WTe}_2$  at  $V_G = 0.1$  V for  $L_{ch} = 5.3$  nm and  $L_{ch} = 28.4$  nm. In the case of the short channel, the increased proximity of the drain backgate, which forces the CB around  $-0.35$  eV in the drain, pulls the channel CB down despite the low gate voltage. The available carriers in the source VB can therefore tunnel and establish current.

While these TMD-based homojunction TFETs yield very weak performance (extremely low ON current and high  $SS$ ) and therefore cannot be used as efficient CMOS transistors, they provided an interesting framework to investigate the overall operation of a TFET, as well as the influence of design parameters such as channel length and backgate voltages, which will be useful when studying the TMD-based in-plane heterojunction TFETs that constitute the main part of my PhD work.

Furthermore, their weak performance will be used as a reference for comparison and will highlight the importance of band alignment in TFETs, as well as the vast potential of the in-plane TMD heterojunctions studied in the coming chapters.



# Chapter 5

## In-plane heterojunction TFETs

In this Chapter, TFETs based on in-plane heterojunctions of TMDs will be investigated. As was detailed in Section 1.4.1, the band alignment between the source and the drain is paramount in TFETs to achieve high performance.

Using TMD heterojunctions should therefore allow us to “mix-and-match” VB and CB from all six TMDs to obtain the most favorable band alignment.

### 5.1 Device architecture

The devices presented here all follow the same design, which is very close to that of the homojunction TFETs presented in Section 4.2.1, the only difference being that two different TMDs are used in the active layer: one in the source and another in the channel and drain.

As a reminder, the device architecture (shown in Figure 65) is as follows:

- SiO<sub>2</sub> buried oxide with thickness  $t_{BOX} = 10 \times a_{device}$  (will depend on the considered heterojunction).
- High- $\kappa$  top gate oxide with equivalent oxide thickness  $EOT = 4 \times a_{device}$ .
- TMD<sub>1</sub> source of length  $L_S$ .
- TMD<sub>2</sub> channel and drain of lengths  $L_{ch}$  and  $L_D$ .
- Source and drain contacts to which voltages  $V_S = 0$  and  $V_D = -eV_{DS}$  are applied and will control the Fermi energies in the contacts.
- A top gate of length  $L_G = L_{ch}$ , to which a voltage  $V_G$  is applied. This gate will control current flow through the device.
- Source and drain backgates to which voltages  $V_{BG-S}$  and  $V_{BG-D}$  are applied. Since the active layer is purely 2D, we can use backgates rather than chemical doping to control charge densities in the contacts.

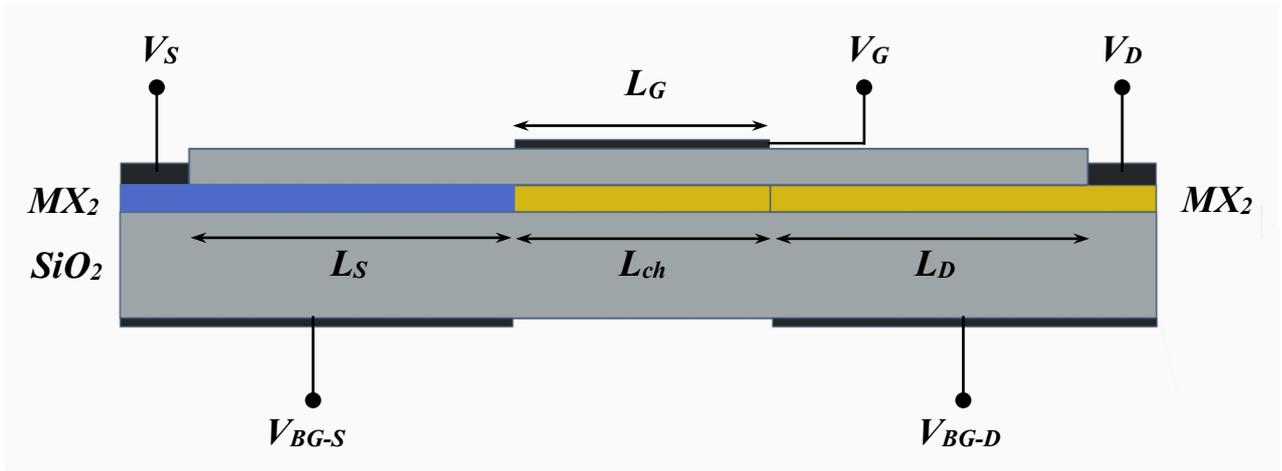


Figure 65. Device architecture for the considered heterojunction TFETs. One TMD acts as the source, and another as the channel/drain.  $\text{SiO}_2$  is used as a buried oxide, and a high- $\kappa$  dielectric as the top gate oxide.

The selection of the TMDs to be used in the source and in the channel/drain region will now be detailed.

## 5.2 Selection of the TMD heterojunctions

As shown in Section 1.4.1, the band alignment in TFETs is a paramount feature, and selecting the correct TMD pair to be used as a heterojunction is therefore extremely important and will strongly impact device performance.

As a reminder, the band alignment of pristine TMDs, as obtained with the TB model used in this work, is shown in Figure 66.

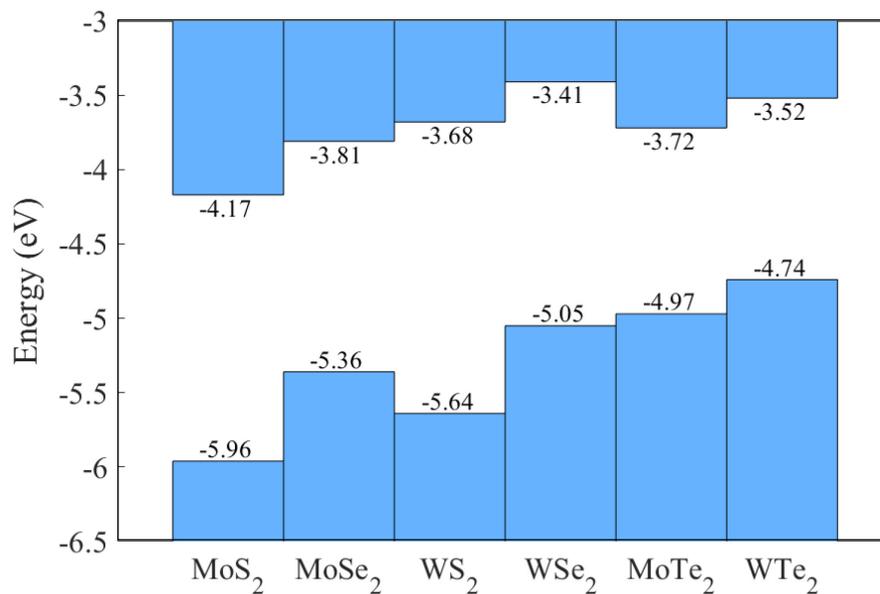


Figure 66. Band alignment in pristine TMDs obtained by using our TB model. The vacuum level is set to 0 eV.

To minimize the length of the depletion region in the considered TFETs, the VB must be as high as possible, while the CB must be as low as possible.

As a result, MoS<sub>2</sub>, which yields the lowest CB, will be used as a channel/drain material in all heterojunction TFETs. The resulting heterojunctions and the strains applied to reach lattice matching at the interface are therefore the following:

- MoSe<sub>2</sub>/MoS<sub>2</sub> and WSe<sub>2</sub>/MoS<sub>2</sub>: in these heterojunctions, ASe<sub>2</sub> is in its pristine form, while a 4.3% tensile strain is applied onto MoS<sub>2</sub> so that a common lattice parameter is reached at  $a_{ASe_2} = 3.31 \text{ \AA}$ . The effects of this strain are detailed in 3.1.5, highlighted in Figure 43 and summed up in Figure 67.
- MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub>: in these heterojunctions, ATe<sub>2</sub> is under a 5.6% compressive strain, while a 5.3% tensile strain is applied onto MoS<sub>2</sub> so that a common lattice parameter is reached at  $a = 3.35 \text{ \AA}$ . The effects of this strain are detailed in 3.1.5, highlighted in Figure 44 and summed up in Figure 67.
- The WS<sub>2</sub>/MoS<sub>2</sub> heterojunction is not considered because it results in a roughly 1.5 eV gap between the source VB and channel CB, which is far too high for TFET operation.

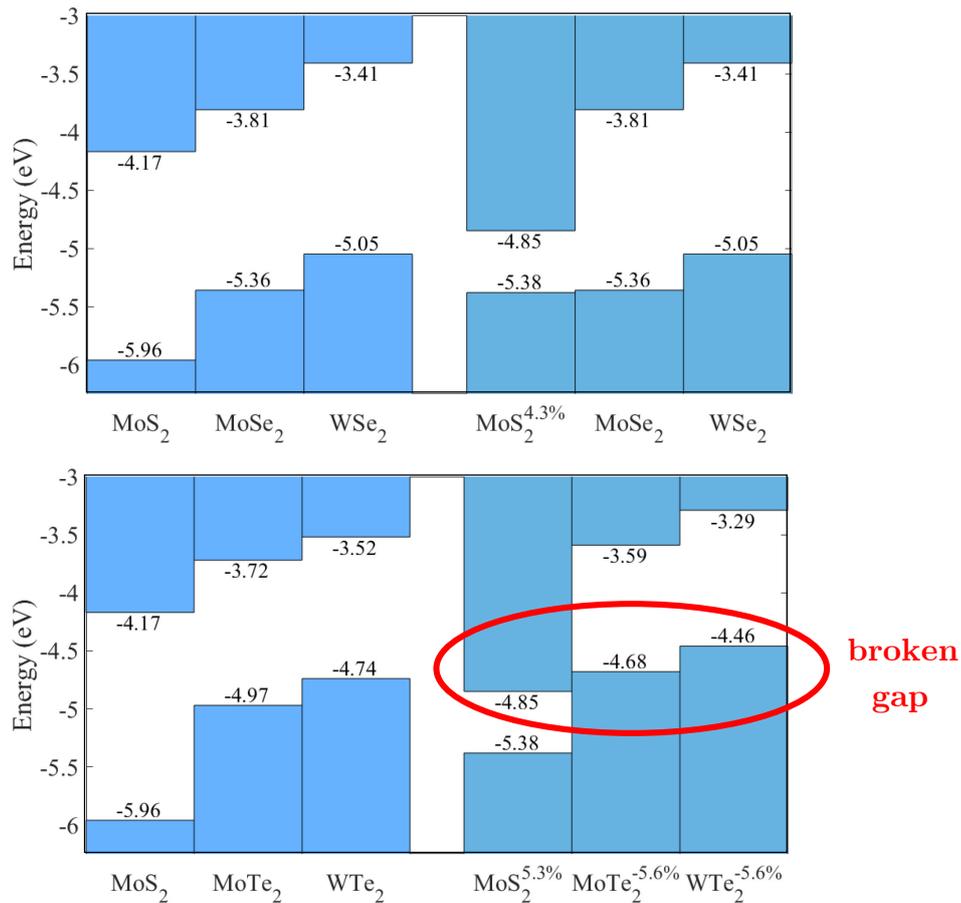


Figure 67. Top: CB and VB of MoS<sub>2</sub>, MoSe<sub>2</sub> and WSe<sub>2</sub> in their pristine form and under the strain applied in the ASe<sub>2</sub>/MoS<sub>2</sub> heterojunctions. Bottom: CB and VB of MoS<sub>2</sub>, MoTe<sub>2</sub> and WTe<sub>2</sub> in their pristine form and under the strain applied in the ATe<sub>2</sub>/MoS<sub>2</sub> heterojunctions.

## 5.3 Electronic transport simulations

The transport code used previously was slightly adapted to accommodate several materials in the active layer, but the transport calculation and overall flowchart remain unchanged.

### 5.3.1 Comparison of all four heterojunctions

Before delving deeper into the influence of design parameters such as contact or channel length, or backgate voltages for instance, let us compare the performance of all four considered TMD heterojunction TFETs.

Their performance was studied for gate voltages ranging from  $V_G = 0$  V to 0.6 V, at  $V_{DS} = 0.3$  V,  $L_{ch} = 80 \times a_{device} \sim 27$  nm,  $L_S = L_D = 50 \times a_{device} \sim 16.5$  nm and backgate voltages depending on the heterojunction considered (the work-function  $W_G$  of the metal used as top-gate and both backgates is also given):

- MoSe<sub>2</sub>/MoS<sub>2</sub>:  $V_{BG-S} = -1$  V,  $V_{BG-D} = 0.5$  V,  $W_G = 4.81$  eV.
- WSe<sub>2</sub>/MoS<sub>2</sub>:  $V_{BG-S} = -0.5$  V,  $V_{BG-D} = 1$  V,  $W_G = 4.91$  eV.
- MoTe<sub>2</sub>/MoS<sub>2</sub>:  $V_{BG-S} = 0.58$  V,  $V_{BG-D} = 0.8$  V,  $W_G = 5.19$  eV.
- WTe<sub>2</sub>/MoS<sub>2</sub>:  $V_{BG-S} = 0.85$  V,  $V_{BG-D} = 1.1$  V,  $W_G = 5.19$  eV.

The resulting current characteristics are shown in Figure 68.

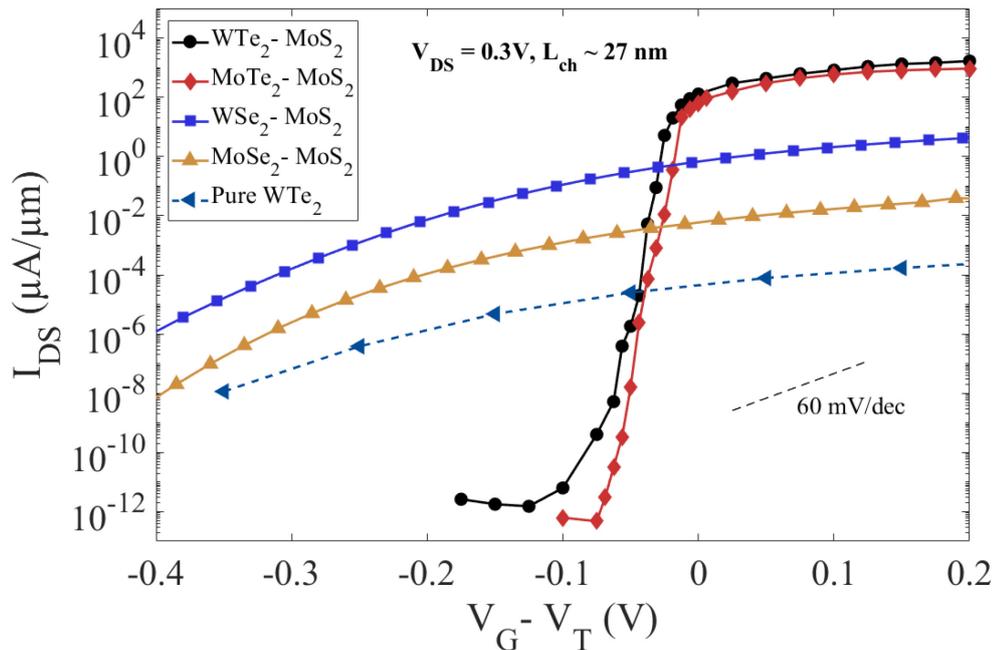


Figure 68.  $I_D$ - $V_G$  characteristics for all four heterojunction TFETs as well as the homojunction WTe<sub>2</sub> TFET at  $L_{ch} \sim 27$  nm,  $V_{DS} = 0.3$  V. The dotted line represents a 60 mV/dec SS.

Due to the band alignment of these TMDs, different ranges of gate voltages have to be applied to observe the OFF-ON transition. Therefore, the current characteristics are plotted against  $V_G - V_T$ , where  $V_T$  is the threshold voltage obtained by the linear approximation of the ON current so that they appear in the same range.

A few things are obvious from the observation of Figure 68:

- In all cases, the heterojunction is beneficial: all heterojunction-based devices yield superior performance compared to the homojunction  $\text{WTe}_2$  TFET, which was by far the highest performing homojunction device. Most notably,  $\text{WSe}_2$  and  $\text{MoSe}_2$ , which could not even function as homojunction TFETs due to their wide band gaps, perform as transistors when used in conjunction with  $\text{MoS}_2$ .
- $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  yield by far the best performance: while the two other devices benefited greatly from the heterojunction and now show transistor-like characteristics, the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  heterojunctions yield incredibly steep transitions from the OFF to the ON state, and far higher ON currents -in the thousands of  $\mu\text{A}/\mu\text{m}$ -.

The large difference in performance between the  $\text{MoSe}_2/\text{MoS}_2$  and  $\text{WSe}_2/\text{MoS}_2$  and the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  devices can be directly explained by the alignment of the bands in those devices.

The band offset (calculated as  $\text{CB}_{\min} - \text{VB}_{\max}$ , see Figure 67) in each of these heterojunctions is given in Table 2 alongside figures of merit such as the length of the depletion region in the ON state,  $I_{\text{ON}}/I_{\text{OFF}}$ , and sub-threshold swing ( $I_{\text{ON}}$  is calculated at  $V_G = V_{\text{OFF}} + V_{\text{DD}}$ , where  $V_{\text{DD}} = 0.3$  V and  $V_{\text{OFF}}$  is  $V_G$  for which  $I_{\text{DS}} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$  and  $SS$  is estimated between  $I_{\text{DS}} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$  and  $I_{\text{DS}} = 10^{-2}$   $\mu\text{A}/\mu\text{m}$ ). This table highlights the strong correlation between the band offset in the considered heterojunction and the performance of the corresponding TFET.

|                                | $\text{MoSe}_2/\text{MoS}_2$ | $\text{WSe}_2/\text{MoS}_2$ | $\text{MoTe}_2/\text{MoS}_2$ | $\text{WTe}_2/\text{MoS}_2$ |
|--------------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|
| Band offset (eV)               | 0.51                         | 0.2                         | -0.17                        | -0.39                       |
| $L_{\text{depletion}}$ (nm)    | 5.3                          | 4.4                         | ~0                           | ~0                          |
| $I_{\text{ON}}/I_{\text{OFF}}$ | $8.7 \times 10^2$            | $2.5 \times 10^4$           | $9.8 \times 10^7$            | $2.0 \times 10^8$           |
| $SS$ (mV/dec)                  | 106                          | 55                          | 4                            | 3                           |

Table 2. Band offset and transport performance (depletion region length in ON state,  $I_{\text{ON}}/I_{\text{OFF}}$  and  $SS$ ) in the four in-plane heterojunction TFETs at  $V_{\text{DD}} = 0.3$  V.

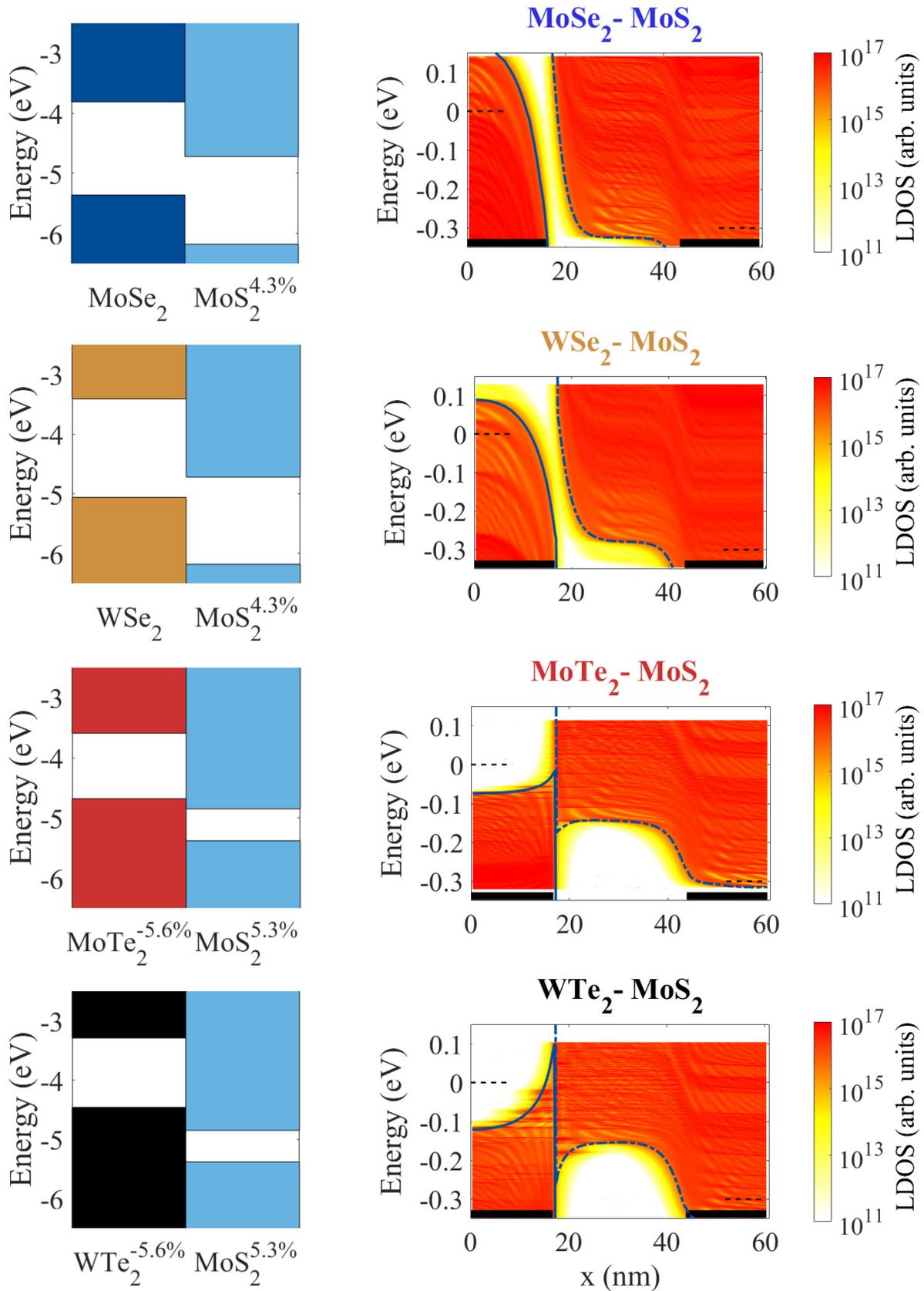


Figure 69. Left: Source VB and channel CB in each heterojunction, highlighting their band alignment. Right: LDOS in the ON state ( $V_G = 0.5$  V) for each heterojunction, highlighting the depletion region through which carriers must tunnel. Full (dotted) blue lines indicate the VB (CB), dotted black lines indicate the Fermi levels in the contacts, and black bars represent the source and drain backgates.

The band alignments and LDOS maps shown in Figure 69 highlight the influence of the band offset on the length of the depletion region, and therefore on the performance of the device. In the case of a broken gap ( $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$ ) the depletion region is almost non-existent, which allows the TFET to yield an extremely steep OFF-ON transition as well as high ON currents in the thousands of  $\mu\text{A}/\mu\text{m}$ , even at a low supply voltage of 0.3 V.

It is worth noting that the performances shown for the  $\text{MoSe}_2/\text{MoS}_2$  and  $\text{WSe}_2/\text{MoS}_2$  devices in Figure 68 were obtained by optimizing contact length, channel length and backgate voltages, and therefore represent the peak performances registered for these devices, both in terms of  $SS$  and ON current. Still, those performances are weak at best, with  $SS$  around or beyond 60 mV/dec and  $I_{ON}/I_{OFF}$  ratios below  $10^5$ .

For this reason, the rest of this chapter and manuscript, will focus solely on the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  heterojunctions, which yield far more promising performances with  $SS$  below 5 mV/dec and  $I_{ON}/I_{OFF}$  around  $10^8$ .

### 5.3.2 Influence of contact length

The length of the source and drain contacts may have a strong influence on the potential in the device and therefore the profile of the bands due to the corresponding backgates. If the contact is too short, the potential cannot adapt as it should, which modifies the profile of the bands in the contacts and possibly even in the channel. As a result, the computed current will be impacted, mainly in the OFF state.

The goal is therefore to identify the shortest contact lengths that do not impact the profile of the bands and the performance of the device. The results presented thereafter were obtained in the  $\text{MoTe}_2/\text{MoS}_2$  heterojunction device with  $V_{DS} = 0.3$  V,  $L_{ch} = 20.1$  nm,  $V_{BG-S} = 0.58$  V and  $V_{BG-D} = 0.8$  V. While the results presented in this section pertain to the  $\text{MoTe}_2/\text{MoS}_2$  device, the same observations were made for the  $\text{WTe}_2/\text{MoS}_2$  device.

We first investigate the influence of the source contact, by modulating its length from 10 nm to 23.5 nm. The resulting  $I_D$ - $V_G$  characteristics, as well as the profile of the highest VB and lowest CB, are shown (for  $L_D = 10.05$  nm) in Figure 70.

It is clear that a 10 nm source is too short:

- Currents in the OFF state increase by a factor of approx.  $10^3$  compared to the devices with longer source contacts.
- The highest VB in the source is not forced at the same energy at  $x = 0$  as in the case of longer contacts.

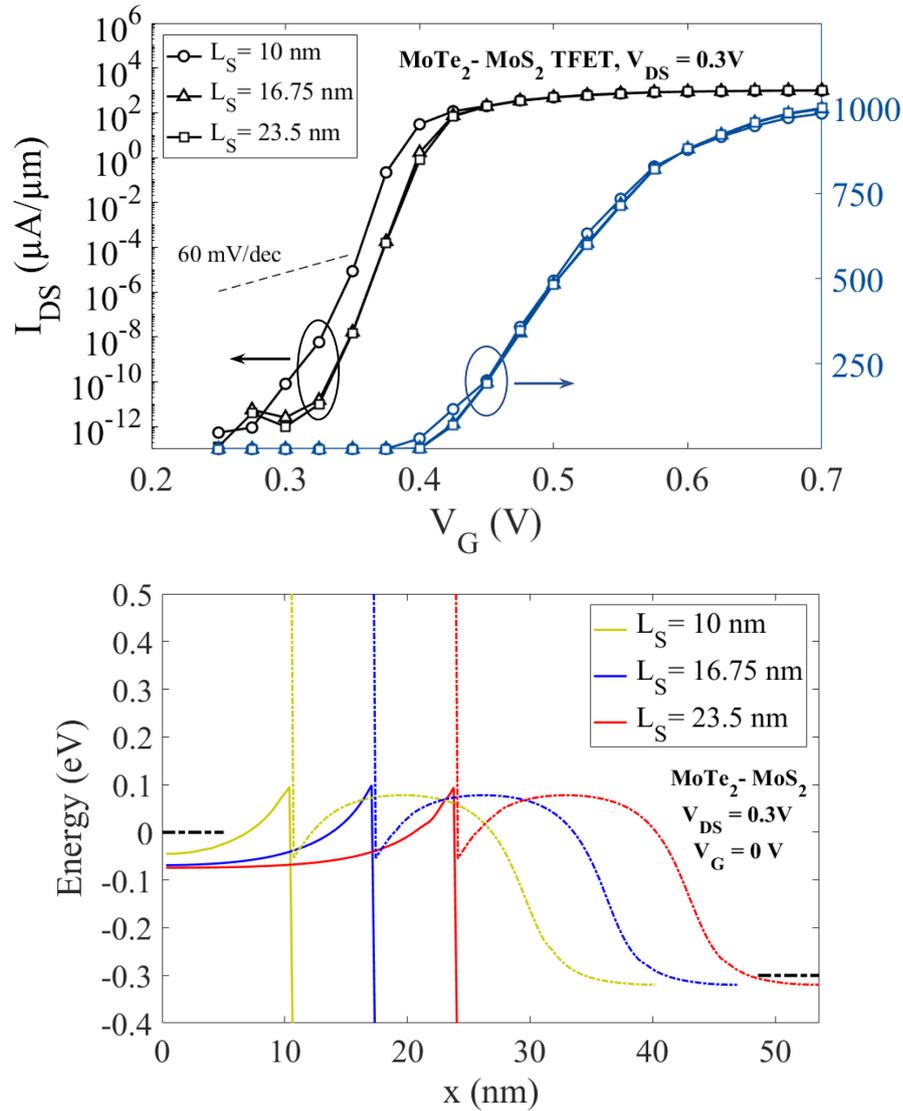


Figure 70. Influence of  $L_S$  on the  $\text{MoTe}_2/\text{MoS}_2$  device. Top:  $I_D$ - $V_G$  characteristics at  $V_{DS} = 0.3\text{V}$ ,  $L_{ch} = 20.1\text{ nm}$ ,  $V_{BG-S} = 0.58\text{ V}$  and  $V_{BG-D} = 0.8\text{ V}$ . Bottom: Highest VB (full lines) and lowest CB (dashed lines) for the same device, at  $V_G = 0\text{ V}$ .

A 16.75 nm source however, seems to be ideal. Compared to the device bearing an even longer source, the currents are not impacted whether in the OFF or the ON state, and the highest VB is also forced at the same energy at  $x = 0$  although barely; this indicates that an even shorter source contact would likely be too short and impact the performance of the device.

As a result, a source length of  $L_S = 16.75\text{ nm}$  will be used in all of the devices investigated. A similar study was performed to identify the appropriate drain contact length.

$I_D$ - $V_G$  characteristics and the profile of the highest VB and lowest CB, are shown for  $L_S = 16.75\text{ nm}$  and  $L_D$  ranging from 6.7 nm to 16.75 nm in Figure 71.

While a drain contact of 6.7 nm does not impact current, the lowest CB in the drain is not forced at the same energy as the devices with longer contacts and, which can be an issue at higher drain backgate voltages.

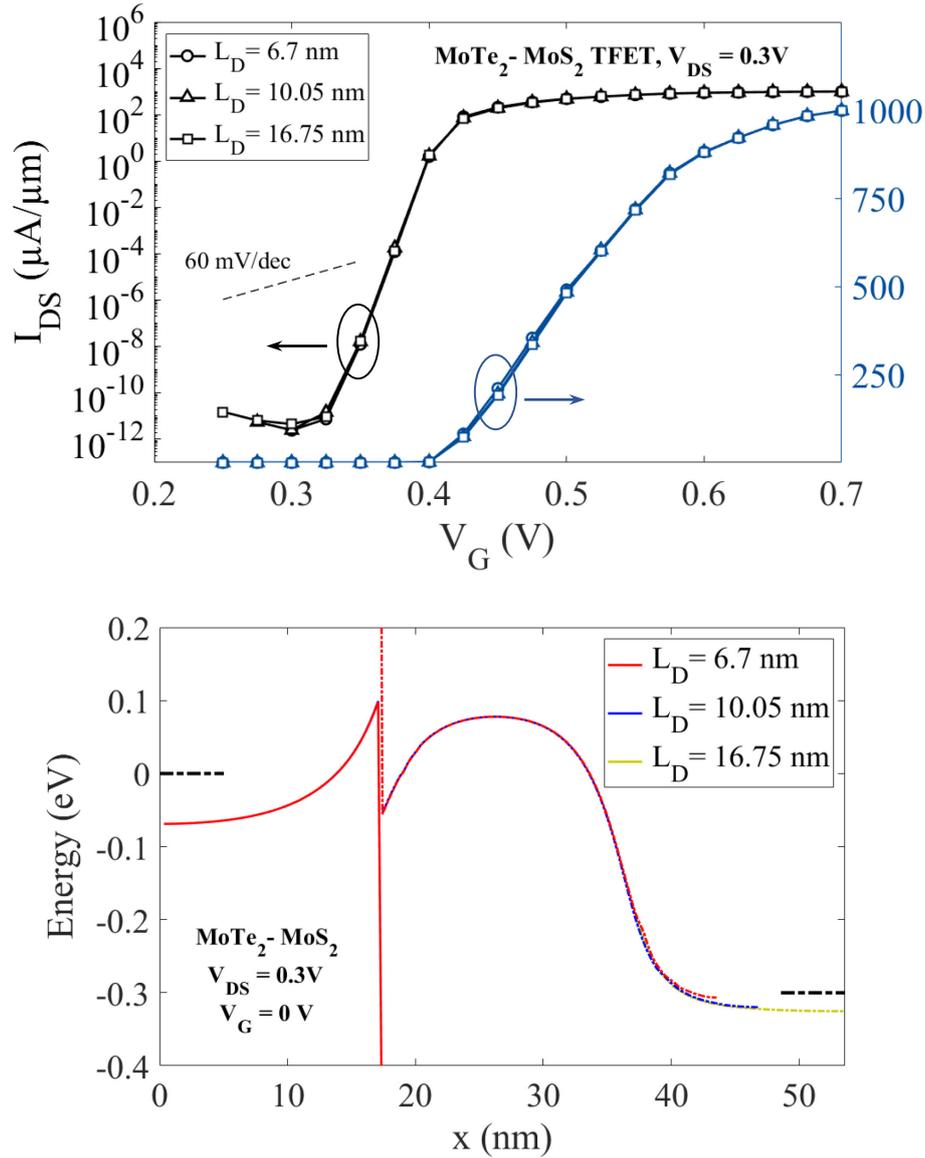


Figure 71. Influence of  $L_D$  on the  $\text{MoTe}_2/\text{MoS}_2$  device. Top:  $I_D$ - $V_G$  characteristics for the at  $V_{DS} = 0.3\text{V}$ ,  $L_{ch} = 20.1\text{ nm}$ ,  $V_{BG-S} = 0.58\text{ V}$  and  $V_{BG-D} = 0.8\text{ V}$ . Bottom: Highest VB (full lines) and lowest CB (dashed lines) for the same device, at  $V_G = 0\text{ V}$ .

Therefore, to make sure the drain will be of an appropriate length no matter the device investigated, I will use a drain contact length of 10.05 nm in all of the devices investigated. Thanks to this quick study of device performance and band profile, I was able to determine contact lengths that ensure a proper resolution of the potential while remaining short nonetheless, so that the need in computational resources is kept at a minimum; while it is not studied here, the negative impact of electron-phonon interactions on device performance will therefore be reduced thanks to this short contact length.

As a reminder,  $L_S = 16.75\text{ nm}$  and  $L_D = 10.05\text{ nm}$  will now be used for all devices. The influence of channel length on device performance will now be studied.

### 5.3.3 Influence of channel length

In Chapter 4, gate length was identified to strongly impact performance both in the case of the TMD MOSFETs and homojunction TMD TFETs. It is therefore expected to influence device performance in these TMD heterojunction devices.

$I_D$ - $V_G$  characteristics for the  $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$  devices at  $V_{DS} = 0.3$  V,  $L_{ch}$  ranging from 5.025 nm to 26.8 nm, and the following backgate voltages:

-  $\text{MoTe}_2/\text{MoS}_2$ :  $V_{BG-S} = 0.58$  V,  $V_{BG-D} = 0.8$  V

-  $\text{WTe}_2/\text{MoS}_2$ :  $V_{BG-S} = 0.85$  V,  $V_{BG-D} = 1.1$  V

are presented in Figure 72.

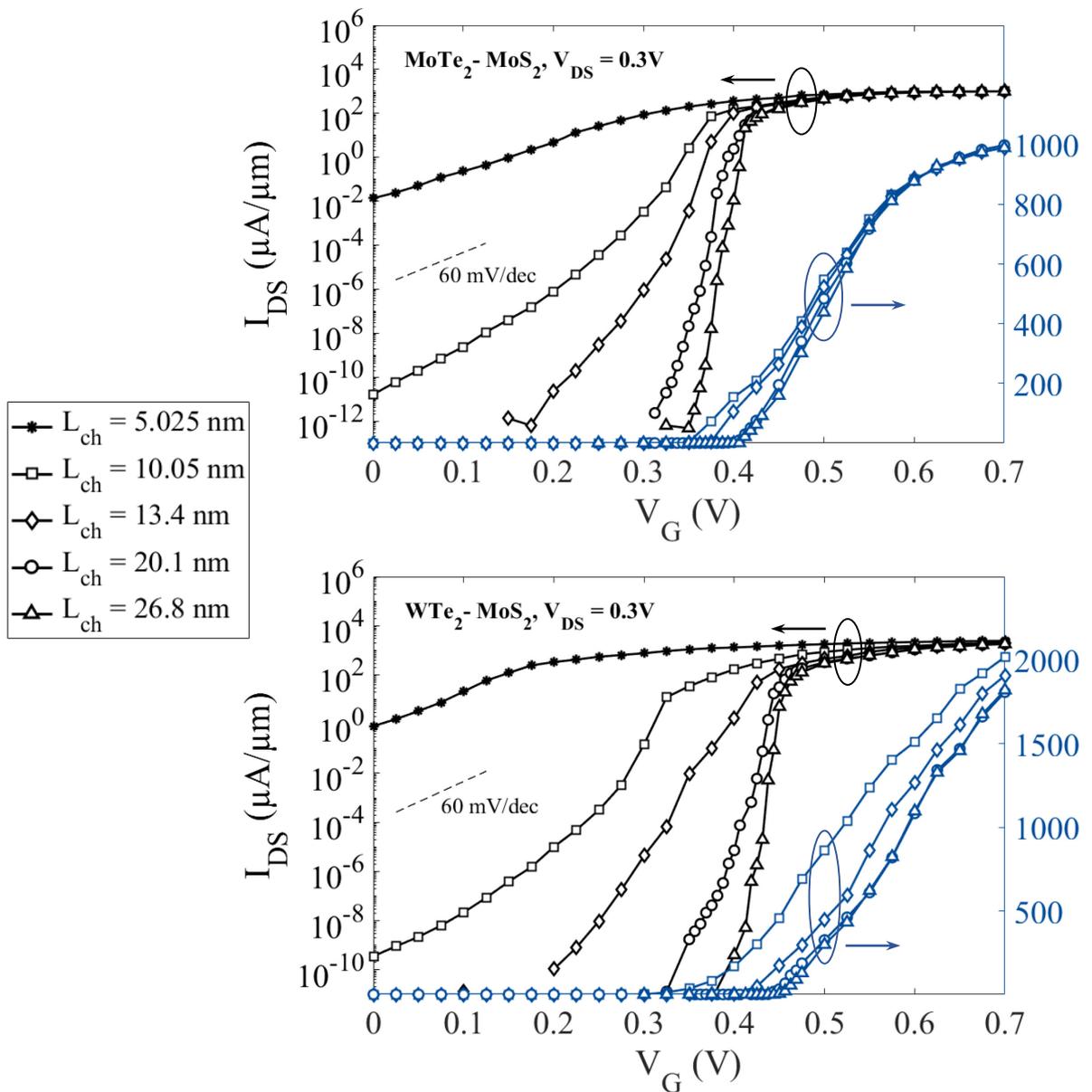


Figure 72.  $I_D$ - $V_G$  characteristics for the heterojunction devices at  $V_{DS} = 0.3$  V,  $L_{ch}$  ranging from 5 nm to 27 nm,  $V_{BG-S} = 0.58$  V and  $V_{BG-D} = 0.8$  V (note that the current at  $L_{ch} = 5.025$  nm is only shown in log scale for clarity purposes).

As expected, channel length has a strong impact on the performance of both heterojunction TFETs. In both devices, increasing  $L_{ch}$  has several major beneficial effects (in the ballistic limit):

- Strong reduction of the OFF-state current: the log scale plots highlight the huge impact of channel length on OFF-state performance. First, if the channel is too short (5.025 nm), the device cannot be switched off due to source-to-drain tunneling and does not behave like a transistor; a 10 nm-channel, however, is sufficient to observe transistor behavior with a clear OFF-ON transition.

As the channel length keeps increasing, device performance in the OFF state can be strongly increased: for instance, a 3.35 nm increase of channel length leads to a reduction of the OFF-current by a factor of approximately  $10^5$  for the WTe<sub>2</sub>/MoS<sub>2</sub> device at low gate voltages ( $V_G = 0.2$  V). Even more impressively, an increase in channel length from 10.05 nm to 26.8 nm allows the MoTe<sub>2</sub>/MoS<sub>2</sub> device to be in a fully OFF state at  $V_G = 0.35$  V, resulting in a reduction of current by a factor beyond  $10^{10}$  (due to both a decrease in leakage current and a slight increase in threshold voltage).

These effects can be explained by the band profiles and current density figures shown in Figure 73 and Figure 74. Much like in Section 4.1.2.2 for MOSFETs, the increased proximity of the drain backgate that comes with a short channel pulls the CB down in the channel region, lowering the barrier to be overcome at a given  $V_G$ . This effect is compounded by the tunneling of carriers through the top of this barrier (see current density figures), further increasing OFF-state leakage currents.

- Strong decrease in sub-threshold swing: along with this strong decrease in OFF state current comes a dramatic increase of the steepness of the slope in the sub-threshold regime. Figure 75 shows the evolution of  $SS$  as a function of channel length in both heterojunction devices. For instance, both devices yield  $SS \sim 60$  mV/dec for  $L_{ch} \sim 7$  nm, compared to  $SS < 5$  mV/dec for  $L_{ch} > 25$  nm.

Once again, this is due to the source-to-drain tunneling that occurs in the case of short channels, which increases OFF-state current and therefore “flattens” the transition from a fully OFF to fully ON state.

This effect is highlighted by the current density figures mentioned earlier (Figure 74). In the case of a short channel, an increasing number of carriers can tunnel through the top of the channel CB as  $V_G$  increases, leading to this steady increase in current. In the case of a long channel however, no such tunneling occurs and the device goes from fully OFF to fully ON state when the threshold voltage is reached.

- Strong increase in  $I_{ON}$  (see Figure 75):  $I_{ON}$  is calculated at  $V_{ON} = V_{OFF} + V_{DD}$  where  $V_{OFF}$  is  $V_G$  for which  $I_{DS} = I_{OFF} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$ . Due to the strong decrease in OFF-state leakage current,  $V_{OFF}$  strongly increases with channel length (from 0.2 V at  $L_{ch} = 10.05$  nm to 0.425 V at  $L_{ch} = 26.8$  nm in the WTe<sub>2</sub>/MoS<sub>2</sub> device) and therefore so does  $V_{ON}$ . Much like  $SS$ ,  $I_{ON}$  saturates for long channels.

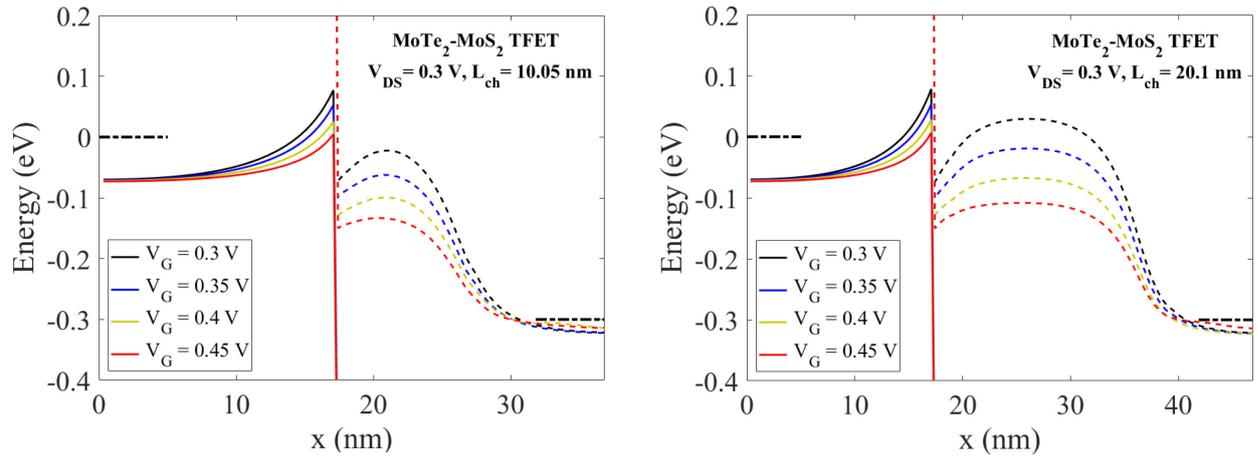


Figure 73. Highest VB (full lines) and lowest CB (dotted lines) during the OFF-ON transition in the MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V and (left)  $L_{ch} = 10.05$  nm (right)  $L_{ch} = 20.1$  nm.

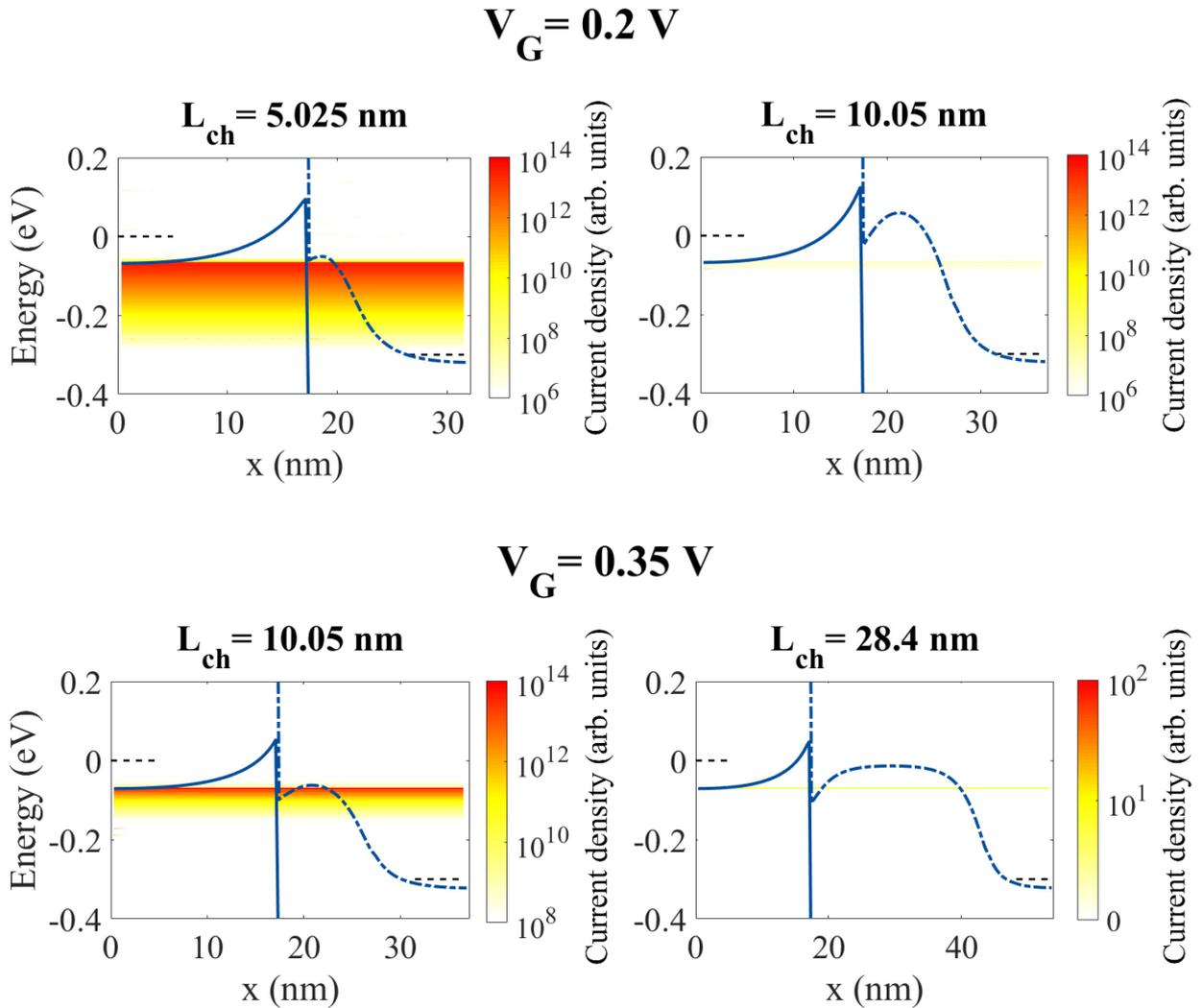


Figure 74. Highest VB (full line) and lowest CB (dotted line) and current density in the MoTe<sub>2</sub>/MoS<sub>2</sub> device at various  $L_{ch}$  and  $V_G$ , and for  $V_{DS} = V_{DD} = 0.3$  V. The top left plot highlights the direct source-to-drain tunneling preventing an actual OFF state to be reached in the device with  $L_{ch} = 5.025$  nm.

The bottom left plot highlights the tunneling through the top of the barrier which degrades  $SS$  in the case of short channels.

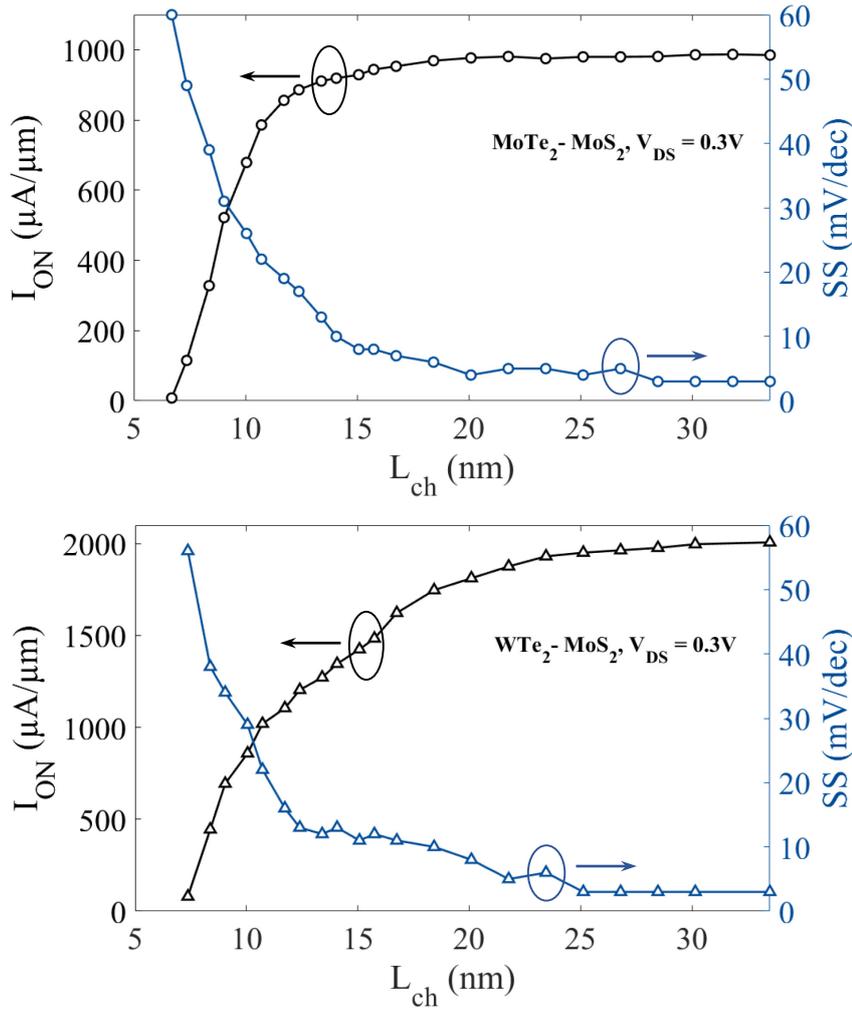


Figure 75. Influence of  $L_{ch}$  on ON current and  $SS$  in (top) the MoTe<sub>2</sub>/MoS<sub>2</sub> device and (bottom) the WTe<sub>2</sub>/MoS<sub>2</sub> device. In both devices, an increase in channel length allows for better performance (lower  $SS$  and higher ON current) up until a certain  $L_{ch}$ , beyond which device performance reaches saturation (20 nm for the MoTe<sub>2</sub>/MoS<sub>2</sub> device and 30 nm for the WTe<sub>2</sub>/MoS<sub>2</sub> device).

From this study, it is clear that the performance of these heterojunction TFETs is intrinsically tied to the length of the channel.

From OFF-state leakage current to  $SS$ , and even ON current, all aspects of device performance are strongly impacted by a change in channel length. In the case of the MoTe<sub>2</sub>/MoS<sub>2</sub> device, a channel length  $> 20$  nm is sufficient to reach peak performance, while a channel length  $> 30$  nm is necessary in the case of the WTe<sub>2</sub>/MoS<sub>2</sub> device.

Nonetheless, promising performance (sub-5 mV/dec  $SS$  and  $I_{ON}/I_{OFF} > 10^8$ ) is observed in both of these devices.

However, electron-phonon interactions (which are not taken into account here) are expected to impact performance more and more as channel length increases: a compromise would therefore need to be found to obtain peak performance in those devices. The influence of the source and drain backgate voltages will now be investigated, as they could allow for further optimization.

### 5.3.4 Influence of backgate voltages

As was shown in Sections 4.1.2.1 and 4.2.2.1, the voltages applied to the source and drain backgates control the potential and band profile in the device, and can therefore strongly impact device performance.

The effect of the backgate voltages on the performance of the MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices with  $V_{DS} = 0.3$  V and  $L_{ch} = 13.4$  nm is studied and analyzed in this section.

Figure 76 shows the influence of  $V_{BG-S}$  and  $V_{BG-D}$  on the  $I_D$ - $V_G$  characteristics and the ON current in MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 13.4$  nm.

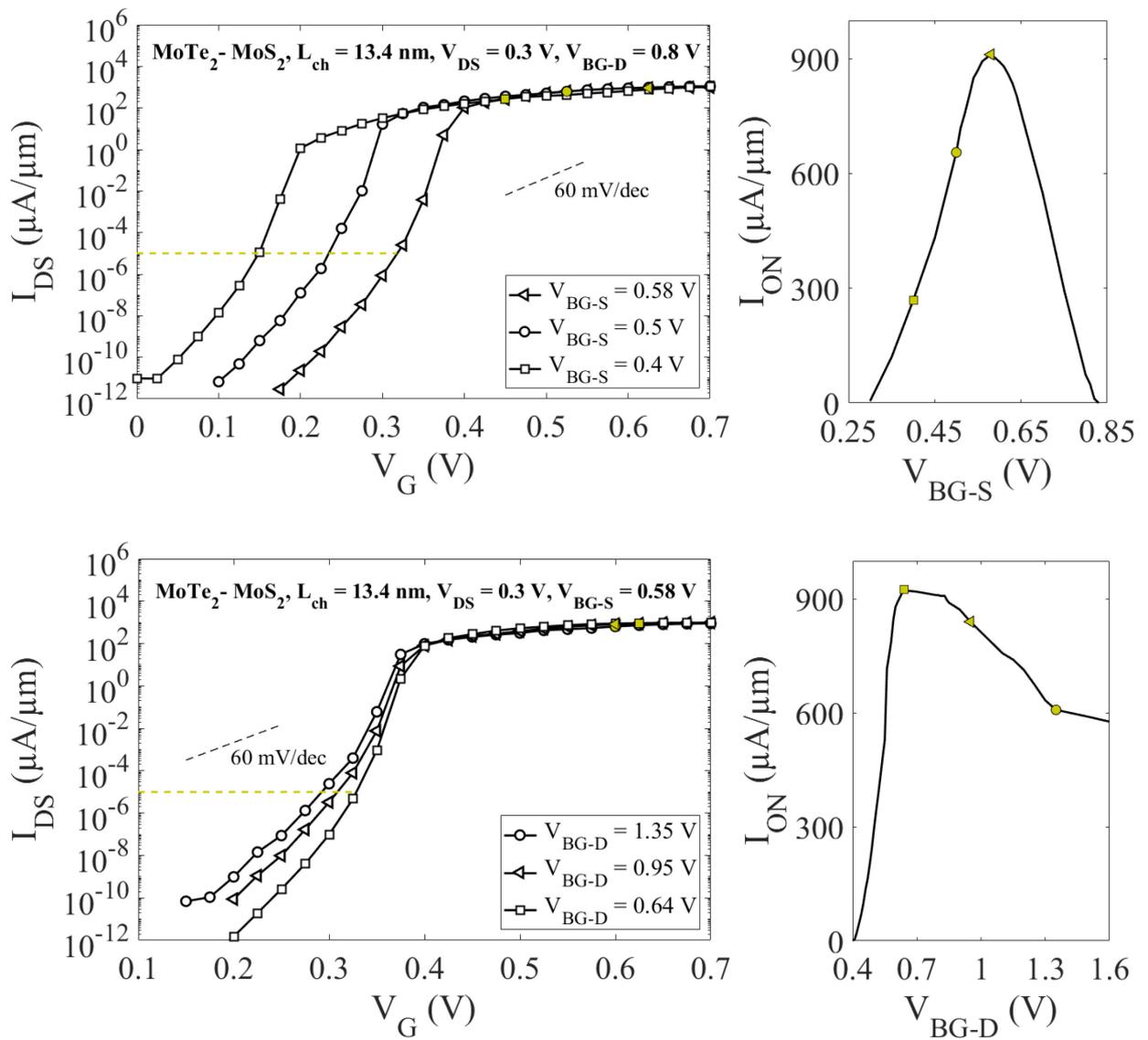


Figure 76. Influence of (top) the source and (bottom) drain backgate voltages on the  $I_D$ - $V_G$  characteristics and the ON current in the MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 13.4$  nm, at  $V_{DS} = V_{DD} = 0.3$  V. The gold dotted line represents the  $I_{OFF} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$  and therefore identifies the corresponding  $V_{OFF}$  for each characteristics.  $I_{ON}$  is then obtained at  $V_{ON} = V_{OFF} + V_{DD}$ , which is highlighted with a gold marker for each characteristic.

Let us now analyze the influence of the backgate voltages:

- Source backgate voltage:  $V_{BG-S}$  strongly impacts both the current characteristics and the ON current of the device. Namely, the threshold voltage is highly affected, dropping from 0.4 V for  $V_{BG-S} = 0.58$  V to 0.25 V for  $V_{BG-S} = 0.4$  V. As is shown in Figure 76, the ON current is highly impacted by the source backgate voltage, and has a somewhat Lorentzian aspect when represented as a function of  $V_{BG-S}$ . The explanations for this behavior differ for either side of the peak.
  - For  $V_{BG-S} < 0.58$  V,  $I_{ON}$  increases with  $V_{BG-S}$ : this behavior is due to the Fermi-Dirac distribution of the carriers in the bands. When  $V_{BG-S}$  is too low, the source VB is forced at energies  $> \mu_S$ , and therefore fewer carriers are available for transport until very high gate voltages are reached. At higher  $V_{BG-S}$  however, the source VB is forced at energies  $< \mu_S$ , and the band is therefore filled with carriers ready for transport. The slope of the current in the ON regime is therefore far steeper (see Figure 77 (left)), and more current flows in the device.
  - For  $V_{BG-S} > 0.58$  V,  $I_{ON}$  decreases with  $V_{BG-S}$ : by increasing  $V_{BG-S}$  further, the source VB is pulled towards even lower energies, gradually narrowing the energy interval between the top of the source VB and the bottom of the channel/drain CB. The band profile shown in Figure 77 for  $V_{BG-S} = 0.75$  V exemplifies this behavior and highlights the narrow energy interval in which current can flow.

From this analysis,  $V_{BG-S} = 0.58$  V is identified as the source backgate voltage for which the MoTe<sub>2</sub>/MoS<sub>2</sub> heterojunction TFET at  $L_{ch} = 13.4$  nm yields peak performance. A similar study is now performed for  $V_{BG-D}$ .

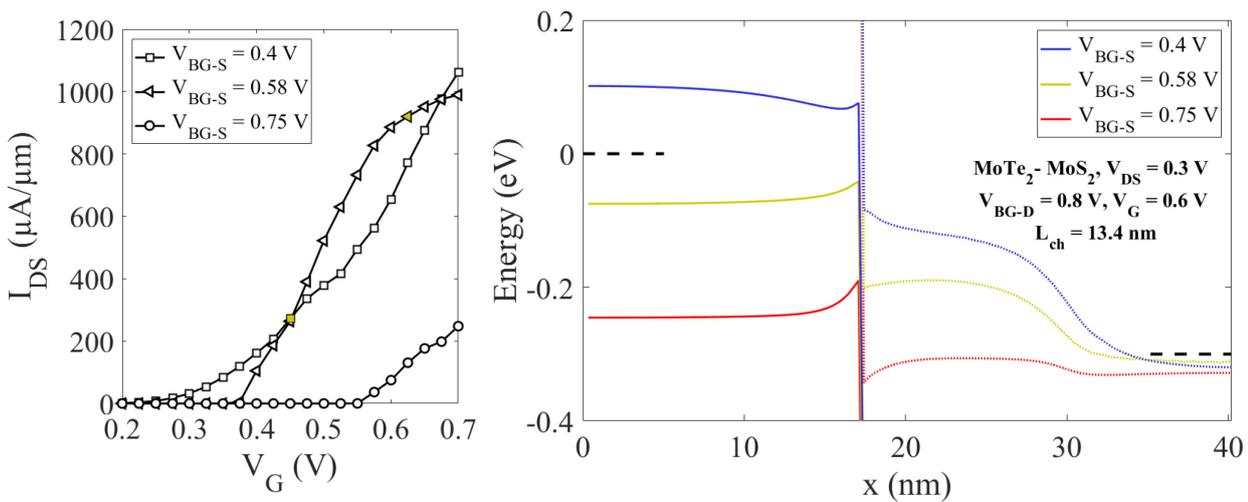


Figure 77. (left)  $I_D$ - $V_G$  characteristics and (right) band profile at  $V_G = 0.6$  V in the MoTe<sub>2</sub>/MoS<sub>2</sub> device at various source backgate voltages ranging from 0.4 V to 0.75 V. The influence of  $V_{BG-S}$  on the threshold voltage  $V_T$  and the steepness of the current in the ON regime is highlighted by the  $I_D$ - $V_G$  characteristics.

The band profiles highlight the impact of  $V_{BG-S}$  on both the position of the source VB with respect to  $\mu_S$ , and the width of the energy interval through which current can flow.

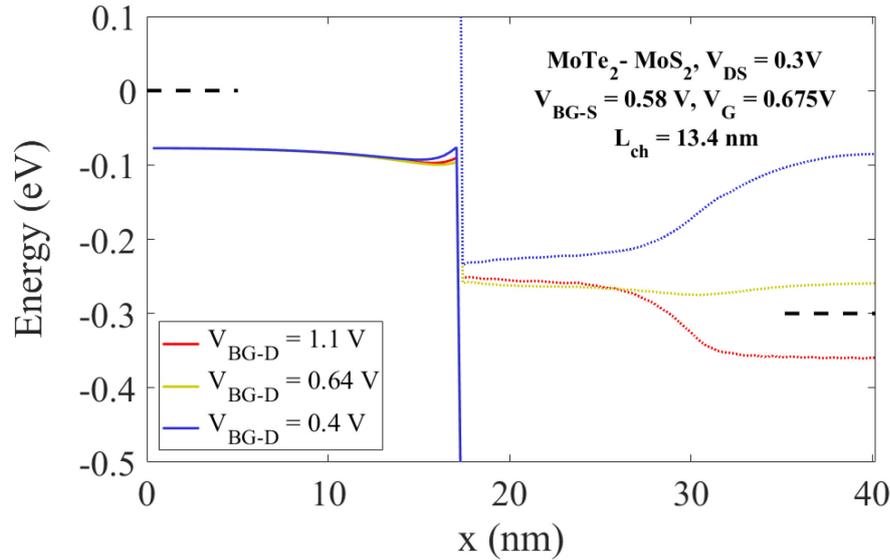


Figure 78. Highest VB (full lines) and lowest CB (dotted lines) in the MoTe<sub>2</sub>/MoS<sub>2</sub> device in the ON state ( $V_G = 0.675\text{ V}$ ) at  $V_{DS} = 0.3\text{ V}$ ,  $L_{ch} = 13.4\text{ nm}$ ,  $V_{BG-S} = 0.58\text{ V}$  and  $V_{BG-D}$  ranging from  $0.4\text{ V}$  to  $1.1\text{ V}$ . When the drain backgate voltage is too low ( $0.4\text{ V}$  here), the CB is forced at higher energies in the drain than the VB in the source and ON current drops dramatically (see Figure 76)

- Drain backgate voltage: much like  $V_{BG-S}$ ,  $V_{BG-D}$  also has an influence on both the current characteristics and the ON current (see Figure 76). As  $V_{BG-D}$  decreases, the steepness of the slope in the sub-threshold regime increases:  $SS$  goes from  $16\text{ mV/dec}$  for  $V_{BG-D} = 1.35\text{ V}$  to  $8\text{ mV/dec}$   $V_{BG-D} = 0.64\text{ V}$  for instance.

The effects of  $V_{BG-D}$  on  $I_{ON}$  can once again be explained by two separate mechanisms:

- For  $V_{BG-D} > 0.64\text{ V}$ : as  $V_{BG-D}$  decreases, the steepness of the slope in the sub-threshold regime increases while  $V_T$  remains unchanged. Therefore,  $V_{OFF}$  ( $V_G$  for which  $I_{DS} = I_{OFF} = 10^{-5}\text{ }\mu\text{A}/\mu\text{m}$ ) increases, and so does  $V_{ON}$ . Finally, since  $I_{ON}$  is calculated at  $V_{ON}$ ,  $I_{ON}$  increases as  $V_{BG-D}$  decreases.
- For  $V_{BG-D} < 0.64\text{ V}$ : as  $V_{BG-D}$  decreases,  $I_{ON}$  plummets, before finally reaching 0 around  $V_{BG-D} = 0.4\text{ V}$ . The band profiles shown in Figure 78 highlight the explanation for this phenomenon: at  $V_{BG-D} = 0.64\text{ V}$ , the CB in the channel and drain is relatively flat (at high  $V_G$ , where  $I_{ON}$  is obtained). By decreasing  $V_{BG-D}$  further, the CB in the drain is pushed towards higher energies, narrowing the energy window in which current can flow. Finally, at  $V_{BG-D} = 0.4\text{ V}$ , the CB in the drain is forced at the same energy than the VB in the source, closing the aforementioned energy window and preventing current flow.

In the end, thanks to this analysis of the influence of source and drain backgate voltages, an optimal set of backgate voltages  $V_{BG-S} = 0.58\text{ V}$  and  $V_{BG-D} = 0.64\text{ V}$  was identified for this MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3\text{ V}$  and  $L_{ch} = 13.4\text{ nm}$ .

A similar study was performed on the  $\text{WTe}_2/\text{MoS}_2$  device at  $L_{ch} = 13.4$  nm (Figure 79), for which optimal backgate voltages of  $V_{BG-S} = 0.85$  V and  $V_{BG-D} = 0.62$  V were identified.

Since some of the mechanisms highlighted here depend on the energy window between the source VB and drain CB, several other optimal sets of  $V_{BG-S}$  and  $V_{BG-D}$  can be found in the same range for both devices. While this study was performed on devices with  $L_{ch} = 13.4$  nm, the backgate voltages identified remain optimal for most channel lengths in the same range. A shift is expected in the case of long channels due to the different profile of the CB in the channel (induced by the decreased proximity of the drain backgate).

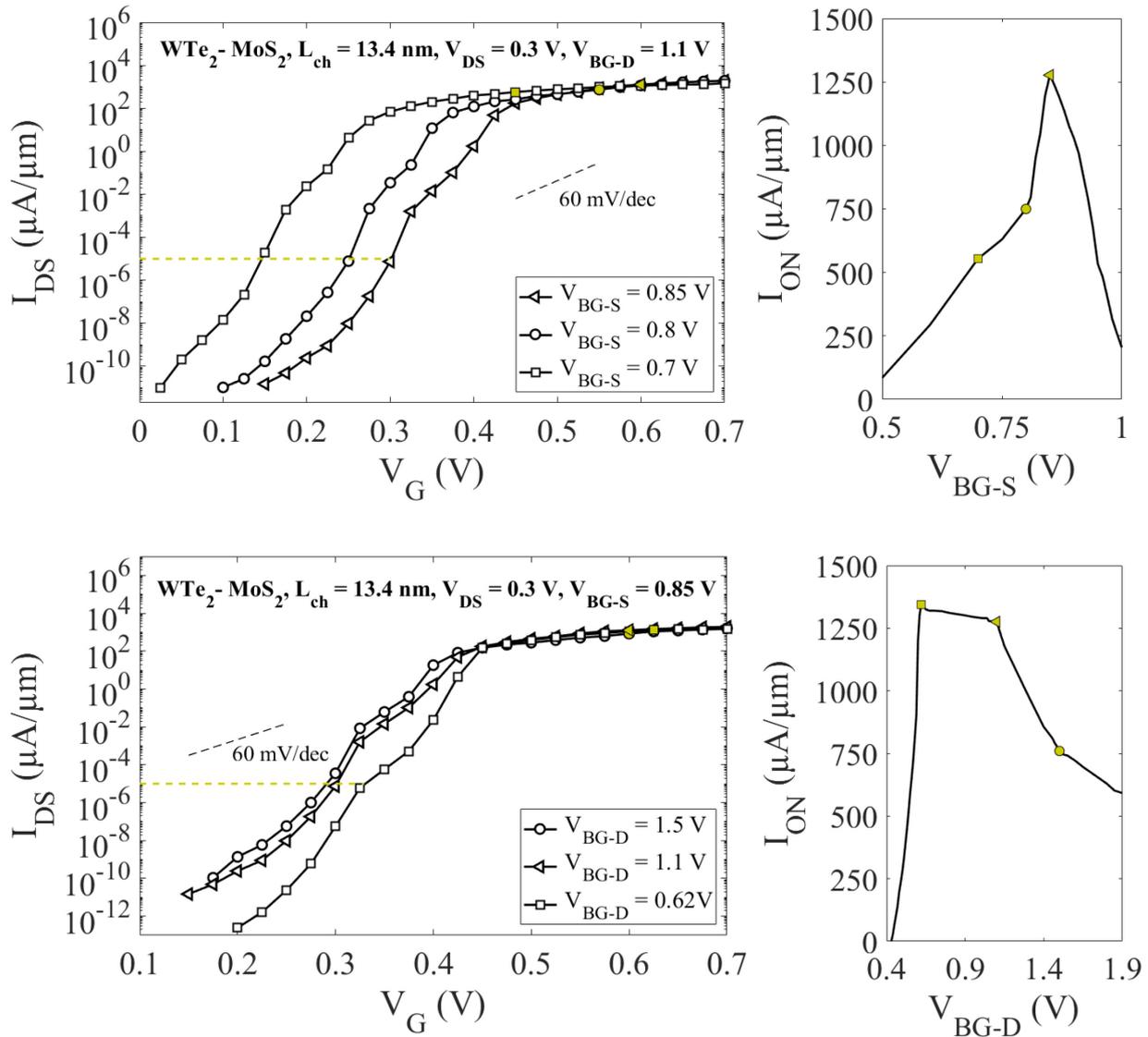


Figure 79. Influence of (top) the source and (bottom) drain backgate voltages on the  $I_D$ - $V_G$  characteristics and the ON current in the  $\text{WTe}_2/\text{MoS}_2$  device at  $L_{ch} = 13.4$  nm and  $V_{DS} = V_{DD} = 0.3$  V. The gold dotted line represents the  $I_{OFF} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$  and therefore identifies the corresponding  $V_{OFF}$  for each characteristics.  $I_{ON}$  is then obtained at  $V_{ON} = V_{OFF} + V_{DD}$ , which is highlighted with a gold marker for each characteristic.

### 5.3.5 Drain voltage characteristics and DITL

In this short section, I will present drain voltage characteristics for the MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices, as well as highlight their robustness against a common short-channel effect that traditionally impedes MOSFETs: drain induced barrier lowering (DIBL).

The  $I_D$ - $V_{DS}$  characteristics for the MoTe<sub>2</sub>/MoS<sub>2</sub> device are shown in Figure 80 at  $L_{ch} = 13.4$  nm,  $V_G$  ranging from 0.45 V to 0.6 V, and various  $V_{BG-S/D}$  sets, to highlight the impact the backgate voltages have on these characteristics.

At  $V_{BG-S} = 0.4$  V and  $V_{BG-D} = 2.85$  V, the characteristics exhibit the behavior expected of a transistor for all  $V_G$ : linear increase in current at low  $V_{DS}$ , followed by a saturation for  $V_{DS} > 0.15$  V. This indicates that this device can operate at full capacity even at very low supply voltages, making its potential for ultra-low power operation even greater.

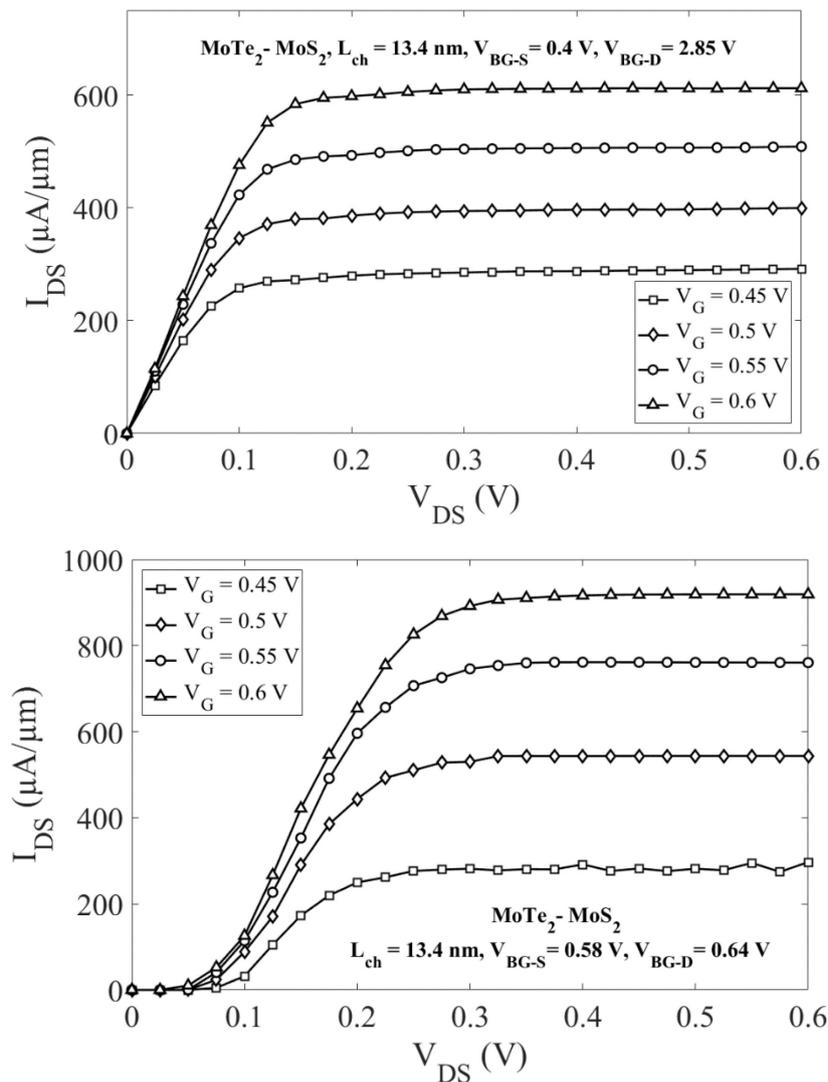


Figure 80.  $I_D$ - $V_{DS}$  characteristics of the MoTe<sub>2</sub>/MoS<sub>2</sub> device for  $V_G$  ranging from 0.45 V to 0.6 V,  $L_{ch} = 13.4$  nm, and two sets of backgates voltages, including the optimal set identified in Section 5.3.4.

At  $V_{BG-S} = 0.58$  V and  $V_{BG-D} = 0.64$  V (the optimal set of backgate voltages for which  $I_{ON}$  is at its peak at  $L_{ch} = 13.4$  nm), the  $I_D$ - $V_{DS}$  characteristics exhibit a different behavior. Instead of a linear increase in current at low  $V_{DS}$ , the current remains around 0 until  $V_{DS} = 0.075$  V, then increases until  $V_{DS} = 0.3$  V after which it saturates.

The origin of this behavior can be understood by investigating the energy levels of the source VB and drain CB presented in Figure 81, which shows the band profile for both of the devices shown above at  $V_G = 0.6$  V and  $V_{DS}$  ranging from 0 V to 0.2 V.

- In the device at  $V_{BG-S} = 0.4$  V and  $V_{BG-D} = 2.85$  V, the drain CB sits at lower energies than the source VB even at  $V_{DS} = 0$  V, and the only factor preventing current flow is that  $\mu_D = \mu_S$ . As soon as  $V_{DS}$  increases,  $\mu_D < \mu_S$  and current flows freely from the source to the drain.
- In the device at  $V_{BG-S} = 0.58$  V and  $V_{BG-D} = 0.64$  V however, the drain CB sits at higher energies than the source VB for all  $V_{DS} < 0.5$  V, and therefore no current flows even though  $\mu_D < \mu_S$ . When  $V_{DS}$  is high enough, the drain CB is forced at lower energies than the source CB and current flows from the source to the drain.

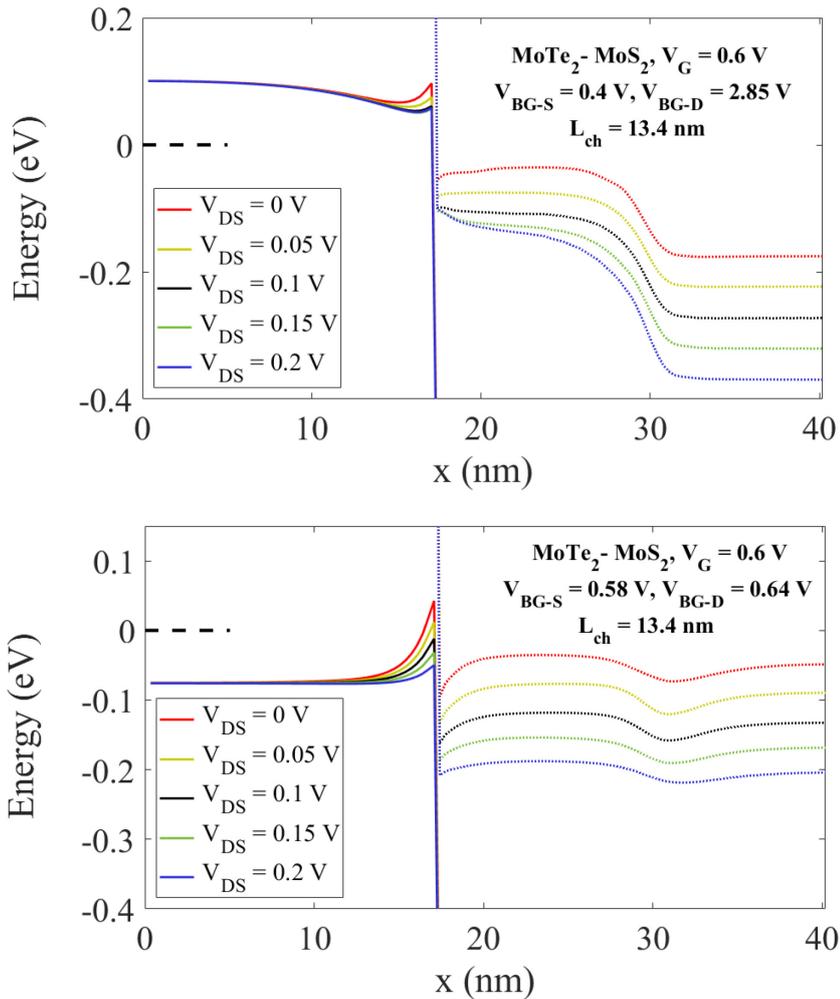


Figure 81. Highest VB (full lines) and lowest CB (dotted lines) in the MoTe<sub>2</sub>/MoS<sub>2</sub> devices studied in Figure 80 at  $V_G = 0.6$  V and  $V_{DS}$  ranging from 0 V to 0.2 V.

However, using this optimal set of backgate voltages allows the device to yield much higher currents (50% higher at high  $V_G$ ) and may therefore be preferable if high  $I_{ON}$  is of prime importance for the targeted application.

Moreover, even though the characteristic may not resemble that of a “classic” transistor, the current saturates nicely at  $V_{DS} > 0.3$  V nonetheless, which is once again extremely promising for ultra-low power operation.

Similar observations can be made for the  $WTe_2/MoS_2$  device, of which the  $I_D$ - $V_{DS}$  characteristics are shown in Figure 82.

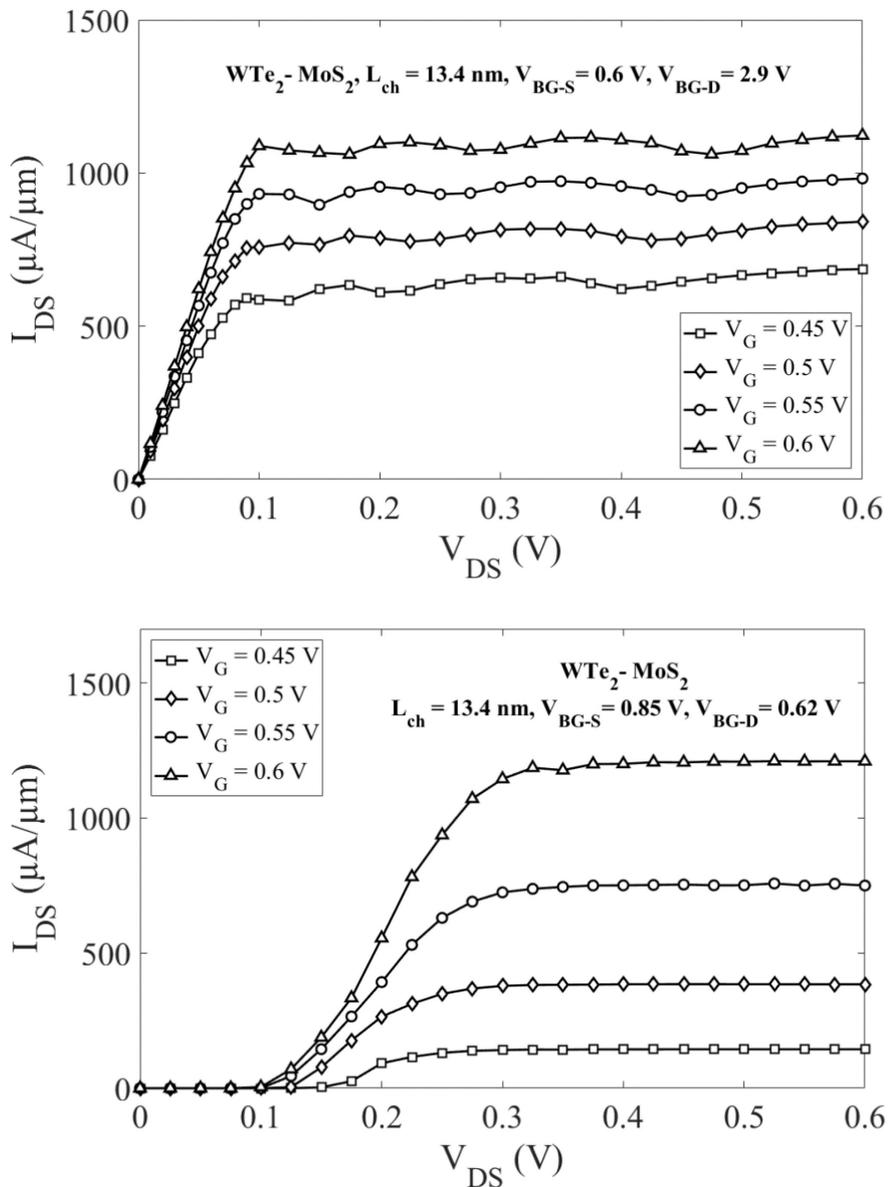


Figure 82.  $I_D$ - $V_{DS}$  characteristics of the  $WTe_2/MoS_2$  device for  $V_G$  ranging from 0.45 V to 0.6 V,  $L_{ch} = 13.4$  nm, and two sets of backgate voltages, including the optimal set identified in Section 5.3.4.

Drain-induced barrier lowering (DIBL) is an SCE commonly found in MOSFETs, and, as its name suggests, describes the influence of the applied supply voltage on the height of the potential barrier. As an SCE, it is increasingly reinforced as channel length is shortened, and is measured in mV/V (shift in  $V_T$  per 1 V increase in  $V_{DS}$ ).

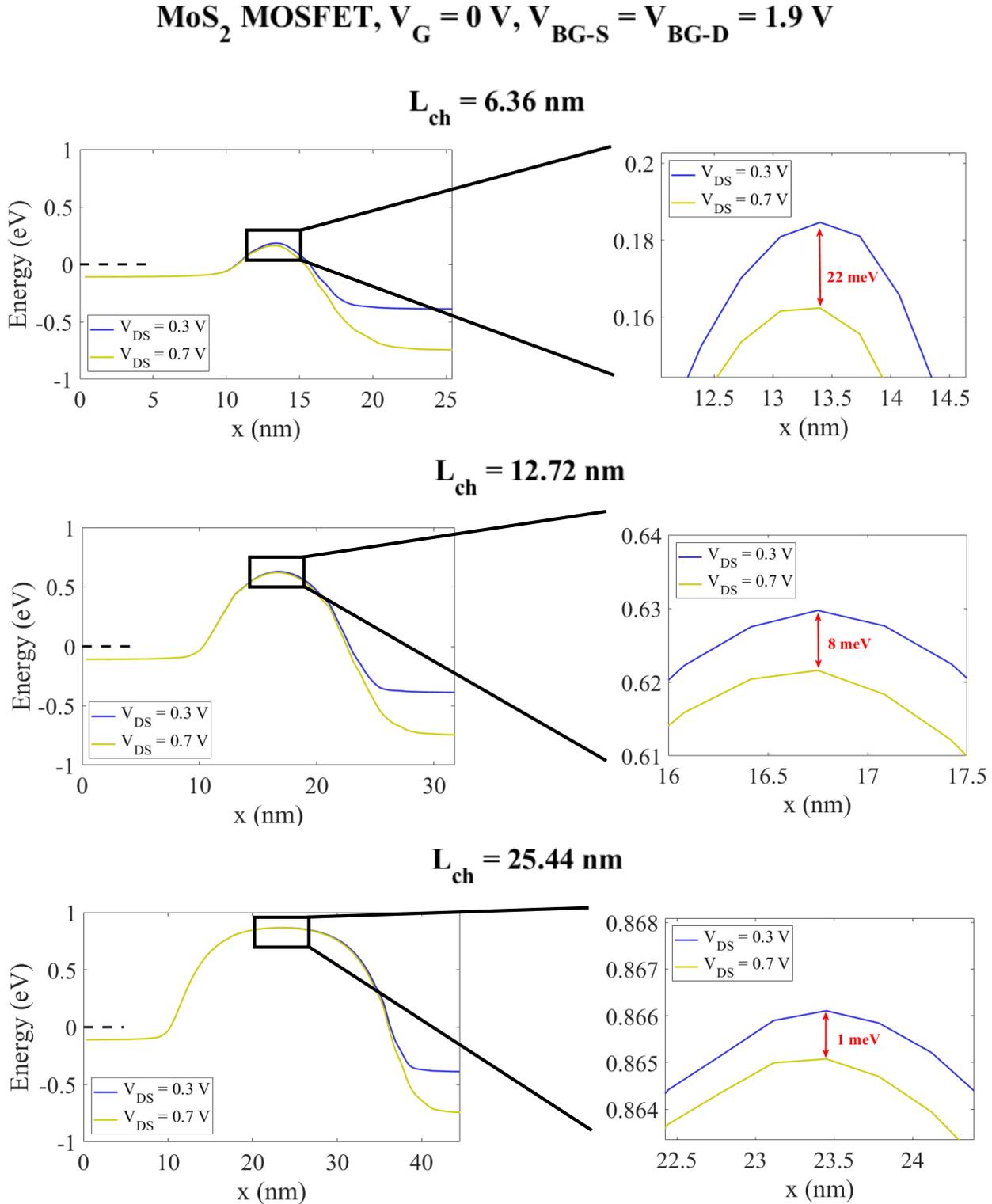


Figure 83. Highest VB in the MoS<sub>2</sub> MOSFET at  $V_G = 0$  V and  $V_{DS} = 0.3$  V and 0.7 V for several channel lengths, highlighting the DIBL in each case (right).

Figure 83 highlights the effects of the DIBL occurring in the MoS<sub>2</sub> MOSFET studied in Section 4.1, and its dependence on channel length. DIBL is often used as a measurement of the susceptibility of a MOSFET to short-channel effects in general.

TFETs, on the other hand, generally do not suffer from this effect since they rely on BTBT rather than thermionic injection over a potential barrier. They can however suffer drain induced threshold lowering (DITL).

Figure 84 highlights the robustness of the MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices against this effect: for  $V_{DS}$  varying from 0.1 to 0.8 V,  $V_T$  remains unchanged. Currents reported at  $V_{DS} = 0.1$  V are lower for all gate voltages due to the position of the energy levels of the bands in the contacts at these backgate voltages (see Figure 81 which highlighted the same issue).

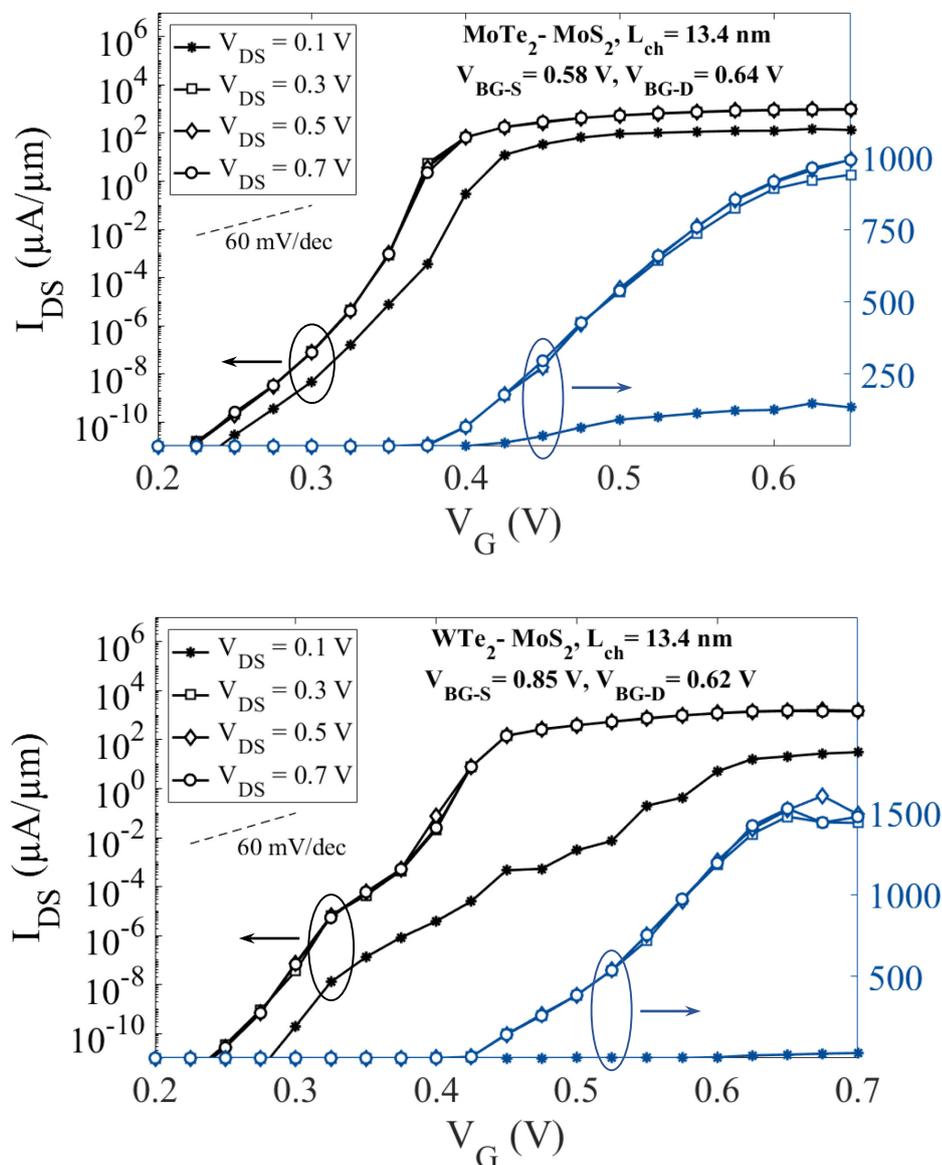


Figure 84.  $I_D$ - $V_G$  characteristics of the MoTe<sub>2</sub>/MoS<sub>2</sub> and the WTe<sub>2</sub>/MoS<sub>2</sub> devices for  $L_{ch} = 13.4$  nm,  $V_{DS}$  ranging from 0.1 V to 0.7 V and the optimal backgate voltages for each device as identified in Section 5.3.4.

Indeed, by using the optimal sets of  $V_{BG-S}$  and  $V_{BG-D}$  identified in Section 5.3.4, the CB in the drain is forced at energy levels higher than the VB in the source at very low  $V_{DS}$  (see Figure 81). Therefore, much like for the  $I_D-V_{DS}$  characteristics shown in Figure 80 and Figure 82, a certain threshold has to be reached by the supply voltage so that the drain CB is forced below the source VB and current can flow. However, at  $V_{DS}$  close to this threshold, the energy window in which current can flow remains narrow compared to higher  $V_{DS}$ , which explains the lower currents reported at low  $V_{DS}$ . Figure 85 highlights the width of the energy window in which current can flow for  $V_{DS} = 0.1$  V and 0.7 V in the MoTe<sub>2</sub>/MoS<sub>2</sub> device.

In the end, the study of these devices under varied supply voltages highlighted their robustness when it comes to DITL as well as their capacity to saturate at low  $V_{DS}$ , which reinforces their strong potential for ultra-low power operation.

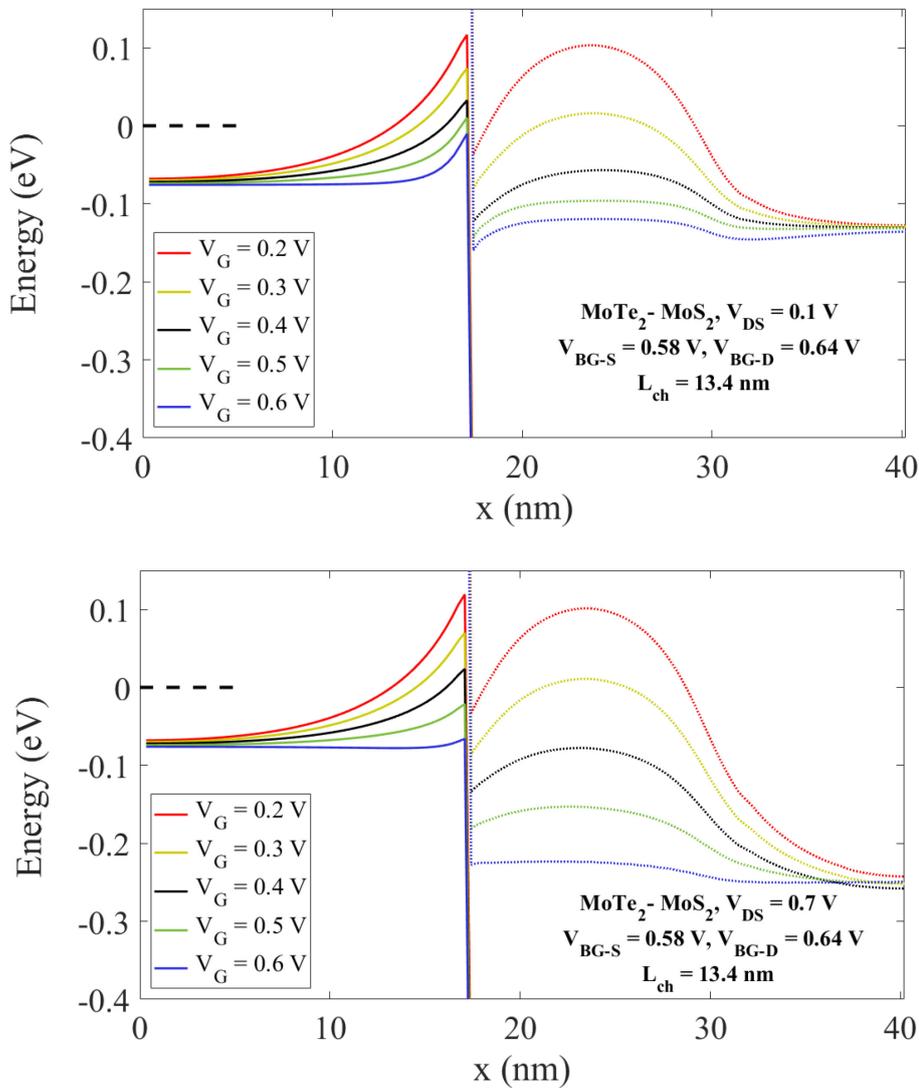


Figure 85. Highest VB (full lines) and lowest CB (dotted lines) in the MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 13.4$  nm,  $V_{BG-S} = 0.58$  V,  $V_{BG-D} = 0.64$  V and (top)  $V_{DS} = 0.1$  V (top)  $V_{DS} = 0.7$  V. At  $V_{DS} = 0.1$  V, the drain CB is at comparable energies than the source VB (see Figure 81), leading to lower currents.

## 5.4 Conclusion on standard in-plane heterojunction TFETs

The MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices studied in this chapter show great promise for ultra-low power operation thanks to several key points:

- **Extremely low SS:** depending on the length of the channel, the devices yield ballistic *SS* ranging from 30 mV/dec in the case of short channels, down to below 5 mV/dec for  $L_{ch} > 20$  nm.
- **High ON/OFF ratio:** depending on the backgate voltages applied to the contacts, ballistic ON/OFF ratios up to  $10^8$  for the MoTe<sub>2</sub>/MoS<sub>2</sub> device and  $2 \times 10^8$  for WTe<sub>2</sub>/MoS<sub>2</sub> device have been reported.
- **Good saturation even at low V<sub>DS</sub>:** both devices saturate nicely at low drain voltages (as low as  $V_{DS} = 0.2$  V) when the optimal backgate voltages are applied. They therefore yield peak performance while remaining energy-efficient, which only strengthens their appeal as ultra-low power electronic switches.

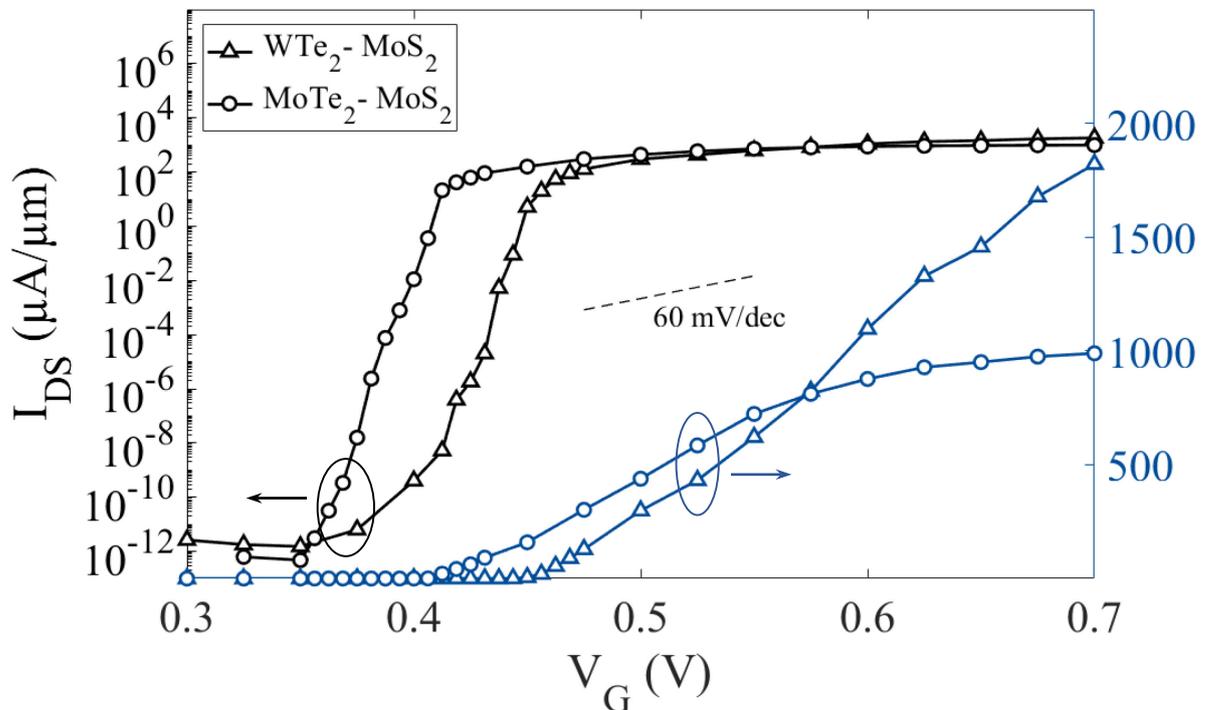


Figure 86.  $I_D$ - $V_G$  characteristics for both devices at  $V_{DS} = 0.3$  V,  $L_{ch} = 26.8$  nm,  $V_{BG-S/D} = 0.58$  V and  $0.64$  V for MoTe<sub>2</sub>/MoS<sub>2</sub> and  $V_{BG-S/D} = 0.85$  V and  $0.62$  V for WTe<sub>2</sub>/MoS<sub>2</sub>.

# Chapter 6

## Drain-backgate-enhanced heterojunction TFETs

### 6.1 Origin and definition

When studying the influence of the source and drain backgate voltages on the performance of the MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices, an idea for a new device derived from the standard in-plane heterojunction based TFET came to us.

By analyzing the impact of the drain backgate voltage on the current in the sub-threshold regime, we observed an interesting phenomenon that could be exploited to our advantage. As  $V_{BG-D}$  increases, the current in the sub-threshold regime also increases (see Figure 87). This is expected and is due to the impact of  $V_{BG-D}$  on the drain CB: the drain CB is pulled down towards lower energies, allowing for more electrons to flow from the source to the drain (see the bands profiles and LDOS shown in Figure 88).

It thus seems relevant to check if this property can be used to improve the device performance: we anticipate that the steepness of the slope in the sub-threshold regime may be dramatically increased by carefully selecting the workfunctions of the various gates and applying the same voltage to the drain backgate and channel gate, so that

$$V_{BG-D} = V_G \quad W_{BG-D} = W_{CG} - \Delta W \quad (53)$$

where  $\Delta W$  is the offset between the work-functions of the metals used as drain-backgate ( $W_{BG-D}$ ) and channel gate/source backgate ( $W_{CG}$ ).

By carefully selecting  $\Delta W$ , the drain CB can be forced at energies higher than the source CB at low  $V_G$ , preventing all current flow in the OFF state. The workfunctions of the metals used as gates in both DBE devices are therefore:

- 5.19 eV for the channel-gate and the source backgate.
- $(5.19 - \Delta W)$  eV for the drain backgate.

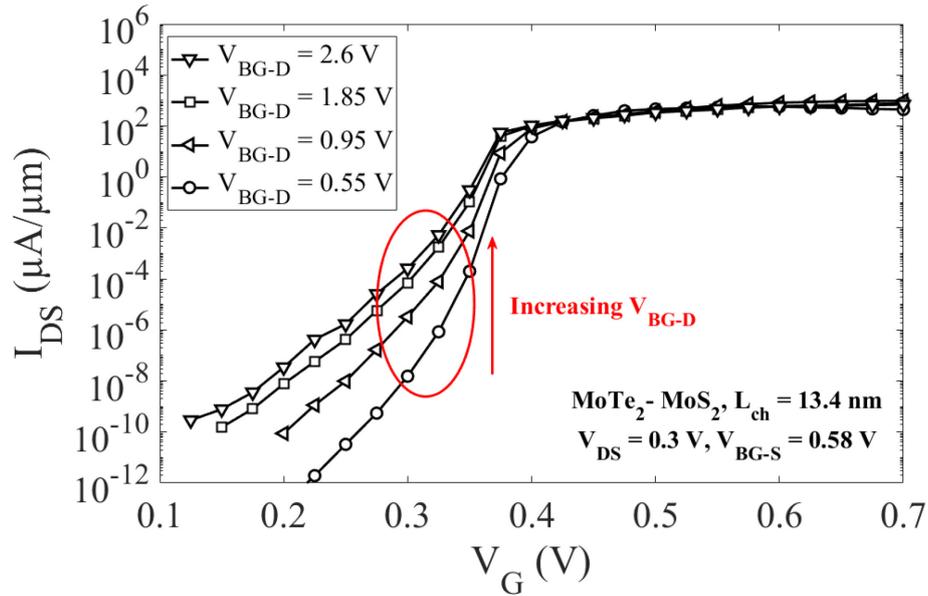


Figure 87.  $I_D$ - $V_G$  characteristics for the MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $L_{ch} = 13.4$  nm,  $V_{BG-S} = 0.58$  V and  $V_{BG-D}$  ranging from 0.55 V to 2.6 V. This figure highlights the increase in OFF current with  $V_{BG-D}$  used in these DBE devices.

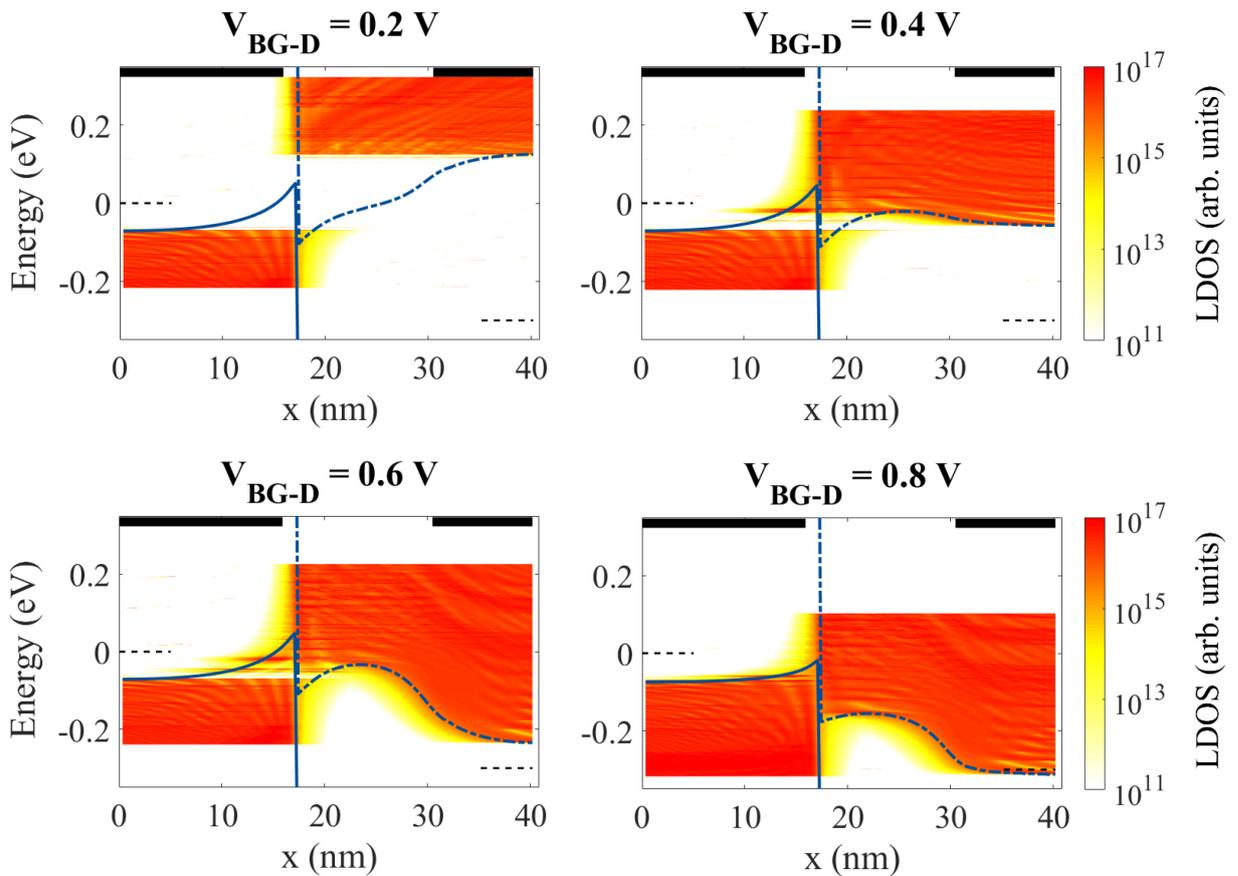


Figure 88. LDOS, highest VB (full lines) and lowest CB (dotted line) at  $V_G = 0.35$  V in the MoTe<sub>2</sub>/MoS<sub>2</sub> device detailed in Figure 89 for  $V_{BG-D}$  increasing from 0.2 V to 0.8 V. This figure highlights the absence of states in the channel/drain to tunnel to at low  $V_{BG-D}$ . As  $V_{BG-D}$  increases, the drain CB is pulled down towards lower energies, and current can start flowing from the source VB to the channel/drain.

## 6.2 Device architecture

The architecture of the drain-backgate-enhanced (DBE) devices investigated is the same as that of the standard TFETs presented in Section 5.1. The only difference is that, as detailed in the previous section, the voltage applied to the drain backgate will be  $V_G$ , the same voltage as the channel-gate.

The source backgate voltage is not modified and behaves as it did in the standard in-plane heterojunction TFETs.

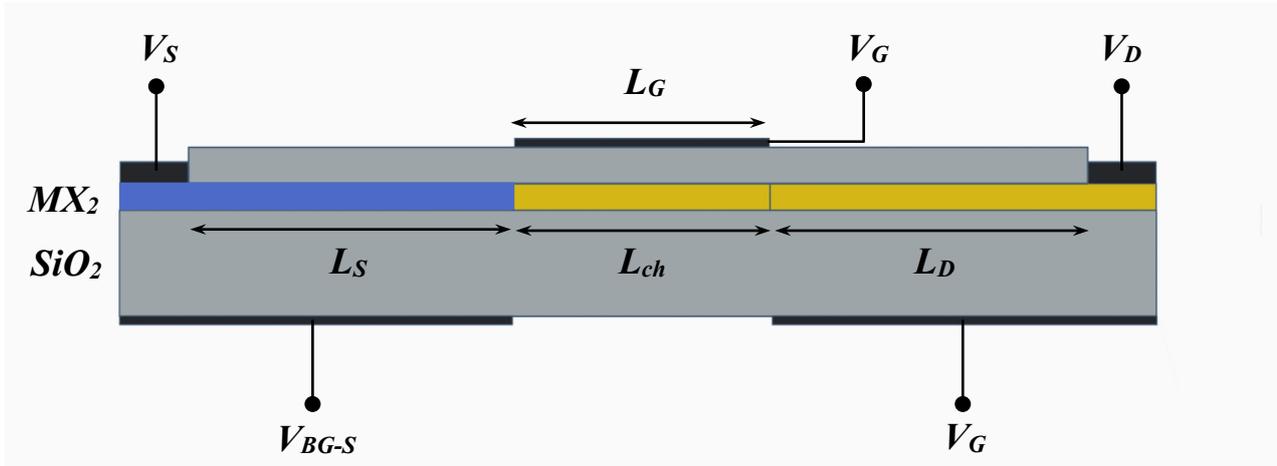


Figure 89. Device architecture for the considered DBE in-plane heterojunction TFETs.

One TMD acts as the source, and another as the channel/drain.  $\text{SiO}_2$  is used as a buried oxide, and a high- $\kappa$  dielectric as the top gate oxide. The same voltage is applied to the drain backgate and the top-gate so that  $V_{BG-D} = V_G$ , while  $W_{BG-D} = W_{CG} - \Delta W$  is the workfunction of the metal used as drain backgate.

## 6.3 Electronic transport simulations

### 6.3.1 Influence of backgate metal workfunction

The first parameter to study in these new devices is of course the backgate work-function difference with respect to the channel gate,  $\Delta W$ , and its influence on device performance. In some of the  $I_D$ - $V_G$  characteristics shown in this section, the behavior of these drain backgate enhanced devices will be shown for several  $\Delta W$  (as full lines), but also compared to that of a standard in-plane heterojunction TFET with a static  $V_{BG-D}$  (which will be shown as dotted lines) in which case  $W_{BG-D} = W_{CG}$ .

$I_D$ - $V_G$  characteristics for both the DBE  $\text{MoTe}_2/\text{MoS}_2$  and the  $\text{WTe}_2/\text{MoS}_2$  devices at  $V_{DS} = 0.3$  V,  $L_{ch} = 10.05$  nm and  $V_{BG-S} = 0.58$  V and 0.85 V (resp.) and various workfunction offsets are shown in Figure 90.

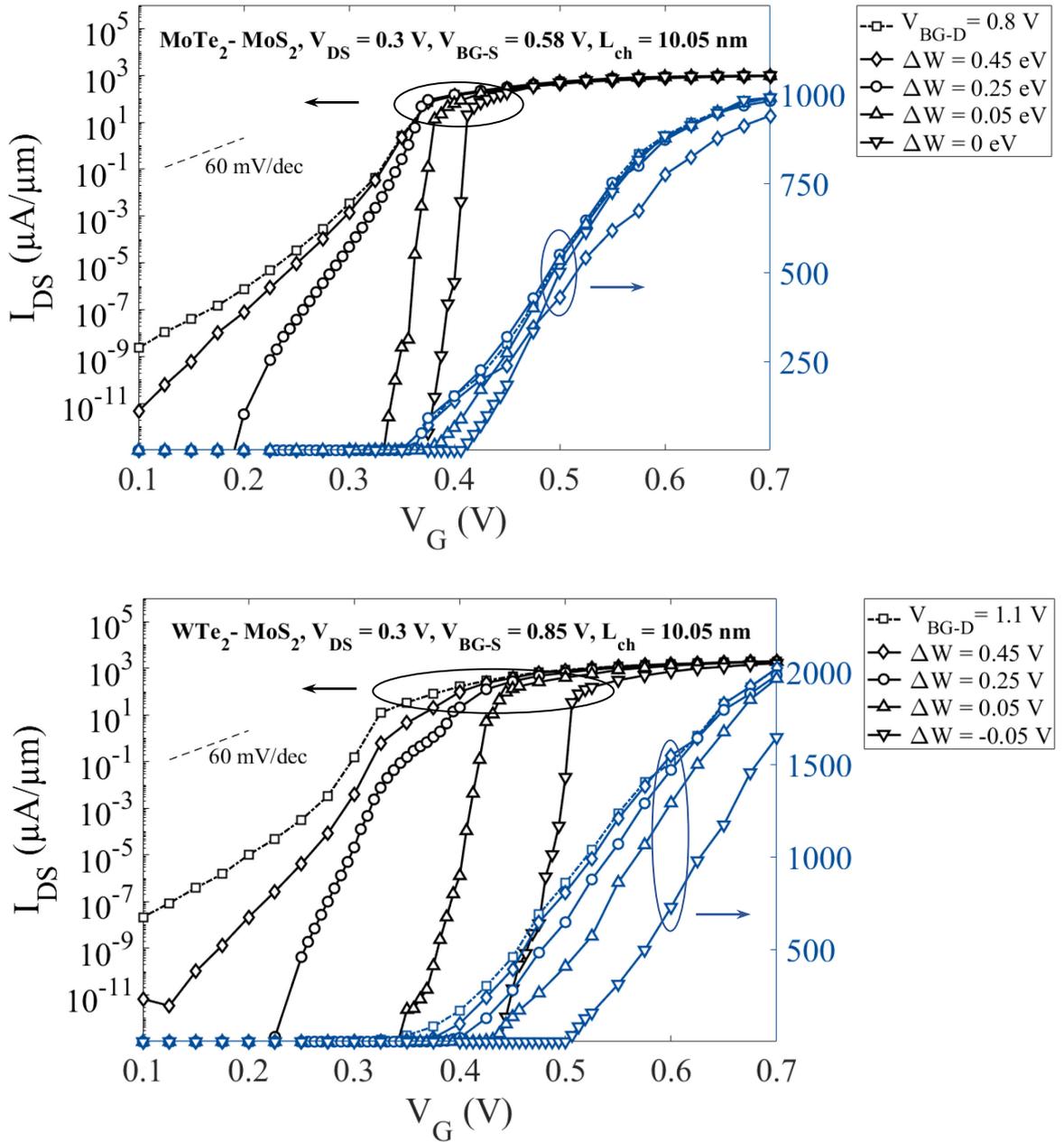


Figure 90.  $I_D$ - $V_G$  characteristics for the MoTe<sub>2</sub>/MoS<sub>2</sub> and the WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $L_{ch} = 10.05$  nm and  $V_{BG-S} = 0.58$  V and 0.85 V (resp.).  $\Delta W$  ranges from  $-0.05$  eV to 0.45 eV for the DBE heterojunction TFETs.

A similar behavior can be observed across both devices: as  $\Delta W$  decreases, the steepness of the slope in the sub-threshold regime strongly increases due to the absence of source-to-drain tunneling (because the CB in the drain is at higher energies than the source VB).  $SS$  is therefore tremendously reduced as  $\Delta W$  decreases: it is for instance reduced from 30 mV/dec in the standard MoTe<sub>2</sub>/MoS<sub>2</sub> device to less than 5 mV/dec in the DBE device for  $\Delta W = 0.05$  V. At this workfunction offset however, minimal  $SS$  has been reached and will not change if  $\Delta W$  is decreased further.

ON current is also strongly affected by  $\Delta W$ : since  $V_{OFF}$  is strongly increased (from 0.25 V in the standard MoTe<sub>2</sub>/MoS<sub>2</sub> device to 0.35 V in the DBE device for  $\Delta W = 0.05$  eV), so is  $V_{ON}$  and therefore  $I_{ON}$ .

Due to the joint influence of  $\Delta W$  and  $V_G$  on the CB in the drain (see Figure 88) and the resulting ability of these devices to completely inhibit source-to-drain tunneling at low  $V_G$ , the limits of channel scaling are completely removed.

As highlighted in Figure 91, DBE devices with channels as short as 1.675 nm (which, in the case of standard TFETs cannot be switched OFF due to source-to-drain tunneling) are shown to reach  $SS$  as low as the 10 nm devices shown previously, and marginally higher ON currents at high  $V_G$  thanks to source-to-drain tunneling.

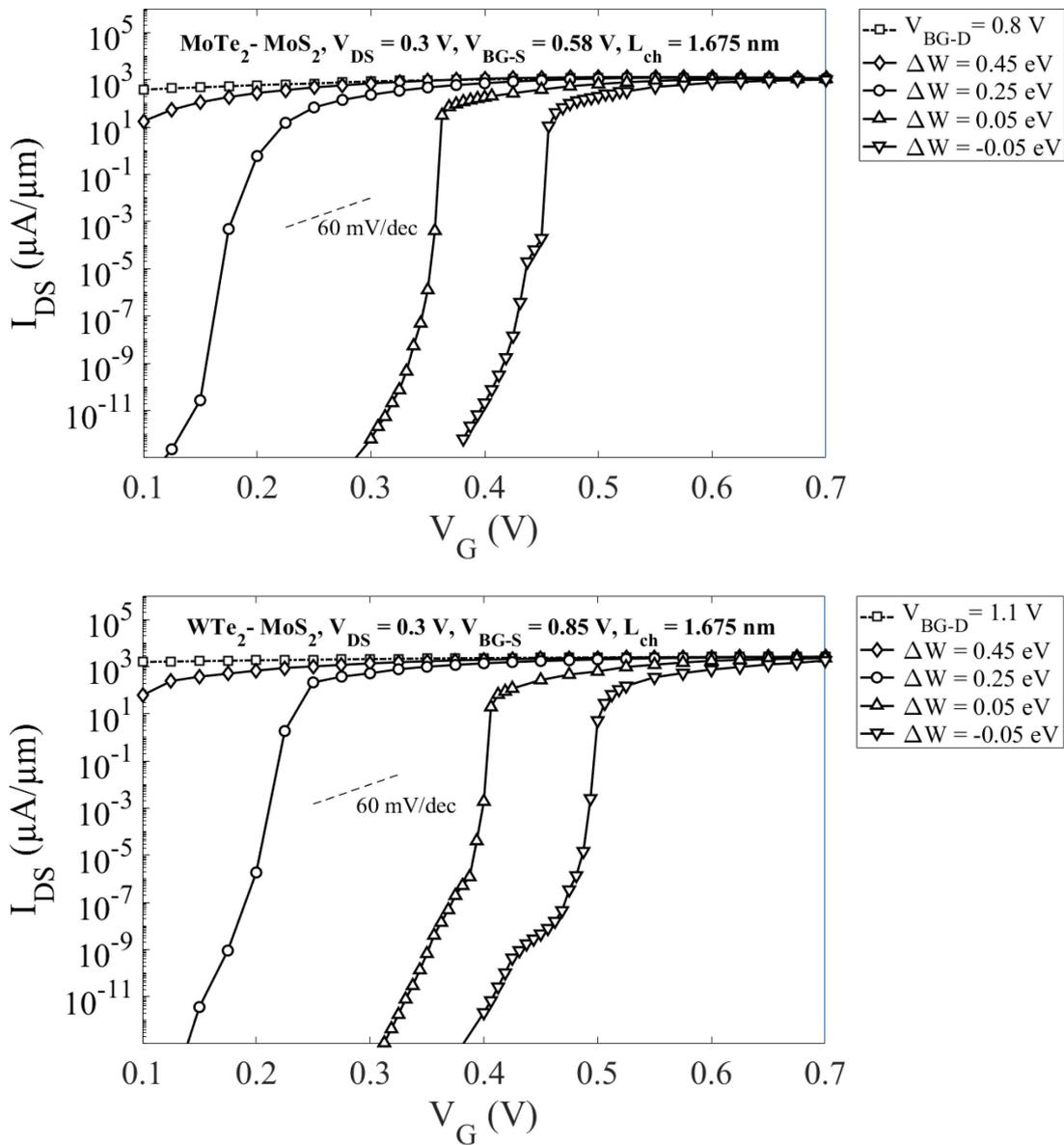


Figure 91.  $I_D$ - $V_G$  characteristics for the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> and the WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $L_{ch} = 1.675$  nm and  $V_{BG-S} = 0.58$  V and 0.85 V (resp.).  $\Delta W$  ranges from  $-0.05$  eV to 0.45 eV for the DBE-TFETs. The current is only shown in log scale to improve readability.

The potential of this DBE devices cannot be understated: the traditional limits of channel scaling are removed, and, in short-channel devices, source-to-drain tunneling actually becomes an advantage at high  $V_G$ , increasing  $I_{ON}$  further. This will be highlighted in Section 6.4, which will investigate the effect of channel length on these DBE devices.

It is now clear that these new devices present tremendous advantages compared to standard TFETs; and their optimal workfunction offset will now be identified.

Figure 92 shows the  $I_D$ - $V_G$  characteristics for the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $L_{ch} = 10.05$  nm,  $V_{BG-S} = 0.58$  V, and  $\Delta W$  ranging from -0.20 eV to 0.05 eV. As mentioned before, it is clear that the maximum steepness is reached at  $\Delta W = 0.05$  eV, and therefore  $SS$  is not modified by decreasing the work-function offset further. Both the threshold voltage and the steepness of the slope in the ON regime are however impacted as  $\Delta W$  decreases further, and the ON current is therefore expected to be modified as well.

Although it is not shown here, similar observations can be made for the DBE WTe<sub>2</sub>/MoS<sub>2</sub> device.

The direct influence of the work-function offset on  $SS$  and  $I_{ON}$  in both the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $L_{ch} = 10.05$  nm,  $V_{DS} = 0.3$  V and  $V_{BG-S} = 0.58$  V and 0.85 V (resp.) is shown in Figure 93.

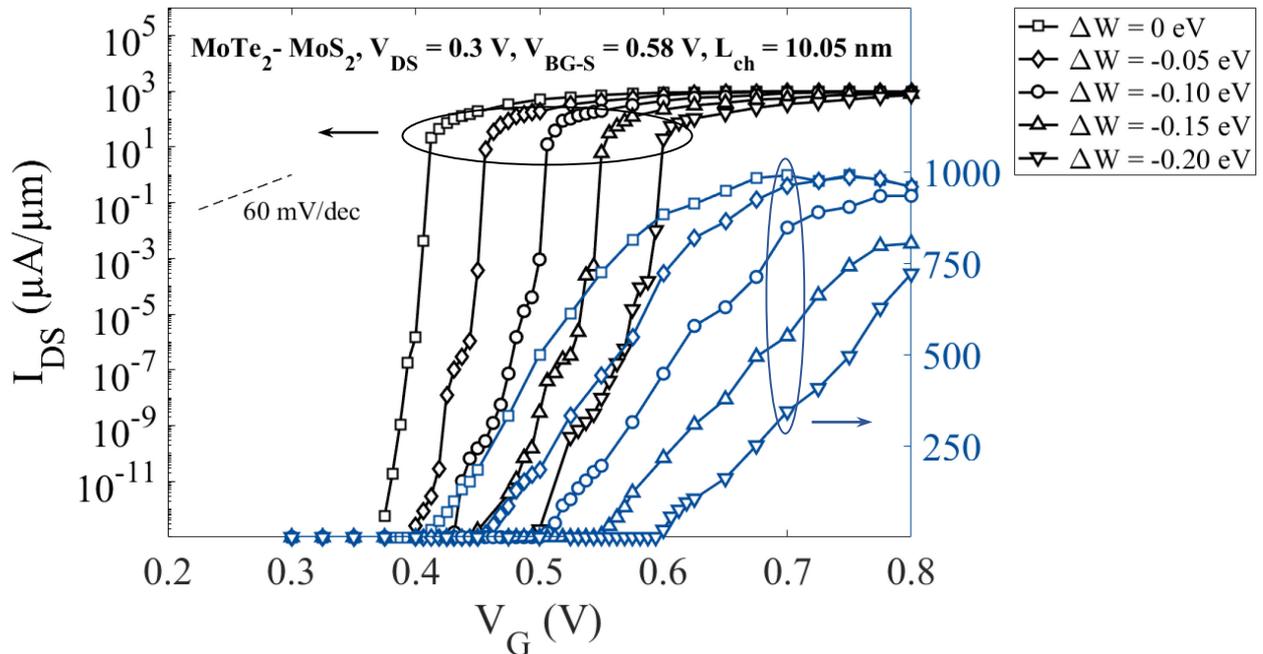


Figure 92.  $I_D$ - $V_G$  characteristics for the backgate-enhanced MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $L_{ch} = 10.05$  nm,  $V_{BG-S} = 0.58$  V, and  $\Delta W$  ranging from -0.20 eV to -0.05 eV.

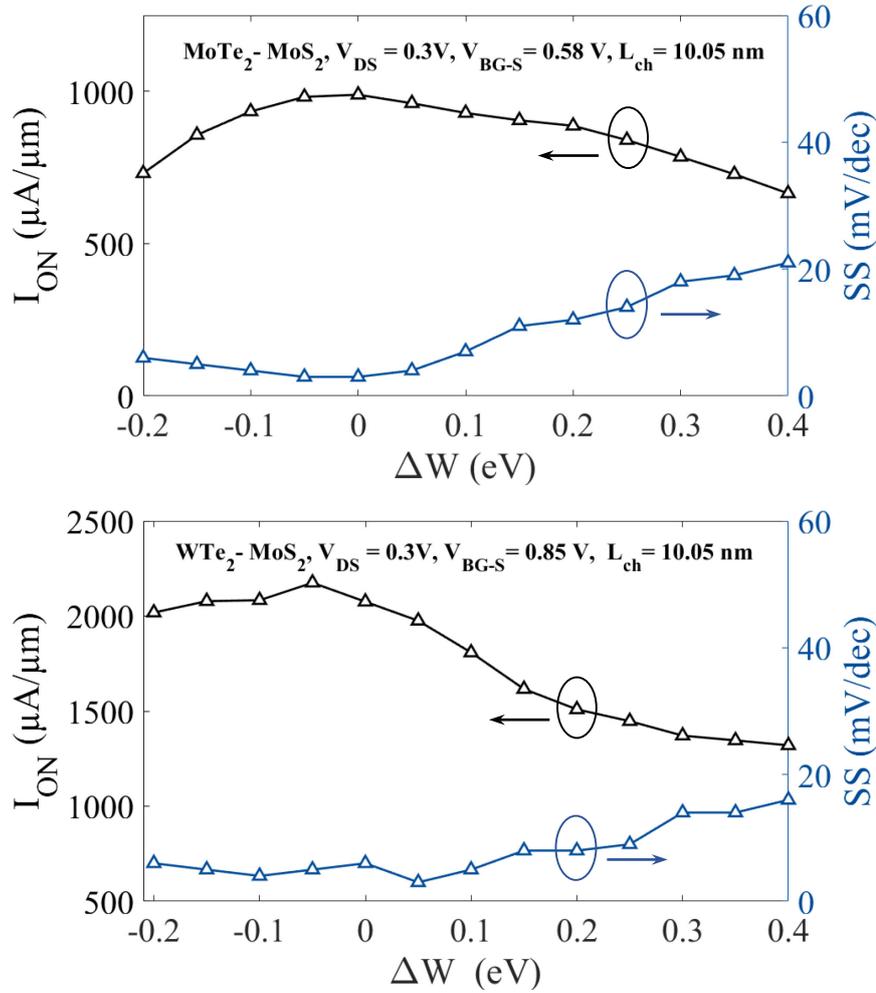


Figure 93. Influence of the workfunction offset on device performance in the DBE (top) MoTe<sub>2</sub>/MoS<sub>2</sub> and (bottom) WTe<sub>2</sub>/MoS<sub>2</sub> devices. In both cases, an optimal range from -0.05 eV to 0.05 eV allowing for peak performance (minimum  $SS$  and maximum  $I_{ON}$ ) can be identified.

The work-function offset has a similar impact in both devices:

- $I_{ON}$ : As  $\Delta W$  decreases, the ON current increases until it reaches a maximum around  $\Delta W = 0$  eV (980  $\mu\text{A}/\mu\text{m}$  for MoTe<sub>2</sub>/MoS<sub>2</sub> and 2175  $\mu\text{A}/\mu\text{m}$  for WTe<sub>2</sub>/MoS<sub>2</sub>) and slightly decreases for  $\Delta W < -0.05$  eV
- $SS$ : As  $\Delta W$  decreases,  $SS$  decreases and stabilizes around 5 mV/dec for  $\Delta W < 0.1$  eV

In both DBE devices, the optimal work-function offset is identified to be  $\Delta W = -0.05$  eV. This is expected since, at this  $\Delta W$ ,  $V_{OFF} \sim 0.415$  V (see Figure 92), therefore  $V_{ON} = V_{OFF} + V_{DS} \sim 0.715$  V.

At this  $V_G$ , the equivalent drain backgate voltage in the standard devices (where  $W_{BG-D} = W_{CG}$ ) is  $V_{BG-D} = \frac{\Delta W}{e} + 0.715 \sim 0.665$  V, which is close to the optimal drain backgate voltages identified in Section 5.3.4 for both devices (0.64 V for MoTe<sub>2</sub>/MoS<sub>2</sub> and 0.62 V for WTe<sub>2</sub>/MoS<sub>2</sub>).

By using the same metal in all gates ( $\Delta W = 0$  eV), great performance can therefore be reached. Note that these observations pertain to the devices with short channels (10.05 nm shown here). In the case of longer channel where standard TFETs already yield peak  $I_{ON}$  and minimum  $SS$  (see Figure 75),  $\Delta W$  has almost no influence on device performance.

### 6.3.2 Influence of channel length

In Section 5.3.3, it was shown that the performance of the standard heterojunction TFETs was strongly influenced by channel length, and that  $L_{ch} > 20$  nm (30 nm) was necessary for the  $\text{MoTe}_2/\text{MoS}_2$  (the  $\text{WTe}_2/\text{MoS}_2$  device) to yield its peak performance both in terms of  $SS$  as well is  $I_{ON}$ .

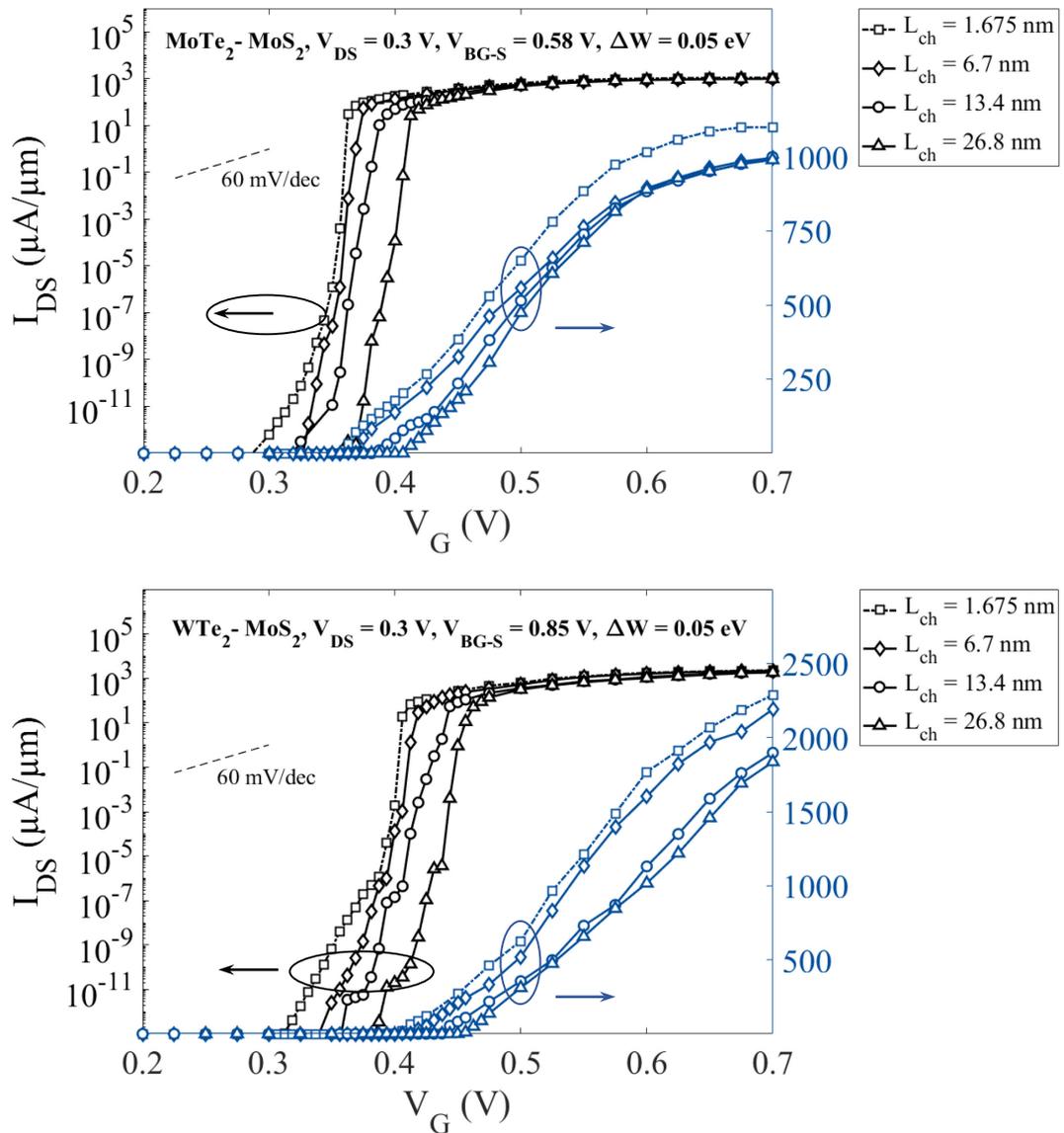


Figure 94.  $I_D$ - $V_G$  characteristics for the DBE  $\text{MoTe}_2/\text{MoS}_2$  and the  $\text{WTe}_2/\text{MoS}_2$  devices at  $V_{DS} = 0.3$  V,  $V_{BG-S} = 0.58$  V and  $0.85$  V (resp.),  $\Delta W = 0.05$  eV and for channel lengths between 1.675 nm and 27 nm.

Figure 94 shows the  $I_D$ - $V_G$  characteristics for the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> and the WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $V_{BG-S} = 0.58$  V and  $0.85$  V (resp.),  $\Delta W = 0.05$  eV and channel lengths ranging from  $1.675$  nm to  $26.8$  nm.

In both devices, it is obvious that channel length does not impact  $SS$  (as a reminder, we estimate  $SS$  between  $I_{DS} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$  and  $10^{-2}$   $\mu\text{A}/\mu\text{m}$ ): no matter the channel length, the transition from a fully OFF to a fully ON state requires only a small increase in  $V_G$  of at most  $0.03$  V.

The direct influence of channel length on  $SS$  and  $I_{ON}$  in the DBE devices is shown in Figure 95. Its impact on the performance of the standard TFETs as studied in Section 5.3.3 is also shown for comparison purposes.

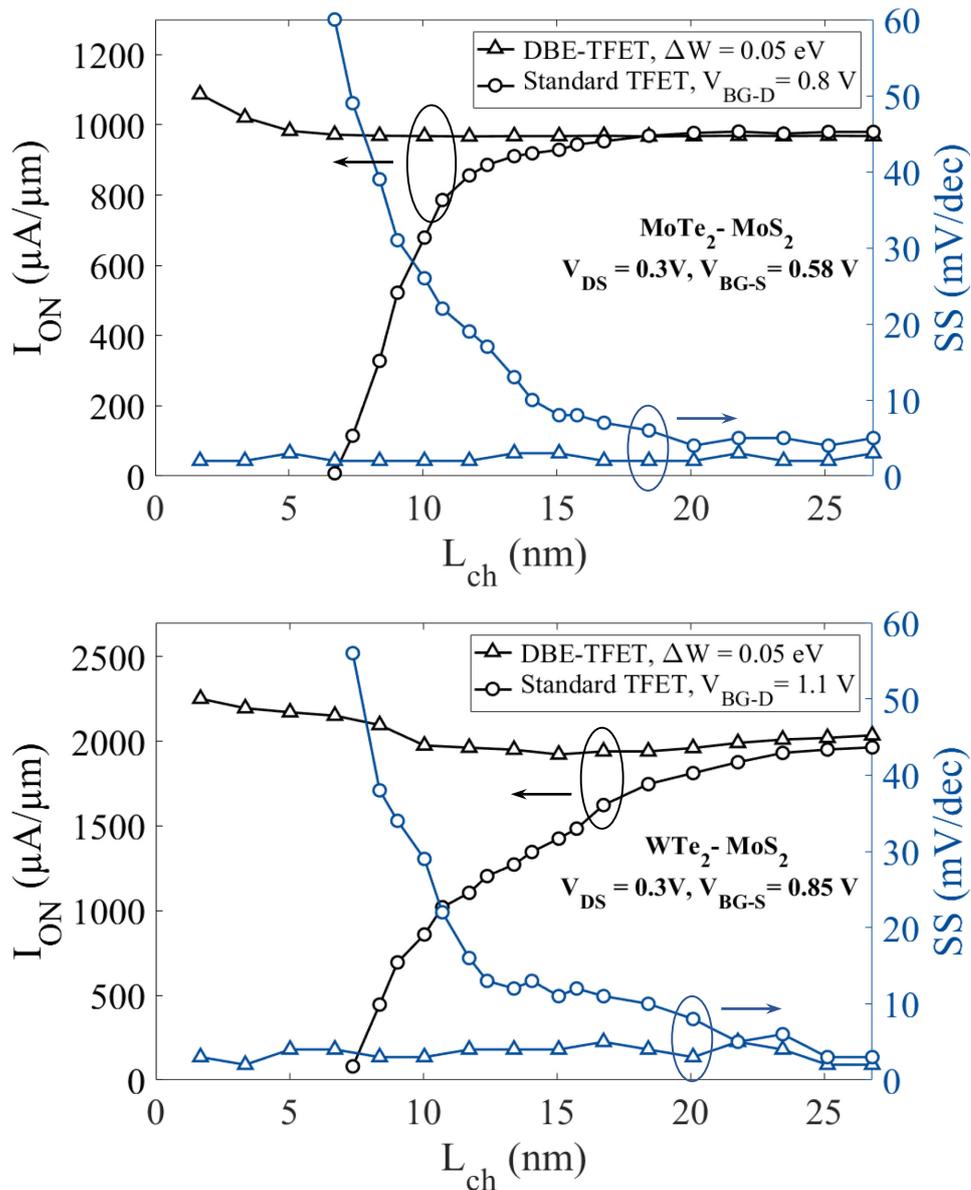


Figure 95. Influence of channel length on both  $SS$  and  $I_{ON}$  in the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V and  $V_{BG-S} = 0.58$  V and  $0.85$  V (resp.), as well as the standard TFETs as studied in Section 5.3.3 and shown in Figure 75.

As expected,  $SS$  is not impacted by  $L_{ch}$  in either device and remains  $< 5$  mV/dec for all channel lengths. The ON current at this  $\Delta W$  is slightly impacted in both devices: it peaks for the shortest channel, then decreases until  $L_{ch} > 7$  nm at which point it stabilizes. This evolution can be explained by two factors highlighted in Figure 96 and Figure 97:

- in short-channel devices, the proximity of the drain backgate pulls the CB down in the channel, widening the energy window in which current can flow.
- in very short-channel devices, carriers can tunnel directly from the source VB to the drain CB, effectively widening the aforementioned energy window even further.

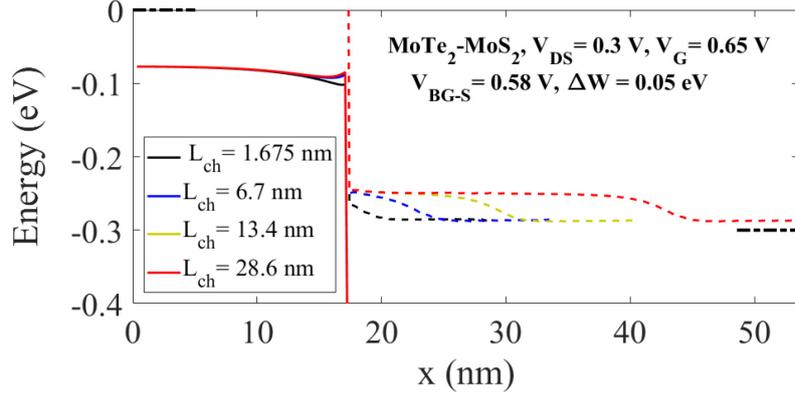


Figure 96. Highest VB (full lines) and lowest CB (dotted lines) in the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $V_G = 0.65$  V,  $V_{BG-S} = 0.58$  V,  $\Delta W = 0.05$  eV and  $L_{ch}$  ranging from 1.675 nm to 26.8 nm, highlighting the impact of  $L_{ch}$  on the CB in the channel.

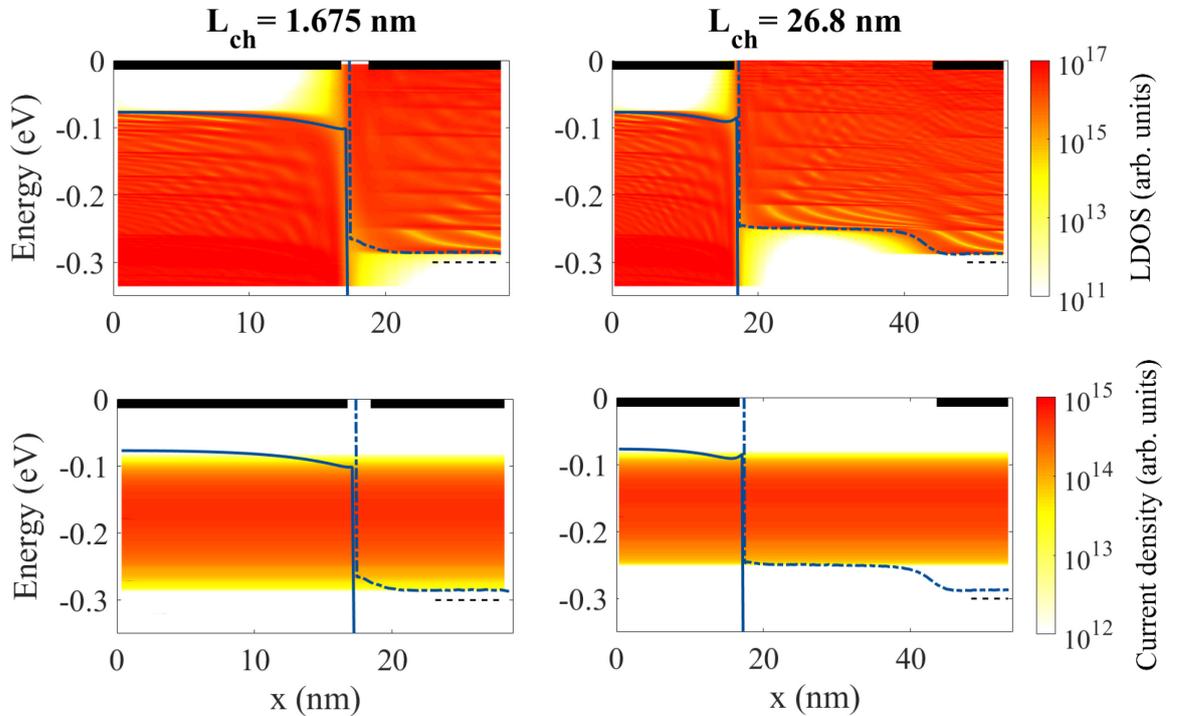


Figure 97. (top) LDOS and (bottom) current density as well as highest VB (full lines) and lowest CB (dotted lines) in the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $V_G = 0.65$  V,  $V_{BG-S} = 0.58$  V,  $\Delta W = 0.05$  eV and (left)  $L_{ch} = 1.675$  nm and (right) 26.8 nm, highlighting the impact of  $L_{ch}$  on source-to-drain tunneling.

However, the main takeaway from Figure 95 is the striking comparison with the standard TFETs, because virtually any dependence on channel length is removed in the DBE devices:

- The performance of standard heterojunction TFETs increases with  $L_{ch}$ , and channel lengths beyond at least 8 nm are necessary for these devices to even be functional. Channel lengths beyond at least 20 nm are necessary for them to yield the promising performances detailed in Chapter 4.
- The performance of the DBE TFETs, no matter the channel length, is always superior to or equal to the peak performance of the standard TFETs. There are no limits to channel scaling, and extremely short channels actually yield marginally higher ON currents (maximum  $I_{ON}$  requires  $L_{ch} < 5$  nm) at the considered  $\Delta W$  (at a lower  $\Delta W$ ,  $L_{ch}$  would not influence  $I_{ON}$ ). Moreover, the negative impact of electron-phonon interactions increases with device length, so keeping the channel short would alleviate these effects.

While they share the same materials, architecture and general principle of operation, the DBE devices allow us to access the peak performance of the already very promising heterojunction TFETs at any channel length.

### 6.3.3 Influence of source backgate voltage

Much like in the standards TFETs studied in Chapter 4, the source backgate voltage is another important tuning parameter, as it controls the potential profile as well as the energy level of the VB in the source contact.

However, since the analysis is very close to that of the standard TFETs performed in Section 5.3.4, this section will be brief and will solely focus on identifying the optimal  $V_{BG-S}$  for each device at  $\Delta W = 0.05$  eV.

The effect of the backgate voltages on the performance of the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $L_{ch} = 10.05$  nm and  $\Delta W = 0.05$  eV and analyzed in this section.

The corresponding  $I_D$ - $V_G$  characteristics for both devices are shown in Figure 98 at several source backgate voltages:

- DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device:  $V_{BG-S} = 0.4$  V, 0.52 V and 0.6 V
- DBE WTe<sub>2</sub>/MoS<sub>2</sub> device:  $V_{BG-S} = 0.7$  V, 0.8 V and 0.85 V

Overall, the impact of the source backgate voltage in these DBE devices is very close to its influence on the performance of the standard TFETS described in Section 5.3.4.

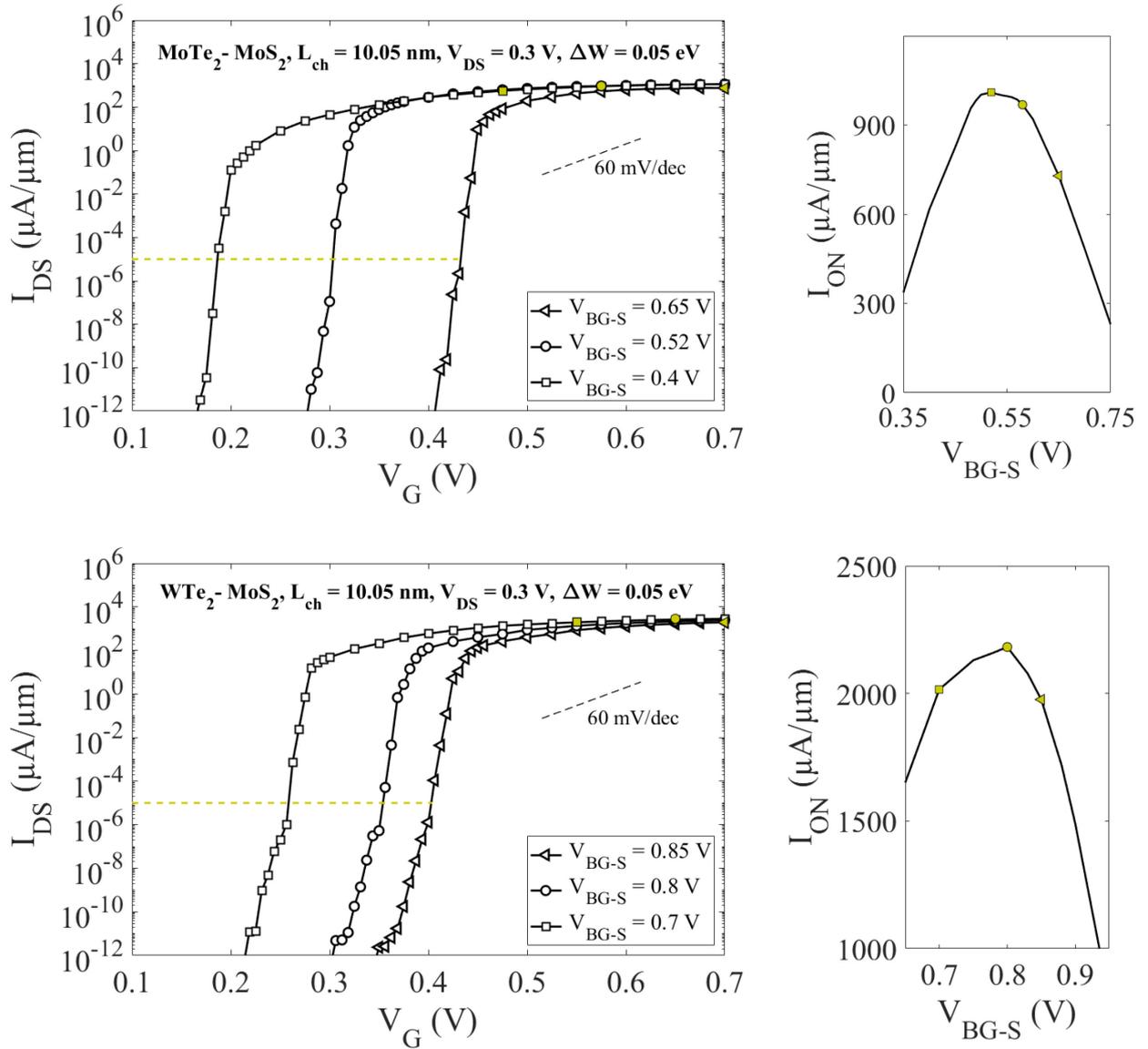


Figure 98. (left)  $I_D$ - $V_G$  characteristics at various  $V_{BG-S}$  and (right) influence of the source backgate voltage on  $I_{ON}$  in the DBE (top) MoTe<sub>2</sub>/MoS<sub>2</sub> and (bottom) WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = V_{DD} = 0.3$  V,  $L_{ch} = 10.05$  nm and  $\Delta W = 0.05$  eV.

As was the case in the standard heterojunction TFETs, the source backgate voltage does not impact  $SS$  in either device, as evidenced by the slope in the sub-threshold regime of the  $I_D$ - $V_G$  characteristics.

The ON current of both devices however, is strongly impacted by  $V_{BG-S}$  as highlighted by in Figure 98 (right). In both cases, a somewhat parabolic evolution of  $I_{ON}$  can be observed, around a peak value of 1011  $\mu\text{A}/\mu\text{m}$  at  $V_{BG-S} = 0.52$  V for the MoTe<sub>2</sub>/MoS<sub>2</sub> device, and 2182  $\mu\text{A}/\mu\text{m}$  at  $V_{BG-S} = 0.8$  V for the WTe<sub>2</sub>/MoS<sub>2</sub> device (at  $L_{ch} = 10.05$  nm).

These optimal backgate voltages remain close to those identified for the standard TFETs in Section 5.3.4, which is expected ( $V_{BG-S} = 0.58$  V for the MoTe<sub>2</sub>/MoS<sub>2</sub> device and  $V_{BG-S} = 0.85$  V for the WTe<sub>2</sub>/MoS<sub>2</sub> device).

### 6.3.4 Drain voltage characteristics and DITL

Another strong feature of the heterojunction TFETs presented in Chapter 4 is the saturation reached at supply voltages as low as 0.2 V. Since these DBE-TFETs rely on the same materials and general principle of operation, they are expected to yield similar performance.

The  $I_D$ - $V_{DS}$  characteristics of the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 13.4$  nm,  $V_G$  ranging from 0.4 V to 0.6 V and  $V_{BG-S} = 0.4$  V and 0.52 V are shown in Figure 99.

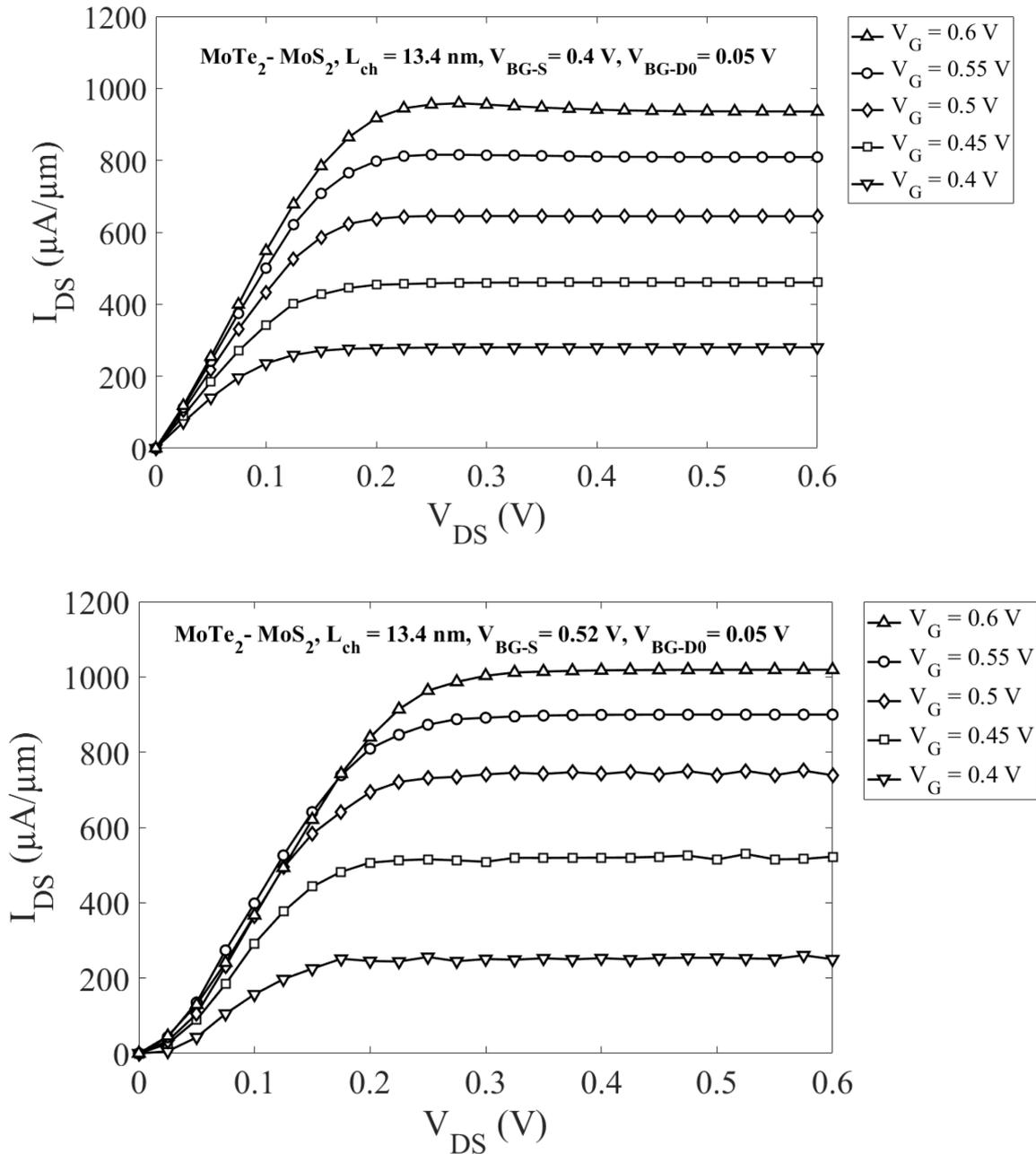


Figure 99.  $I_D$ - $V_{DS}$  characteristics of the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 13.4$  nm,  $\Delta W = 0.05$  eV and (top)  $V_{BG-S} = 0.4$  V (bottom)  $V_{BG-S} = 0.52$  V.

The characteristics are, as expected, similar to those of the standard in-plane heterojunction TFETs:

- at the optimal  $V_{BG-S} = 0.52$  V, the drain CB is forced at energies higher than the source CB for  $V_{DS} < 0.015$  V (see Figure 81), therefore the current is established only once this threshold drain voltage is reached. The current then follows a linear increase until saturation is reached around  $V_{DS} = 0.25$  V
- at  $V_{BG-S} = 0.4$  V, the characteristic is that of a standard transistor. The current increases linearly from  $V_{DS} = 0$ , and reaches saturation around  $V_{DS} = 0.2$  V.

Although  $V_{BG-S} = 0.52$  V has been identified as yielding the maximum  $I_{ON}$  for the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device, the currents reported in Figure 99 at a given  $V_G$  are in the same range as those obtained at  $V_{BG-S} = 0.4$  V.

This can be explained by the strong shift in threshold voltage (from 0.3 V to 0.35 V) and  $V_{OFF}$  (from 0.19 V to 0.3 V) which are both highlighted by the  $I_D$ - $V_G$  characteristics shown in Figure 100.

Even though the current at any given  $V_G$  is comparable between the two considered source backgate voltages, the ON current is calculated at

- $V_{ON} = V_{OFF} + V_{DD} = 0.19 + 0.3 = 0.49$  V for  $V_{BG-S} = 0.4$  V.
- $V_{ON} = V_{OFF} + V_{DD} = 0.3 + 0.3 = 0.6$  V for  $V_{BG-S} = 0.58$  V.

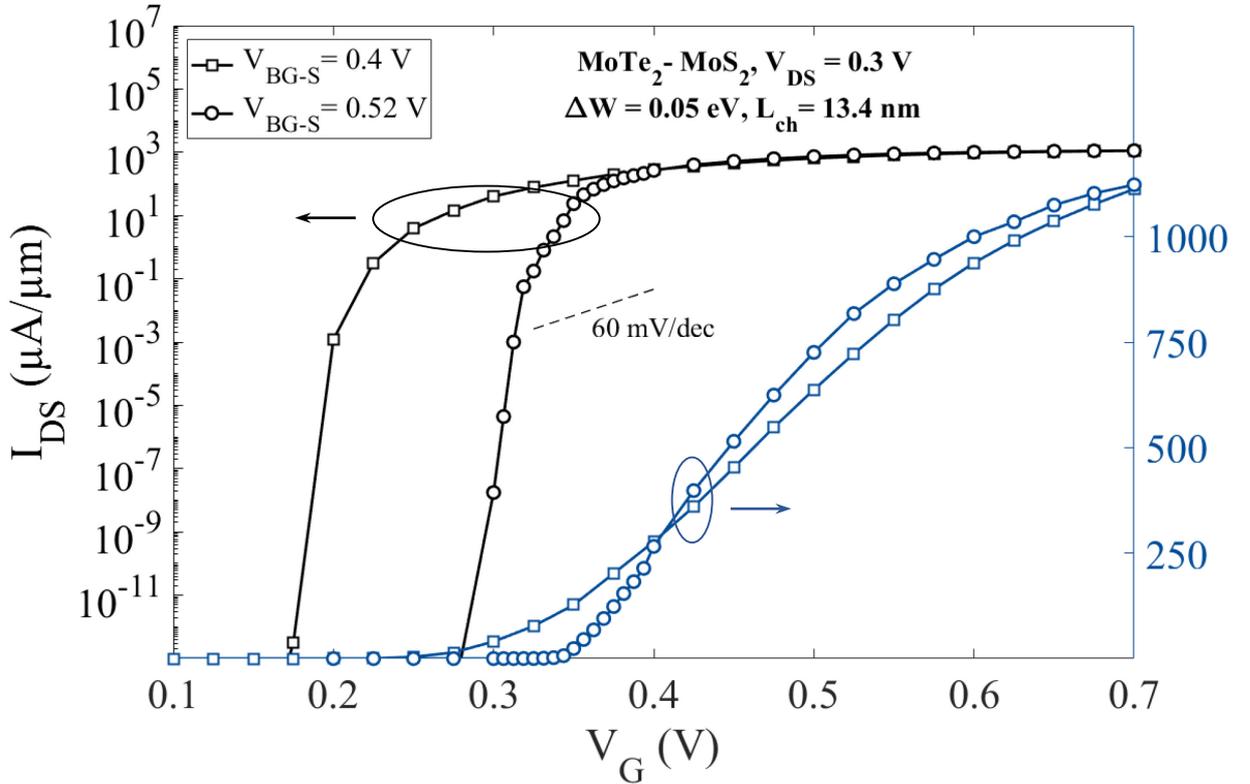


Figure 100.  $I_D$ - $V_G$  characteristics of the DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $L_{ch} = 13.4$  nm,  $\Delta W = 0.05$  eV and  $V_{BG-S} = 0.4$  V and 0.52 V. The strong shift in both  $V_{OFF}$  and  $V_T$  is highlighted here.

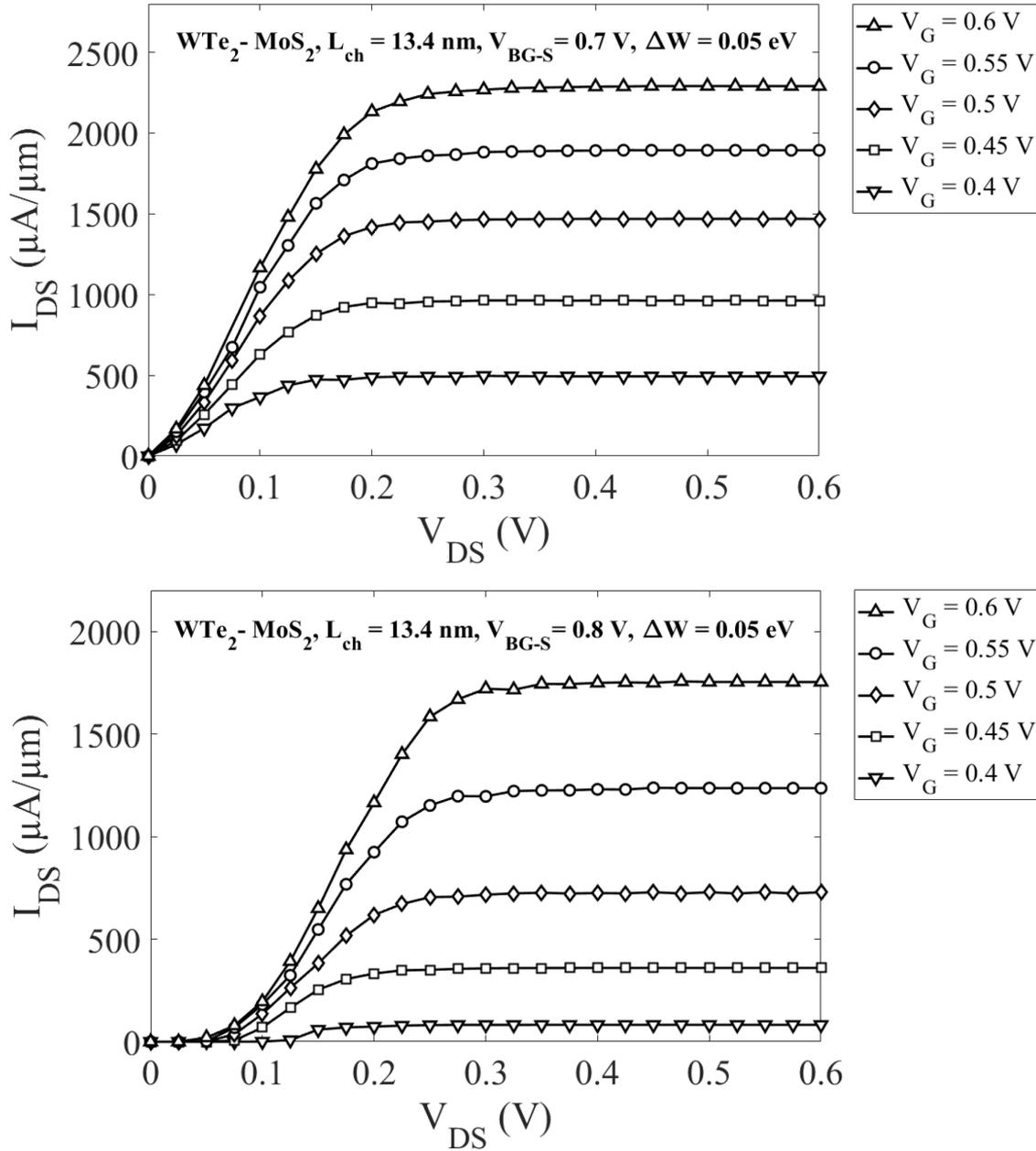


Figure 101.  $I_D$ - $V_{DS}$  characteristics of the DBE  $WTe_2/MoS_2$  device at  $L_{ch} = 13.4$  nm,  $\Delta W = 0.05$  V and (top)  $V_{BG-S} = 0.7$  V (bottom)  $V_{BG-S} = 0.8$  V.

Similar observations can be made about the  $I_D$ - $V_{DS}$  characteristics for the  $WTe_2/MoS_2$  device shown in Figure 101.

In both the DBE  $MoTe_2/MoS_2$  and  $WTe_2/MoS_2$  devices, much like in the standard heterojunction TFETs, current saturation is reached at drain voltages as low as  $V_{DS} = 0.2$  V; this peak performance reached at low  $V_{DS}$  highlights the potential of these DBE in-plane heterojunctions TFETs for ultra-low power operation.

Figure 102 shows the  $I_D$ - $V_G$  characteristics of the  $MoTe_2/MoS_2$  and the  $WTe_2/MoS_2$  devices for  $L_{ch} = 13.4$  nm,  $V_{DS}$  ranging from 0.1 V to 0.7 V and the optimal  $V_{BG-S}$  and  $\Delta W$  identified for each device, and highlights the absence of DITL in these devices.

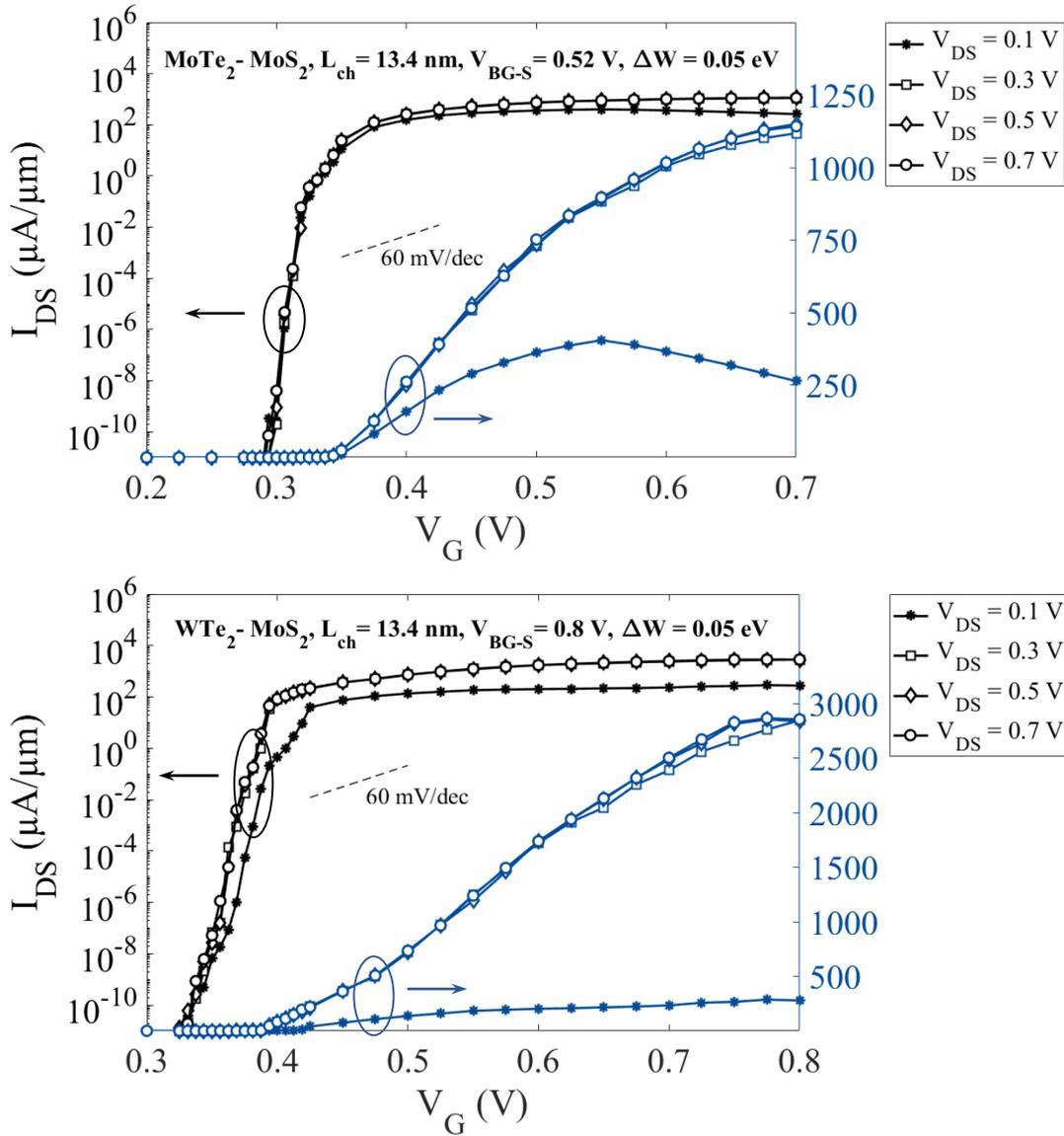


Figure 102.  $I_D$ - $V_G$  characteristics of the DBE  $\text{MoTe}_2/\text{MoS}_2$  and the  $\text{WTe}_2/\text{MoS}_2$  devices for  $L_{\text{ch}} = 13.4$  nm,  $V_{\text{DS}}$  ranging from 0.1 V to 0.7 V, and the optimal  $V_{\text{BG-S}}$  and  $\Delta W$  for each device as identified in Sections 6.3.1 and 6.3.3.

Once again, the behavior of these DBE devices is close to that of the standard TFETs: at very low  $V_{\text{DS}}$ , the drain CB lies at energies close to the source CB, and less current can flow; at higher  $V_{\text{DS}}$  however, both OFF and ON-state behaviors are unaffected by the drain voltage.

The current decrease observed at  $V_G > 0.55$  V at  $V_{\text{DS}} = 0.1$  V in the  $\text{MoTe}_2/\text{MoS}_2$  device is due to the effect of the gate voltage on the source VB: at high  $V_G$ , the source VB at the source channel/interface is pulled down towards lower energies, narrowing the energy window in which current can flow. At higher  $V_{\text{DS}}$ , the drain CB lies at far lower energies, allowing for a wider energy interval in which the current saturates and therefore is not impacted by the marginal lowering of the source VB due to the gate voltage.

## 6.4 Conclusion on DBE in-plane heterojunction TFETs

The DBE MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices studied in this chapter, while being only a minor variation from the standard TFETs studied in Chapter 4, show even greater promise for ultra-low power operation and device scaling. By using the same metal in all gates and applying  $V_{BG-D} = V_G$ , performance far superior to that of the standard TFETs can be reached.

- **Gate length scaling does not impact:**  $SS$  is unaffected by channel length, and the ON current only slightly increases in the case of very short channels (down to  $< 2$  nm) for the considered workfunction offset. Such short channels would strongly alleviate most negative effects due to electron-phonon scattering.
- **Extremely low SS:** no matter the length of the channel, the devices yield ballistic  $SS$  below 7 mV/dec when the optimal workfunction offset is applied, and ballistic  $SS$  as low as 3 mV/dec were observed in some short channel devices
- **High ON/OFF ratio:** depending on the source backgate voltage applied to the device, ballistic ON/OFF ratios beyond  $10^7$  for the MoTe<sub>2</sub>/MoS<sub>2</sub> device and  $2 \times 10^8$  for WTe<sub>2</sub>/MoS<sub>2</sub> device have been reported, no matter the channel length. For channel lengths below 10 nm, ballistic ON currents of  $1.2 \times 10^3$  for the MoTe<sub>2</sub>/MoS<sub>2</sub> device and  $2.4 \times 10^3$  for WTe<sub>2</sub>/MoS<sub>2</sub> device can be reached.
- **Good saturation even at low  $V_{DS}$ :** both devices saturate at drain voltages as low as  $V_{DS} = 0.3$  V when the optimal backgate voltages are applied. Once again, this only strengthens their appeal as ultra-low power electronic switches.

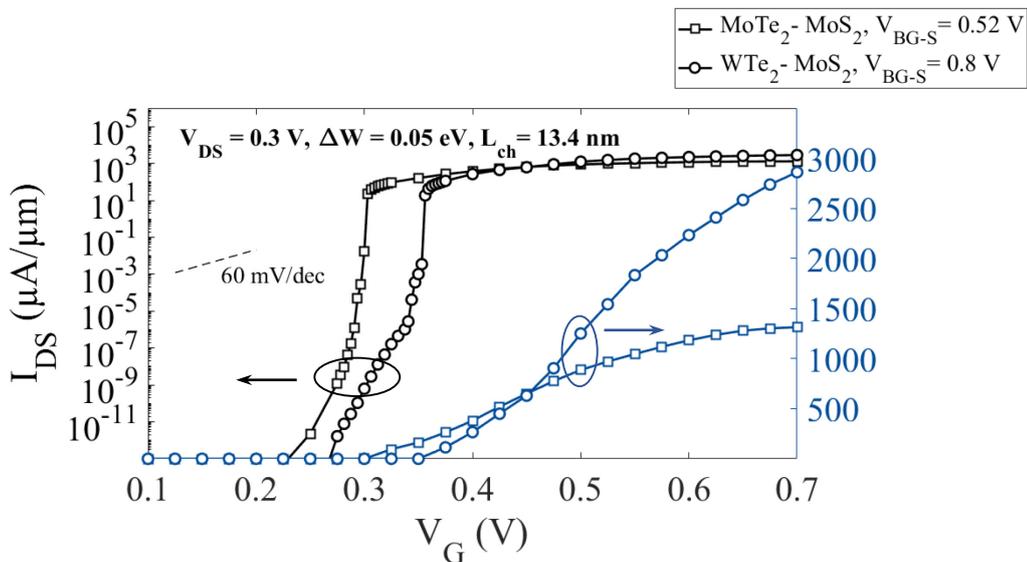


Figure 103.  $I_D$ - $V_G$  characteristics of the backgate-enhanced MoTe<sub>2</sub>/MoS<sub>2</sub> and the WTe<sub>2</sub>/MoS<sub>2</sub> devices for  $L_{ch} = 1.675$  nm,  $V_{DS} = 0.3$  V, and the optimal  $V_{BG-S}$  and  $\Delta W$  for each device.

# Chapter 7

## Ungated-channel in-plane heterojunction TFETs

### 7.1 Introduction

The DBE devices investigated in Chapter 6 relied on the influence of the drain backgate on the CB in the drain contact to increase the performance of the standard MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> heterojunction TFETs.

However, in those devices, a top-gate was still used to control the potential in the channel and, in conjunction with the drain backgate, control current flow in the device.

From the study of these devices came an idea for yet another device design based on these in-plane heterojunction TFETs: **since the drain backgate is used to force the energy level of the CB in the drain, is a channel gate truly necessary for these devices to operate well and achieve good performance ?**

As the results presented and analyzed in this chapter will show, these devices are fully able to operate without a channel gate. Current flow is therefore only controlled by the drain backgate voltage  $V_{BG-D}$ .

From an experimental standpoint, foregoing the top-gate would be extremely beneficial and streamline the material deposition and fabrication processes.

Much like the DBE devices presented in Chapter 6, this innovative device design is made possible by the 2D nature of the materials used in the active layer. If traditional, bulk materials were used instead, standard chemical doping would have to be used instead of the electrostatic doping used in this work; this electrostatic doping via backgates affords us the active control of the band profile and potential in the contacts necessary for the DBE and “ungated-channel” (UC) devices to function.

These DBE and UC devices therefore make full use of the 2D nature of the materials considered in this work.

## 7.2 Device architecture

The architecture of the UC devices (as shown in Figure 104) is extremely close to that of the DBE devices presented previously.

The only difference is that these devices operate without a top-gate and that current flow is therefore controlled solely via the drain backgate voltage  $V_{BG-D}$ . In these devices, the workfunction of both backgates is 5.13 eV for both the MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices.

The overall structure of the device is unchanged, with either MoTe<sub>2</sub> or WTe<sub>2</sub> being used as source material, and MoS<sub>2</sub> being used in the channel and drain. The channel, usually defined by the top-gate, is instead defined here as the region separating the source and drain backgates.

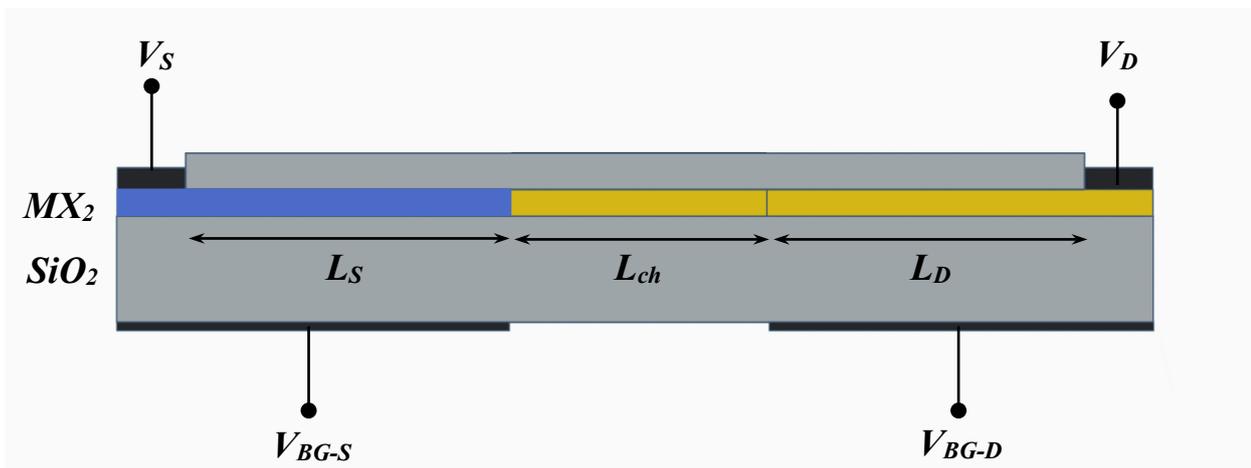


Figure 104. Device architecture for the considered ungated-channel in-plane heterojunction TFETs. One TMD acts as the source, and another as the channel/drain. SiO<sub>2</sub> is used as a buried oxide, and a high- $\kappa$  dielectric as the top gate oxide. The voltage applied to the drain backgate is used to control current flow in the device, while the source backgate voltage remains constant.

## 7.3 Electronic transport simulations

As was the case for the TFETs studied in the previous chapters, overall performance as well as the influence of design parameters will be analyzed. Namely, the impact of the channel length and the source backgate voltage on figures of merit such as  $SS$  and  $I_{ON}$  will be investigated.

Since the drain backgate voltage is used to control current flow in lieu of a traditional top-gate,  $I_D$ - $V_{BG-D}$  characteristics will be shown instead of  $I_D$ - $V_G$  characteristics.

### 7.3.1 Principle of operation

In this short section, I will highlight the principle of operation of these UC devices. While the examples presented here pertain to the MoTe<sub>2</sub>/MoS<sub>2</sub> device, the mode of operation is the same in the WTe<sub>2</sub>/MoS<sub>2</sub> device.

The  $I_D$ - $V_{BG-D}$  characteristic of a UC MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $L_{ch} = 13.4$  nm and  $V_{BG-S} = 0.53$  V is shown in Figure 105.

The first observation to make is that the device indeed behaves as a transistor: at low  $V_{BG-D}$  the device is in the OFF state where no current flows; once a threshold  $V_{BG-D}$  is reached however, the device goes to the ON state and current flows in the device. The transition from the OFF state to the ON state is extremely steep, requiring only a small increase in  $V_{BG-D}$  below 0.02 V, which leads to a sub-threshold swing of roughly 3 mV/dec.

In this device,  $V_{OFF}$  (at which  $I_{DS} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$ )  $\sim 0.35$  V, therefore  $V_{ON} \sim 0.65$  V, which leads to an ON current of roughly 750  $\mu\text{A}/\mu\text{m}$ .

The performances of this initial transistor are already very promising, rivaling those of the DBE devices and of the very best standard TFETs analyzed in Chapters 5 and 6.

In order to highlight the principle of operation of these UC devices, Figure 106 shows the evolution of the highest VB and lowest CB in an UC device and a standard device during the OFF/ON transition, while Figure 107 shows the LDOS in the device at  $V_G = 0.3$  V, 0.35 V, 0.3625 V and 0.5 V (red ellipses in Figure 105).

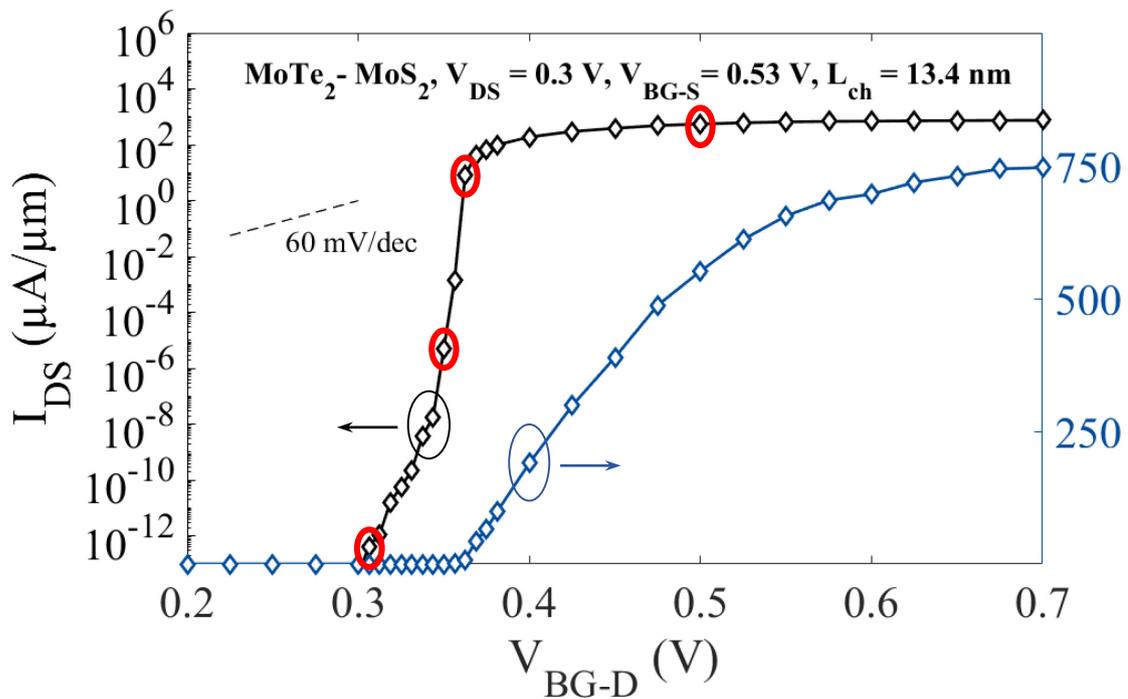


Figure 105.  $I_D$ - $V_{BG-D}$  characteristic of a UC MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $V_{DS} = 0.3$  V,  $L_{ch} = 13.4$  nm and  $V_{BG-S} = 0.53$  V.

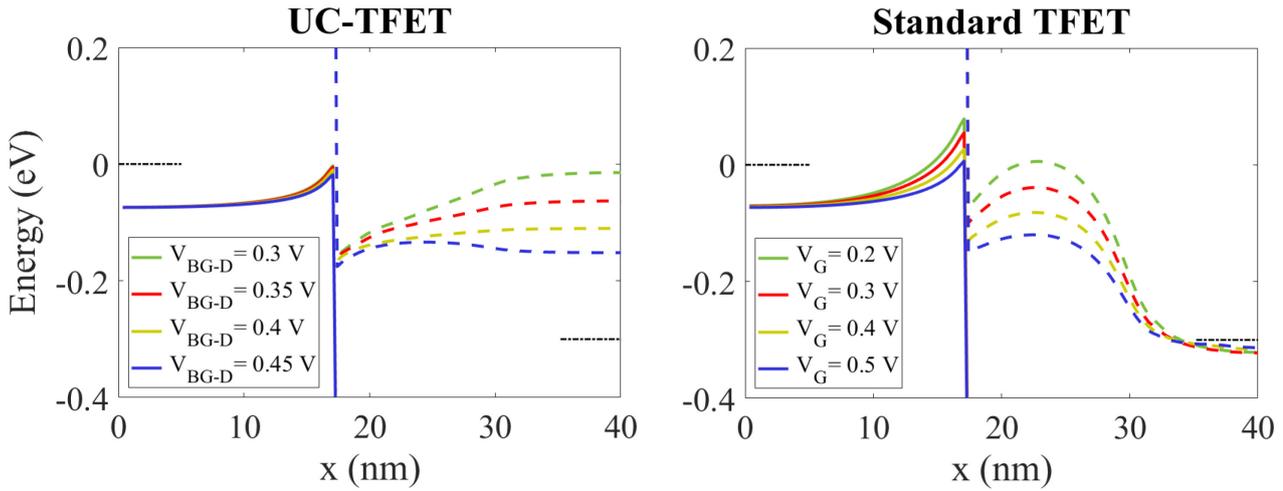


Figure 106. Highest VB (full lines) and lowest CB (dotted lines) highlighting the OFF/ON transition in (left) a UC-TFET and (right) a classic TFET.

The black dashed lines represent the Fermi energies in the contacts.

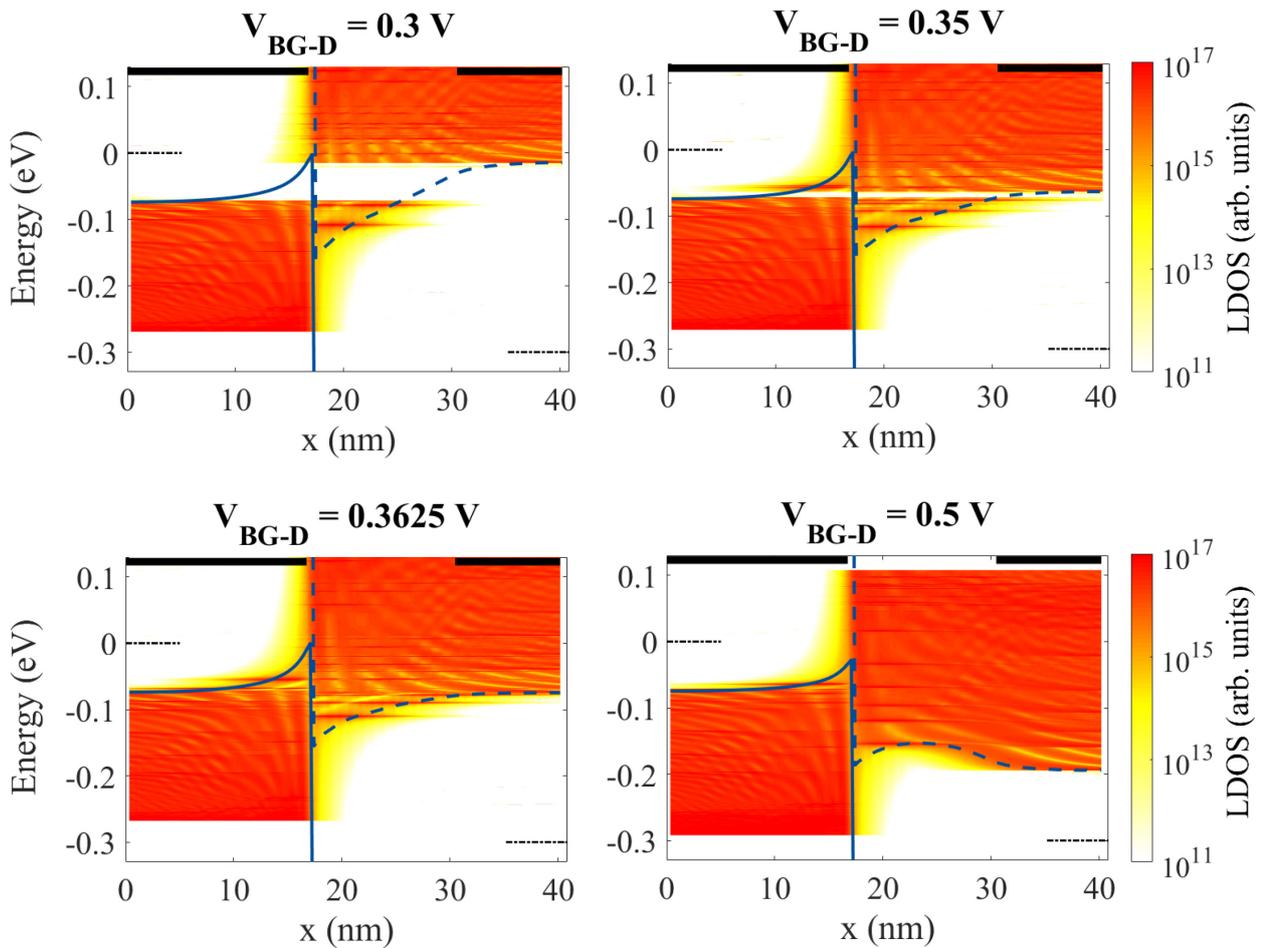


Figure 107. LDOS in the UC MoTe<sub>2</sub>/MoS<sub>2</sub> device at the drain backgate voltages highlighted with red ellipses shown in Figure 105. The highest VB (full lines), lowest CB (dotted lines), and Fermi levels in the source and drain contacts (dashed black lines) are also represented.

These LDOS figures highlight that the UC devices operate solely by modulating the energy of the CB in the drain contact.

The band profiles represented in Figure 106 highlight how the working principle of these UC devices differs from that of a standard TFET:

- Standard TFET: the static source and drain backgate voltages force the potential and the energy level of the bands in the contacts. The top-gate voltage is used to control the profile of the bands in the channel: as  $V_G$  increases, the channel CB is pushed towards lower energies, allowing carriers to flow from source to drain.
- UC TFET: only the source backgate voltage is static, and it forces the energy level of the band in the source contact. The drain backgate voltage dynamically controls the energy level of the band in the drain: as it increases, the drain CB is pushed down towards lower energies. As soon as  $E_{CB-drain} < E_{VB-source}$ , current flows freely from the source to the drain, and the transistor turns ON (see the current densities shown in Figure 108).

As was the case for the DBE devices, this radically different working principle frees the UC devices from traditional FET shortcomings such as source-to-drain tunneling and other short-channel effects: since no states are available to tunnel to at low  $V_{BG-D}$ , the device is in a true OFF state where no current can occur, no matter  $L_{ch}$ .

As soon as a high enough  $V_{BG-D}$  is reached however, the broken gap heterojunction formed by the carefully selected strained TMDs ensures that carriers can flow from the source VB to the channel/drain CB unabated.

The influence of the length of the channel on the performance of these UC devices will now be investigated.

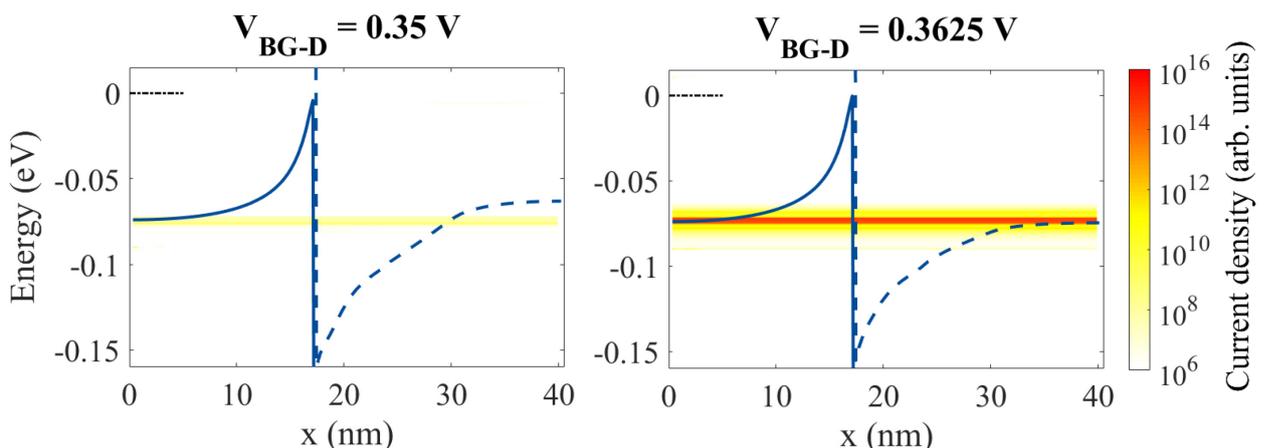


Figure 108. Current density in the UC  $\text{MoTe}_2/\text{MoS}_2$  device at  $V_{BG-D} = 0.35$  V and  $V_{BG-D} = 0.3625$  V. The highest VB (full lines), lowest CB (dotted lines), and Fermi levels in the source and drain contacts (dashed black lines) are also represented. These current density figures highlight the infinitesimal increase in  $V_{BG-D}$  (0.0125 V) required to transition from the OFF to the ON state.

### 7.3.2 Influence of channel length

While channel length had a strong impact on the performance of the standard TFETs studied in Chapters 5, the DBE devices studied in Chapter 6 were largely impervious to the influence of  $L_{ch}$  (except in the case of very short channels).

In this section, the influence of channel length in these UC devices will be analyzed in discussed.

$I_D$ - $V_{BG-D}$  characteristics for both the UC MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $V_{BG-S} = 0.53$  V and 0.8 V (resp.) and channel lengths ranging from 1.675 nm to 26.8 nm are shown in Figure 109.

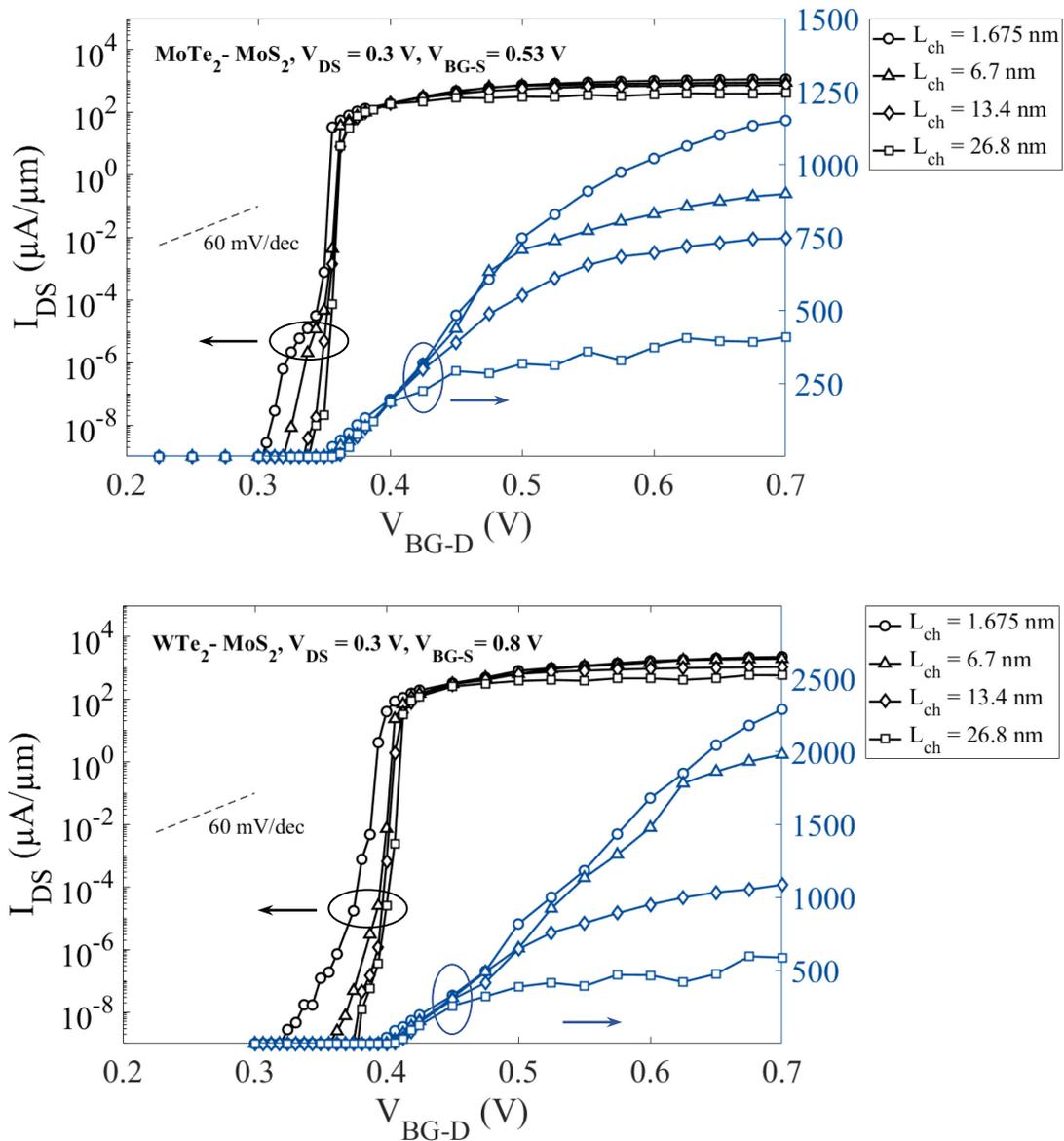


Figure 109.  $I_D$ - $V_{BG-D}$  characteristics for both the UC (top) MoTe<sub>2</sub>/MoS<sub>2</sub> and (bottom) WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $V_{BG-S} = 0.53$  V and 0.8 V (resp.) and channel lengths ranging from 1.675 nm to 26.8 nm. Although it has no effect on  $SS$  and  $V_T$ , channel length strongly impacts the behavior at high  $V_{BG-D}$  and therefore  $I_{ON}$ .

From these  $I_D$ - $V_{BG-D}$  characteristics, two main observations applying to both devices can be made:

- $SS$  is not influenced by channel length: whether  $L_{ch} = 1.675$  nm or 26.8 nm, the steepness of the slope in the sub-threshold regime remains constant. Both devices yield  $SS \sim 3$  mV/dec across all channel lengths.
- The ON-state is strongly impacted by channel length: for  $V_{BG-D} > 0.45$  V, the current in the ON-state decreases as  $L_{ch}$  increases. For instance, in the MoTe<sub>2</sub>/MoS<sub>2</sub> device, current at  $V_{BG-D} = 0.6$  V drops from 1030  $\mu\text{A}/\mu\text{m}$  for a 1.675 nm channel to 450  $\mu\text{A}/\mu\text{m}$  for a 26.8 nm;  $I_{ON}$  is therefore strongly impacted.

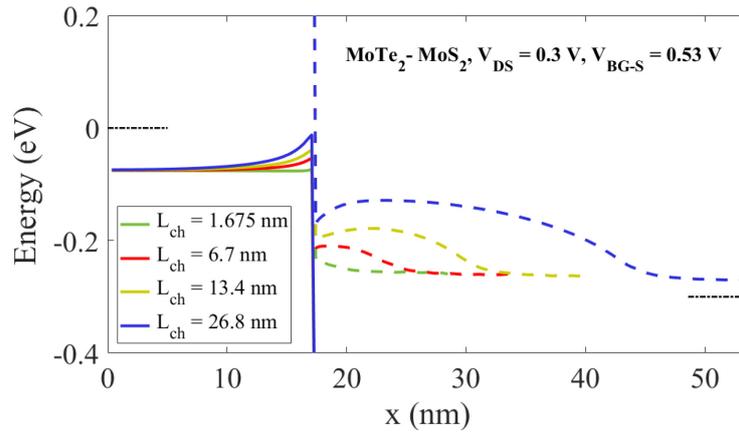


Figure 110. Highest VB (full lines) and lowest CB (dotted lines) in the UC MoTe<sub>2</sub> device in the ON state for channel lengths ranging from 1.675 nm to 26.8 nm. As  $L_{ch}$  increases, the impact of the drain backgate voltage on the CB in the channel is reduced, and the band can reach higher energies.

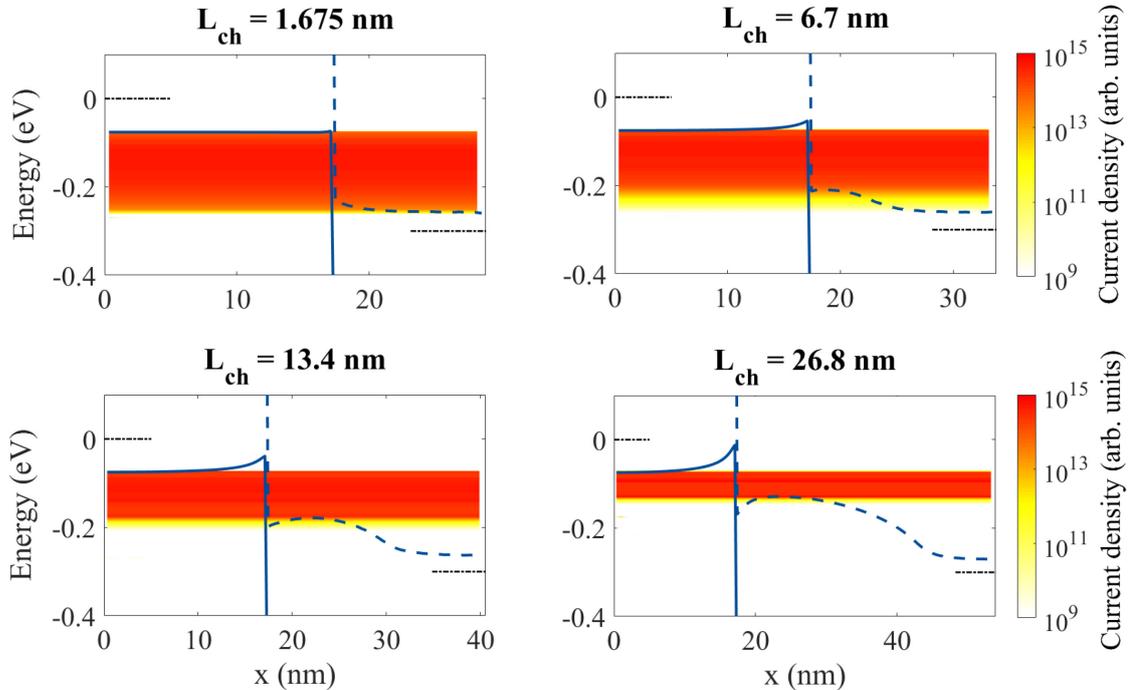


Figure 111. Current density, highest VB (full line) and lowest CB (dotted line) in the UC MoTe<sub>2</sub> device in the ON state for channel lengths ranging from 1.675 nm to 26.8 nm. As  $L_{ch}$  increases, the width of the energy window in which current can flow is drastically reduced, impacting the ON current.

These figures confirm the observations made from the  $I_D$ - $V_{BG-D}$  characteristics shown in Figure 109:  $SS$  is not affected by  $L_{ch}$  and remains  $< 5$  mV/dec in both devices;  $I_{ON}$  however is strongly affected by channel length, and is reduced by over 50% (75%) when  $L_{ch}$  increases from 2 nm to 26.8 nm in the MoTe<sub>2</sub>/MoS<sub>2</sub> (WTe<sub>2</sub>/MoS<sub>2</sub>) device; finally, due to the absence of a top-gate, the threshold voltage  $V_T$  is not influenced by  $L_{ch}$ , unlike in the standard and DBE devices. As soon as  $V_{BG-D}$  induces  $E_{CB-D} < E_{VB-S}$ , the device switches ON, no matter the channel length.

The band profiles and current densities shown in Figure 110 and Figure 111 highlight the origin of the strong decrease of  $I_{ON}$  when the channel length increases.

As the channel length increases, the influence of the drain backgate voltage on the CB in the channel is reduced. Therefore, even though at a given  $V_{BG-D}$  the energy level of the band in the drain is the same for all channel lengths, the channel CB can reach higher energies, narrowing the width of the energy window in which current flows.

This phenomenon is especially apparent in the current density figures shown for several channel lengths (see Figure 111).

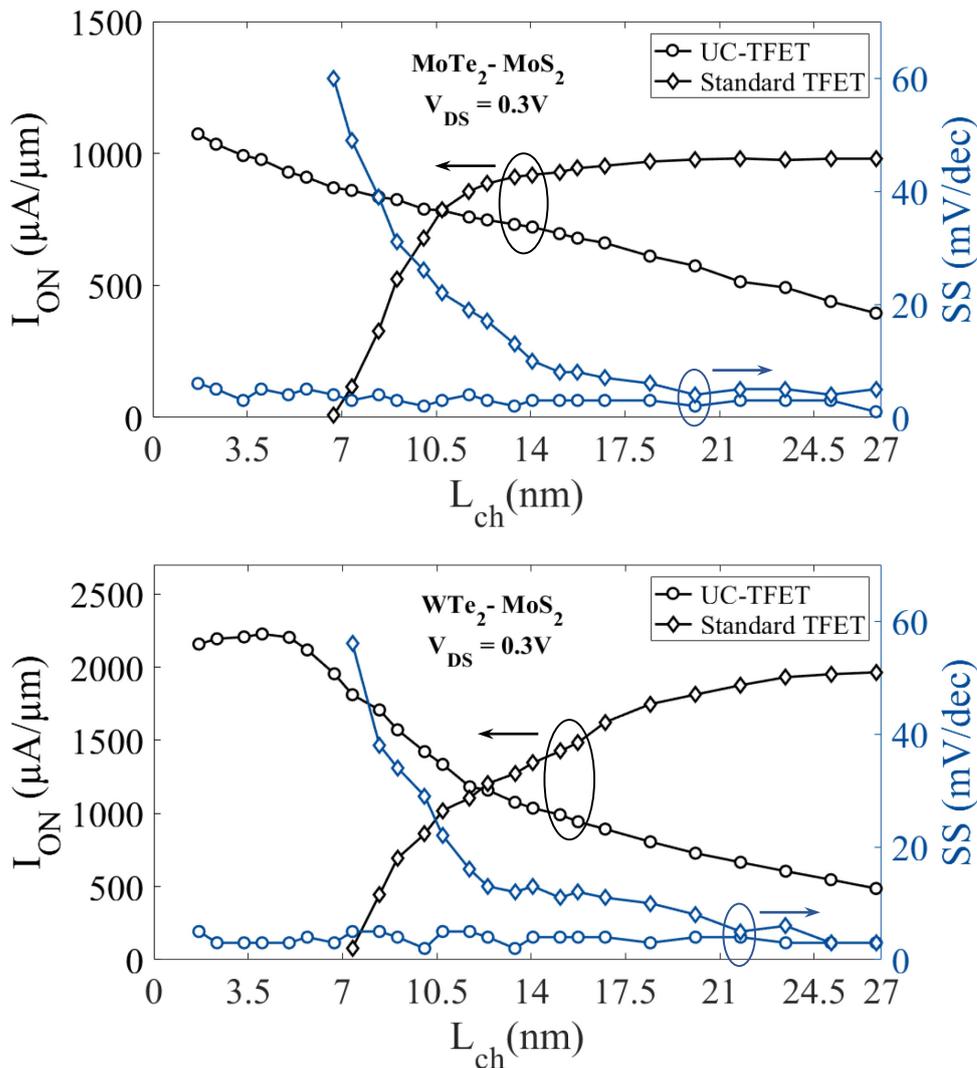


Figure 112. Influence of the channel length on  $SS$  and  $I_{ON}$  in the UC and standard (top) MoTe<sub>2</sub>/MoS<sub>2</sub> and (bottom) WTe<sub>2</sub>/MoS<sub>2</sub> devices.

The direct influence of channel length on  $I_{ON}$  and  $SS$  in these UC devices is shown in Figure 112, alongside its impact on the same figures of merit in the standard TFETs for comparison purposes.

Although these devices yield peak performance when the channel is kept short (preferably below 10 nm), they have a strong advantage compared the standard TFETs: they switch from the OFF to the ON state with a minimal increase in  $V_{BG-D}$  thanks to their  $< 5$  mV/dec  $SS$  no matter the channel length. The standard TFETs, on the other hand, require a channel length  $> 20$  nm to reach this kind of performance.

However, when compared to the DBE TFETs, in which both  $SS$  and  $I_{ON}$  remain constant and optimal no matter the channel length, this strong decrease in  $I_{ON}$  puts the UC devices at a disadvantage.

In the case of extremely short channels, the devices yield similar performance; however, for channel lengths beyond 5 nm the DBE devices yield far higher ON currents as is evidenced by Figure 113.

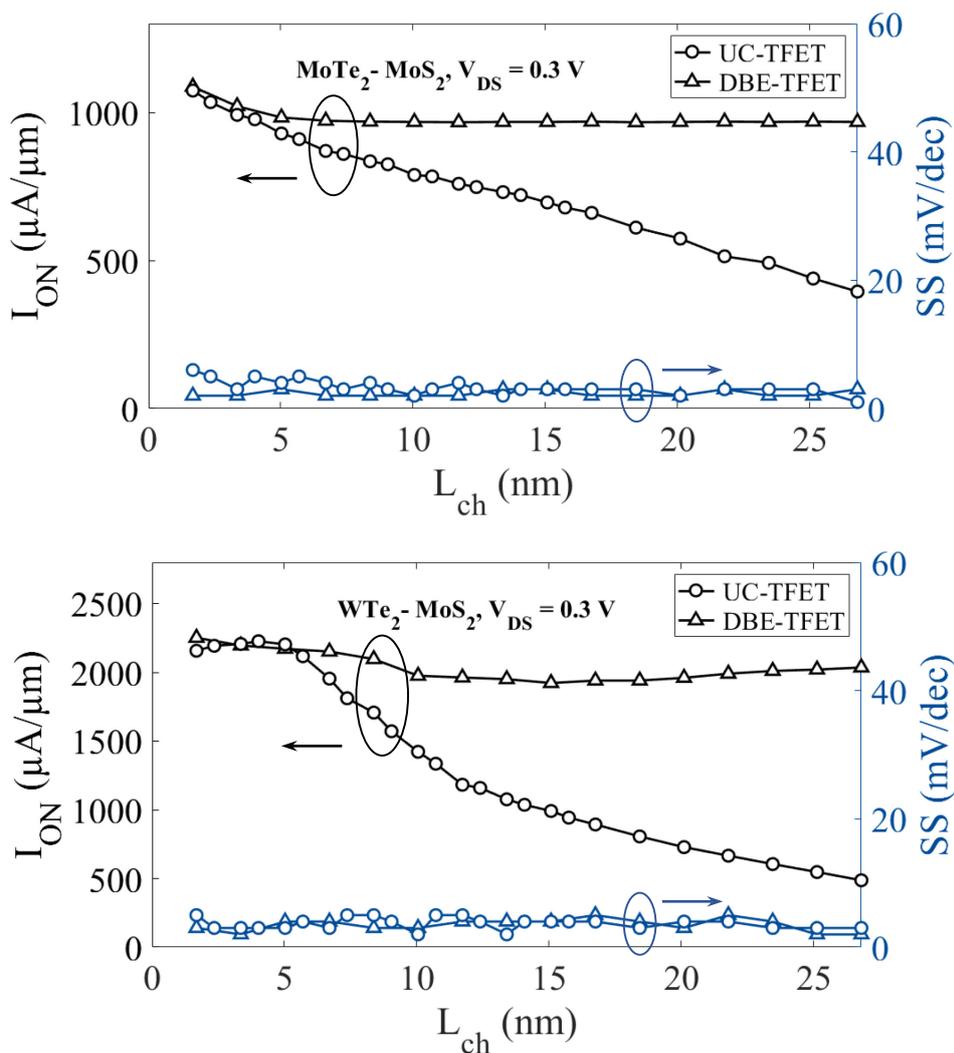


Figure 113. Influence of the channel length on  $SS$  and  $I_{ON}$  in the UC and DBE (top) MoTe<sub>2</sub>/MoS<sub>2</sub> and (bottom) WTe<sub>2</sub>/MoS<sub>2</sub> devices.

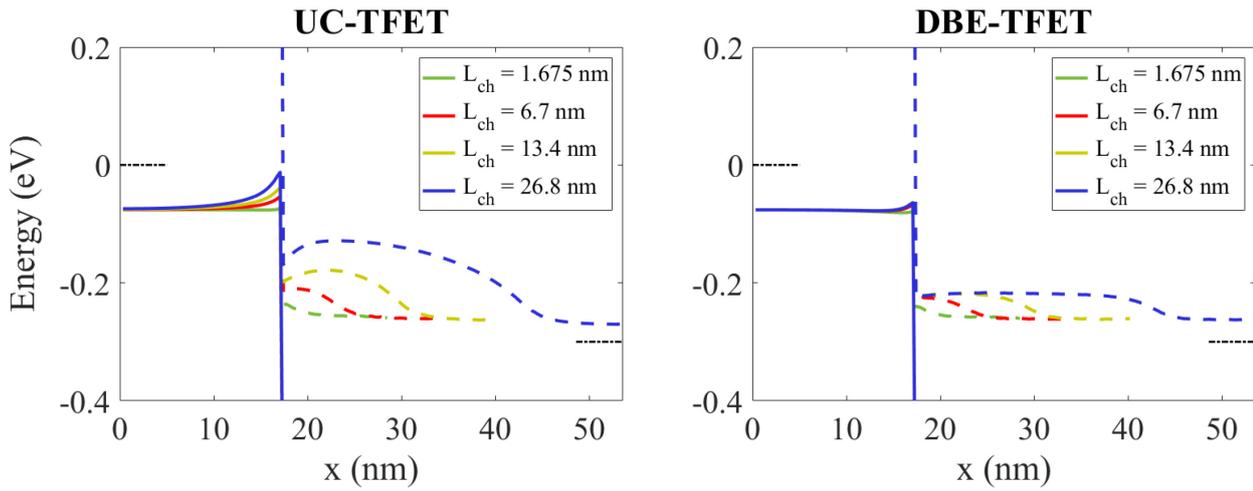


Figure 114. Highest VB (full lines) and lowest CB (dotted lines) in the (left) UC and (right) DBE MoTe<sub>2</sub>/MoS<sub>2</sub> device in the ON state, for channel lengths ranging from 1.675 nm to 26.8 nm. In the DBE device, the voltage applied to the top-gate forces the energy level of the CB in the channel, preventing it from being modified by channel length.

The band profiles of both the UC and DBE MoTe<sub>2</sub>/MoS<sub>2</sub> devices shown in Figure 114 highlight the origin of this difference in behavior regarding channel length:

- In the UC device, as explained earlier, the influence of  $V_{BG-D}$  on the channel CB is reduced as channel length increases, and the band can therefore adapt to the potential over a longer distance, gradually narrowing the width of the energy window in which current can flow.
- In the DBE device however, the electric field generated by the top-gate forces the level of the CB in the channel at the same energy no matter the channel length, and  $I_{ON}$  is therefore not impacted (except in the case of very short channels).

These UC devices therefore have a surprising relationship with channel lengths: their performance strongly increases when  $L_{ch}$  is shortened.

In standard FETs, channel scaling tends to strongly degrade performance and, when too aggressive, prevents the device from operating as a transistor altogether. In these devices however, channel scaling is very much encouraged as it actually favors performance, even in the case of extremely short channels ( $< 2$  nm), and would strongly reduce the impact of electron-phonon scattering on device performance.

Although very short channels are required to reach peak performance in these UC devices, high ON/OFF ratios (beyond  $5 \times 10^7$ ) are nonetheless observed in both devices at  $L_{ch} \sim 20$  nm, which remains extremely promising.

### 7.3.3 Influence of source backgate voltage

As was the case in both the standard and DBE TFETs, the source backgate voltage (which controls the potential profile and the energy level of the bands in the source contact) has a strong influence on the performance of these UC devices.

Figure 115 shows the  $I_D$ - $V_{BG-D}$  characteristics of the UC MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = 0.3$  V,  $L_{ch} = 13.4$  nm and various  $V_{BG-S}$  as well as the direct influence of the source backgate voltage on the ON current in each device.

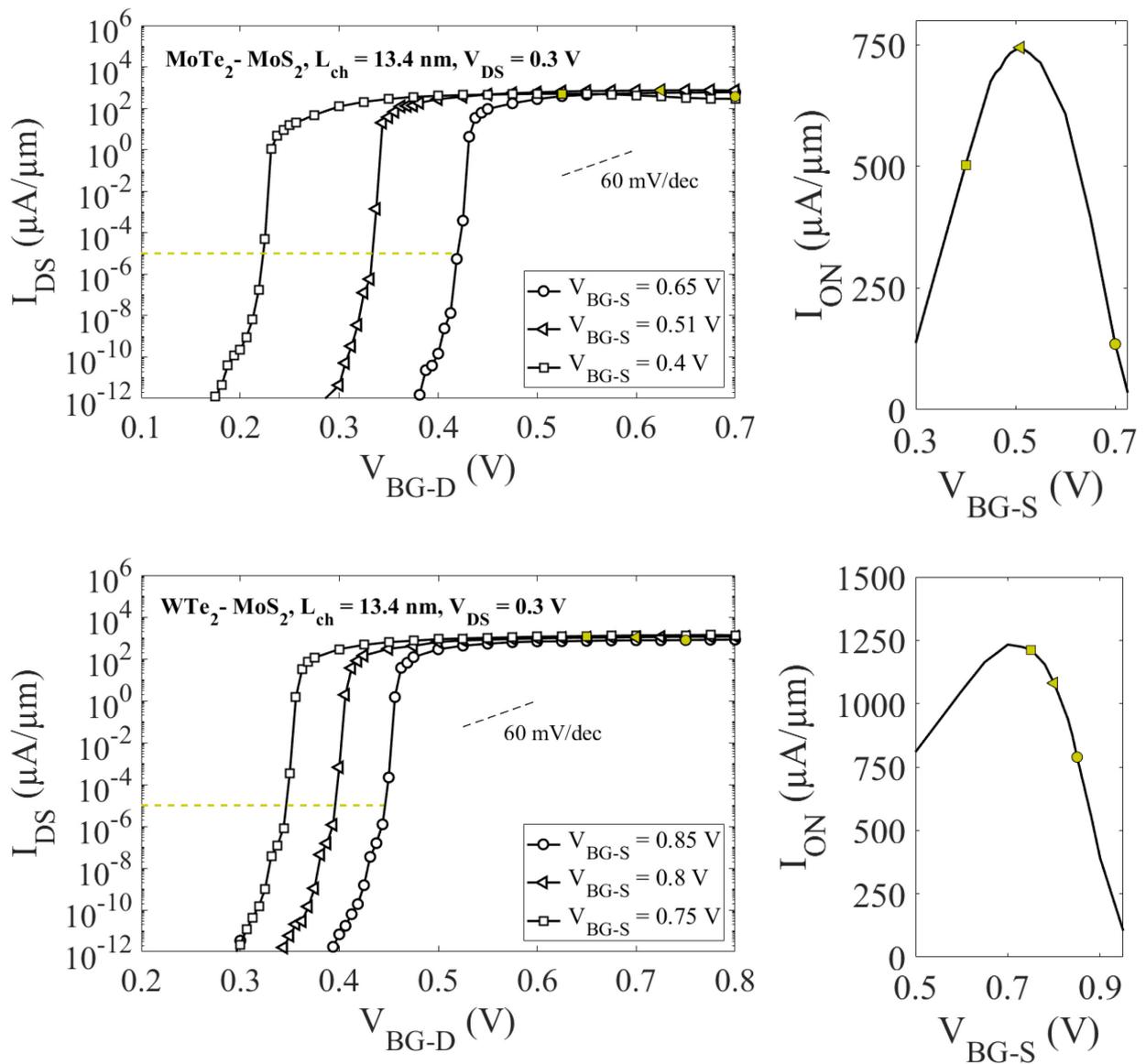


Figure 115. Left:  $I_D$ - $V_{BG-D}$  characteristics of the UC (top) MoTe<sub>2</sub>/MoS<sub>2</sub> and (bottom) WTe<sub>2</sub>/MoS<sub>2</sub> devices at  $V_{DS} = V_{DD} = 0.3$  V,  $L_{ch} = 13.4$  nm and various  $V_{BG-S}$ . The gold dotted line represents  $I_{OFF} = 10^{-5}$   $\mu\text{A}/\mu\text{m}$ , and the gold markers highlight the resulting  $I_{ON}$  measured at  $V_{BG-D} = V_{ON} = V_{OFF} + V_{DD}$ . Right: Influence of  $V_{BG-S}$  on the ON current in the device.

The source backgate voltage has a similar influence on these devices than on both the standard and DBE TFETs shown in Sections 5.3.4 and 6.3.3:  $SS$  is not impacted, and  $I_{ON}$  follows a somewhat parabolic evolution around an optimal value of  $V_{BG-S}$  in both devices.

The reason for this evolution is the same as in the devices previously studied, and was detailed in Section 5.3.4 in the case of the standard TFETs.

Thanks to this study, the optimal source backgate voltages (at  $V_{DS} = 0.3$  V and  $L_{ch} = 13.4$  nm) can be identified as:

- $V_{BG-S} = 0.51$  V for the UC MoTe<sub>2</sub>/MoS<sub>2</sub> device.
- $V_{BG-S} = 0.73$  V for the UC WTe<sub>2</sub>/MoS<sub>2</sub> device.

### 7.3.4 Drain voltage characteristics and DITL

Both the standard and DBE devices have exhibited current saturation for drain voltages for supply voltages as low as 0.2 V, and strong resistance to DITL; both of these features are very promising for ultra-low voltage operation. Similar behavior can be expected in the UC devices thanks to their strong resemblance to these devices.

$I_D$ - $V_{DS}$  characteristics for the UC MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 10.05$  nm and  $V_{BG-S} = 0.35$  V at various  $V_{BG-D}$  are shown in Figure 116. Standard transistor behavior can be observed; the relatively low currents (which range from 200  $\mu\text{A}/\mu\text{m}$  to 360  $\mu\text{A}/\mu\text{m}$ ) observed are due to the channel length: as shown in Section 7.3.2, even shorter channels are required for these UC devices to yield peak performance.

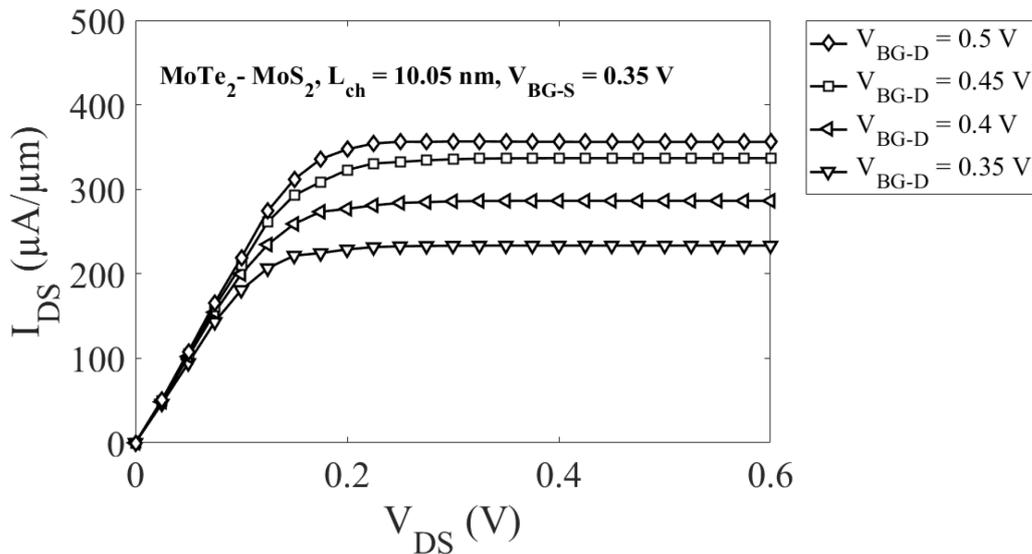


Figure 116.  $I_D$ - $V_{DS}$  characteristics for the UC MoTe<sub>2</sub>/MoS<sub>2</sub> device at  $L_{ch} = 10.05$  nm,  $V_{BG-S} = 0.35$  V and  $V_{BG-D}$  ranging from 0.35 V to 0.5 V; standard transistor behavior can be observed.

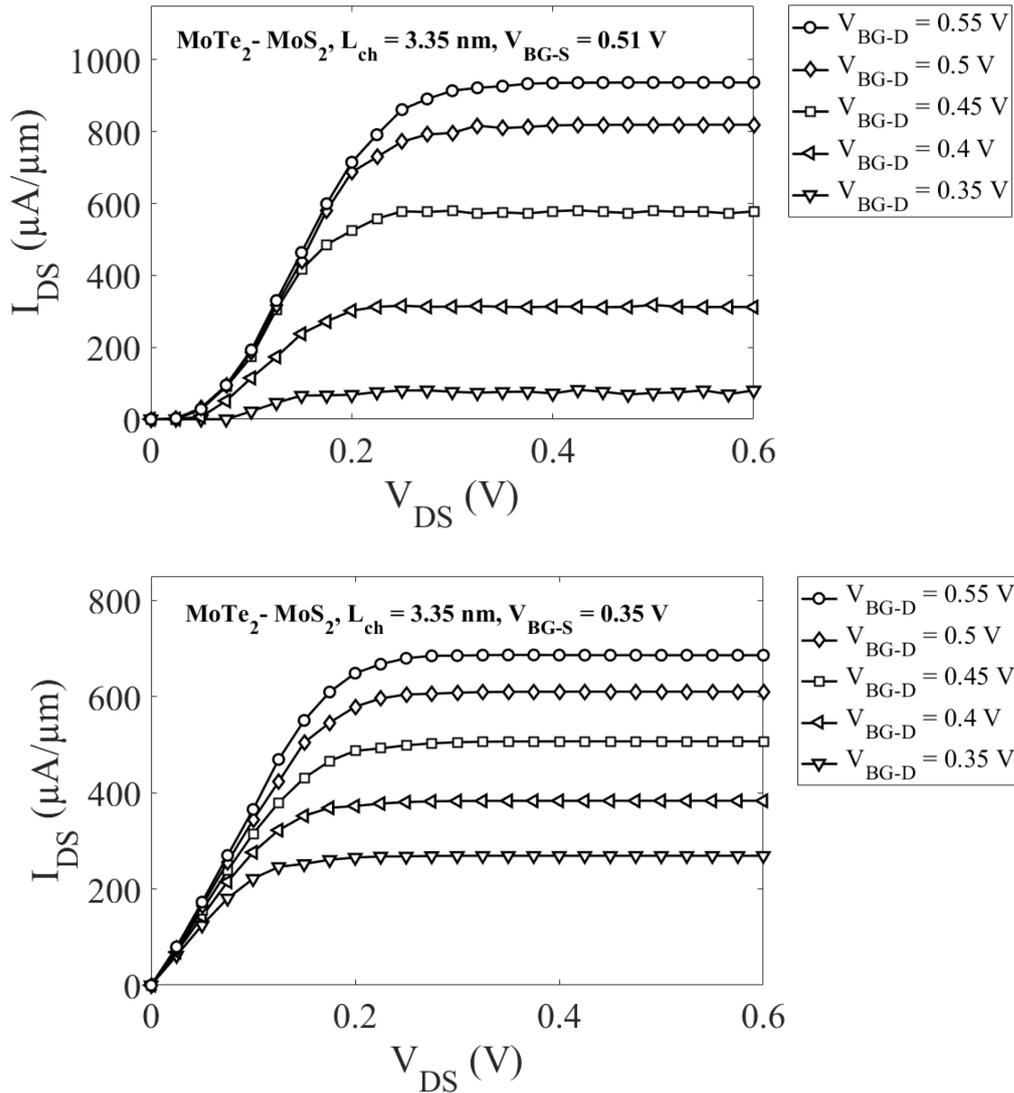


Figure 117.  $I_D$ - $V_{DS}$  characteristics for the UC  $\text{MoTe}_2/\text{MoS}_2$  device at  $L_{ch} = 3.35$  nm,  $V_{BG-D}$  ranging from 0.35 V to 0.5 V and (top)  $V_{BG-S} = 0.51$  V (bottom)  $V_{BG-S} = 0.35$  V.

$I_D$ - $V_{DS}$  characteristics for the UC  $\text{MoTe}_2/\text{MoS}_2$  device at a shorter channel length of 3.35 nm at  $V_{BG-S} = 0.35$  V as well as  $V_{BG-S} = 0.51$  V (the optimal source backgate voltage identified in Section 7.3.3) are shown in Figure 117.

As was the case for all previous transistors, standard transistor behavior can be observed at low  $V_{BG-S}$  while, at the optimal  $V_{BG-S}$ , a threshold  $V_{DS}$  (0.05 V in this case) has to be reached before current can be established. As explained in the previous chapters, at this source backgate voltage the drain CB is forced at higher energies than the source VB at very low  $V_{DS}$  which explains the absence of current. Much higher currents (up to 1000  $\mu\text{A}/\mu\text{m}$ ) are reached in these devices, thanks to their very short channel which favors performance in these UC devices. In all cases, the current saturates at  $V_{DS} \sim 0.225$  V, much like in the DBE and standard devices. Similar observations can be made about the  $\text{WTe}_2/\text{MoS}_2$  device, for which  $I_D$ - $V_{DS}$  characteristics are shown in Figure 118.

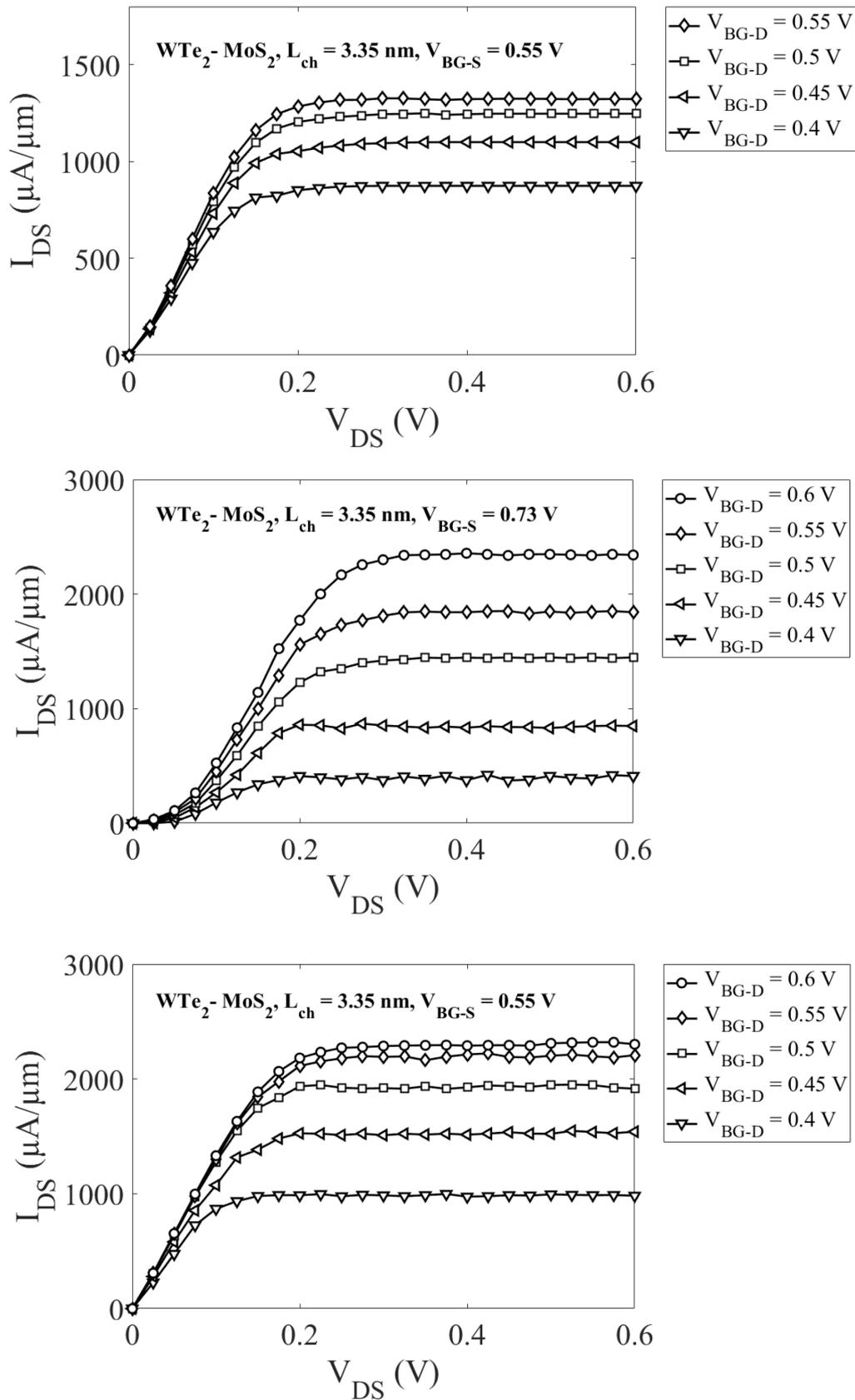


Figure 118.  $I_D$ - $V_{DS}$  characteristics for the UC  $WTe_2/MoS_2$  device at  $V_{BG-D}$  ranging from 0.35 V to 0.5 V and (top)  $L_{ch} = 10.05$  nm,  $V_{BG-S} = 0.55$  V, (middle)  $L_{ch} = 3.35$  nm,  $V_{BG-S} = 0.73$  V, (bottom)  $L_{ch} = 3.35$  nm,  $V_{BG-S} = 0.55$  V.

$I_D$ - $V_{BG-D}$  characteristics for both UC devices at  $V_{DS}$  ranging from 0.1 V to 0.7 V,  $L_{ch} = 3.35$  nm and the optimal source backgate voltage as identified for each device in Section 7.3.3 are shown in Figure 119.

Much like the standard and DBE TFETs presented previously, these UC devices are insensitive to DITL: threshold voltage is not impacted for supply voltages ranging from 0.1 V to 0.7 V, and behavior in both the OFF and ON state is unchanged for  $V_{DS}$  ranging from 0.3 V to 0.7 V.

As was the case in the previous devices, lower currents are observed at  $V_{DS} = 0.1$  V due to the source backgate voltage used: the  $V_{BG-S}$  identified as optimal to maximize ON current forces the source VB to energy levels higher than the drain CB at very low  $V_{DS}$  (a more detailed explanation is given in Section 5.3.5 and band profiles are shown in Figure 81).

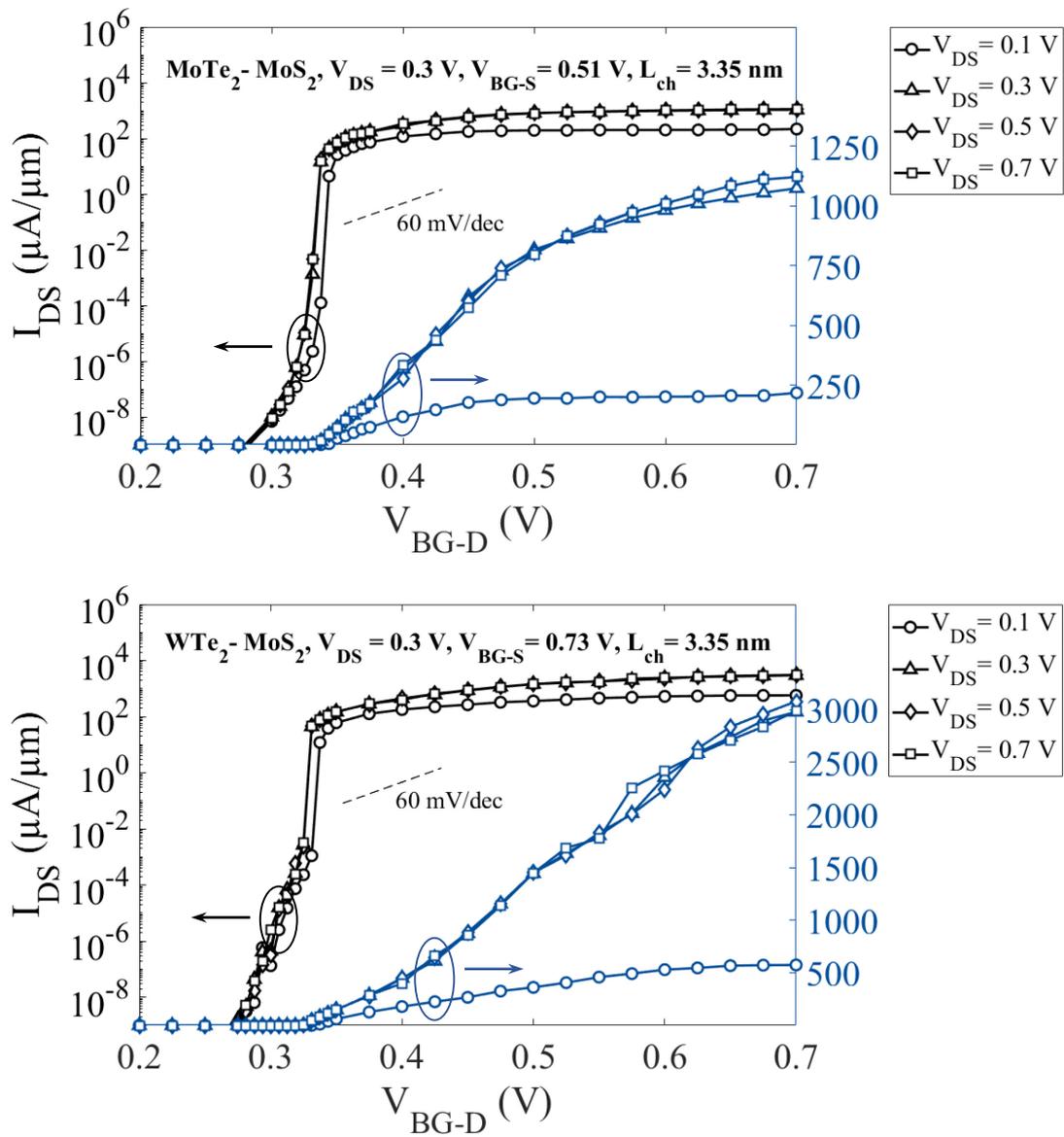


Figure 119.  $I_D$ - $V_{BG-D}$  characteristics of the UC  $\text{MoTe}_2/\text{MoS}_2$  and the  $\text{WTe}_2/\text{MoS}_2$  devices for  $L_{ch} = 3.35$  nm,  $V_{DS}$  ranging from 0.1 V to 0.7 V, and the optimal  $V_{BG-S}$  for each device.

## 7.4 Conclusion on ungated-channel in-plane heterojunction devices

The UC MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub> devices studied in this chapter share many of the traits exhibited in both the standard and especially the DBE devices studied in Chapters 5 and 6. They exhibit the following properties:

- **Device scaling strongly favors performance:**  $SS$  is unaffected by the channel length variation, and ON current strongly increases as the channel is shortened, yielding  $I_{ON}$  comparable to that of the DBE devices in very short channel devices.
- **Extremely low  $SS$ :** no matter the length of the channel and  $V_{BG-S}$  applied, the devices yield  $SS < 5$  mV/dec. As a result, a minuscule 0.0125 V increase in  $V_{BG-D}$  is enough for the device to transition from a fully OFF to fully ON state.
- **High ON/OFF ratio:** depending on the source backgate voltage applied to the device, ballistic ON currents of  $1.2 \times 10^3$  for the MoTe<sub>2</sub>/MoS<sub>2</sub> device and  $2.4 \times 10^3$  for the WTe<sub>2</sub>/MoS<sub>2</sub> device can be reached in the case of very short channels ( $< 5$  nm). Although  $I_{ON}$  decreases as channel length increases, promising ballistic ON/OFF ratios of  $7 \times 10^7$  are obtained for  $L_{ch} \sim 20$  nm in both devices.
- **Good saturation even at low  $V_{DS}$ :** both UC devices are shown to saturate at very low drain voltages ( $V_{DS} = 0.25$  V). Peak performance can therefore be reached at minimal supply voltage, which is promising for ultra-low power operation.
- **No top-gate is required to operate these devices,** which would facilitate and streamline the fabrication process.

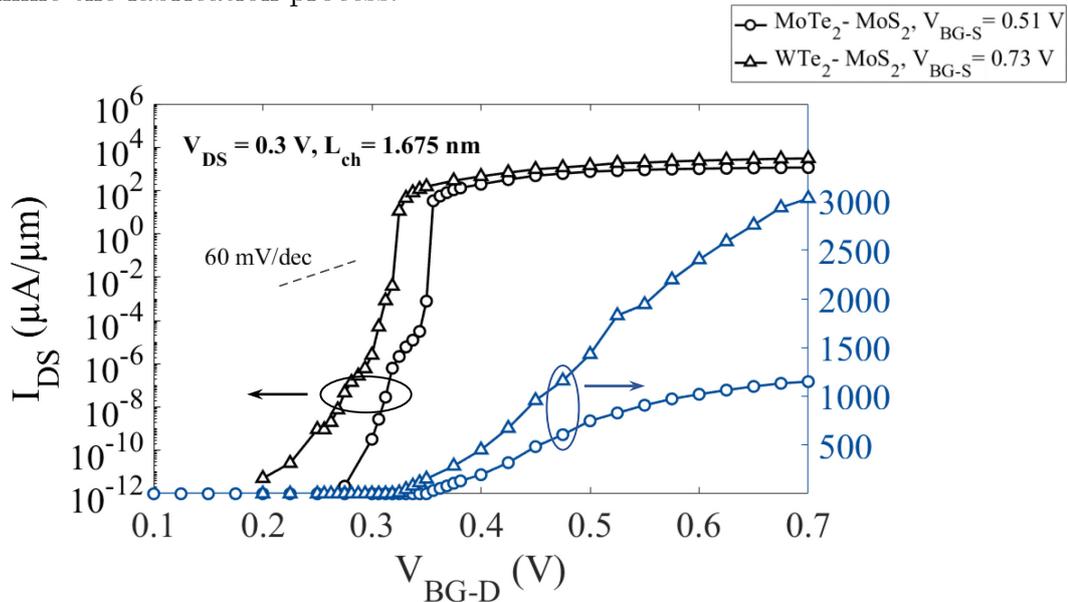


Figure 120.  $I_D$ - $V_G$  characteristics of the UC MoTe<sub>2</sub>/MoS<sub>2</sub> and the WTe<sub>2</sub>/MoS<sub>2</sub> devices for  $L_{ch} = 1.675$  nm,  $V_{DS} = 0.3$  V, and the optimal  $V_{BG-S}$  for each device.

# Chapter 8

## Summary and outlook

In this thesis, an in-depth study of in-plane heterojunctions of transition metal dichalcogenides and their potential for use in nanoelectronics (namely TFETs) was performed, and innovative device architectures taking advantage of the 2D nature of the considered materials were proposed.

Full quantum simulations showed that in the ballistic limit, the resulting devices yield high ON/OFF ratios ( $> 10^8$ ) and extremely low sub-threshold swings ( $< 5$  mV/dec) at low supply voltages ( $V_{DD} = 0.3$  V).

In Chapter 1 a quick outline of the history of the transistor was given, before an introduction on MOSFETs outlining its working principle as well as the limits of the scaling of traditional, silicon-based MOSFETs was presented. Indeed, due to their intrinsic working mechanism (thermionic injection over a potential barrier), the power supply cannot be reduced without deteriorating device performance; nonetheless, the resulting heat dissipated by the billions of transistors found in microprocessors today prevents further miniaturization and severely hampers the future prospects of Si-MOSFET technology, which has ruled over the market for over four decades. A detailed introduction on TFETs was then given: thanks to their reliance on band-to-band tunneling and the resulting low sub-threshold swings, these devices are identified by the ITRS as amongst the best candidates to solve the supply voltage scaling issue.

In Chapter 2, the other main facet of this thesis work was brought to light: ever since 2004 and the experimental isolation of graphene by Geim and Novoselov, scientific interest in graphene and other so-called 2D materials has soared. Motivated by the unheard-of electronic and mechanical properties of graphene, dozens of other one-atom (or few-atom) thick materials were discovered and studied, in the hopes of bringing about a 2D revolution that could extend to all aspects of technology. General information as well as a rundown of their electronic properties were given for the most prominent 2D materials, ranging from graphene to hBN, transition metal dichalcogenide monolayers (TMDs) or silicene, just to name a few. Potential applications spaces for these materials (in electronics, photonics, sensing ...) as well as the current state of 2D material synthesis were quickly presented, to provide a full picture of the research field.

In Chapter 3, the physical models used in this work were detailed, along with information about the computational techniques used to investigate electronic transport in TFETs. First, the tight-binding approach was broadly presented, before the TB model used to describe the properties of the considered TMDs, along with the changes made upon it so that it would fit our needs, were detailed. A short overview of non-equilibrium Green's function theory, its use in nanoelectronics and, more specifically, quantum transport simulation was then given. Finally, a detailed explanation of the implementation of these two approaches in the code used to model ballistic quantum transport in field-effect transistors was presented.

Finally, simulation results were highlighted and analyzed in Chapters 4 through 7.

In Chapter 4, a brief study of the potential (or rather lack thereof) of TMDs for use in MOSFET technology was performed, highlighting their high  $SS$  and low ON current. TFETs based on in-plane heterojunctions of strained TMDs were studied in Chapter 5, and the paramount importance of band alignment in these devices was shown. Out of all the studied heterojunctions, the two bearing a “broken-gap” configuration ( $\text{MoTe}_2/\text{MoS}_2$  and  $\text{WTe}_2/\text{MoS}_2$ ) were shown to yield vastly superior performance (lower  $SS$  and higher  $I_{ON}$ ) than the others. An in-depth study of these devices was then performed to identify the influence of design parameters such as contact length, channel length, as well as the voltages applied to the source and drain backgates (used instead of the traditional chemical doping, thanks to the 2D nature of the materials used). Namely, channel lengths beyond 20 nm were identified as a requirement to obtain peak performance from these devices. By optimizing the aforementioned parameters, these TFETs were shown to yield ballistic  $SS$  as low as 3 mV/dec and ballistic  $I_{ON}$  in excess of  $10^3 \mu\text{A}/\mu\text{m}$  at a low supply voltage  $V_{DD} = 0.3 \text{ V}$ .

Chapter 6 introduced DBE-TFETs: a device architecture derived from the classic TFET design studied in the previous chapter, based on observations made when studying the influence of the drain backgate voltage. By applying the same voltage to the drain backgate and the top-gate, the efficiency of the device was strongly improved, and all limits to channel scaling were removed: peak performance was shown to be achieved in devices with channels as short as 1.675 nm. A study of the impact of design parameters was also performed, as to identify prime conditions to operate the DBE-TFETs.

In Chapter 7 another innovative device design was introduced, the UC-TFET. In this device, the top-gate was completely removed, and the drain backgate (which determines the potential in the drain) was used to control current flow in the device. Foregoing the top-gate would be a strong advantage from a technological standpoint, as the manufacturing process could be streamlined and simplified. The influence of design parameters on the performance of the UC devices was analyzed, and similarly outstanding ballistic performance was reported ( $SS < 5 \text{ mV/dec}$  and  $I_{ON} > 10^3 \mu\text{A}/\mu\text{m}$ ), especially in the case of short channels ( $< 7 \text{ nm}$ ).

Some work remains, however: in these devices, strain is applied to the entirety of the material, including the contacts. A more accurate approach would be to model the gradual relaxation of the strain as the distance from the interface increases, and to consider pristine contacts.

From a simulation and computation standpoint, this is hardly feasible: considering a strain relaxation pattern similar to that observed in experimental works (see Section 3.3.3) would entail several key points:

- Dramatically increase the device length: as shown in Figure 50, a relatively small strain of 1.2% requires several hundreds of nanometers for the material to recover its pristine condition. The strong 5% strains applied in our case would therefore require device lengths well in the  $\mu\text{m}$  range to allow for the recovery of pristine behavior in the left and right semi-infinite contacts (as categorized in the NEGF method). The models and methods used in this work are in no way meant to be used to simulate such a high number of atoms, and the computational cost would therefore skyrocket.
- Consider a near-infinite amount of Hamiltonians to describe the TMDs: if such a strain relaxation pattern is to be adopted, the layer Hamiltonians and coupling Hamiltonians between successive layers would depend on their distance to the interface. For the sake of argument, let us assume a device length of  $2\ \mu\text{m}$  (one micron from each side of the interface, which is very conservative considering the data shown in Figure 50): in which the average distance between consecutive layers is  $3.36\ \text{\AA}$ : a total number of  $2000/0.336 \sim 6000$  unique layer Hamiltonians (and as many coupling Hamiltonians) would be necessary to model the system. Once again, this is simply not feasible from a computational standpoint.

While not totally accurate, the uniform strain patterns considered in this work allowed me to study these in-plane TMD heterojunctions and highlight their potential for TFET operation.

Similarly, the electron-phonon interaction was not taken into account in this work, and the ballistic results obtained therefore represent the best case scenario for each device. Both figures of merit ( $SS$  and  $I_{ON}$ ) are expected to be negatively impacted by phonon scattering mechanisms to various degrees, as shown in [109], [466], [467].

$SS$  is expected to be increased no matter the channel length, due to phonon absorption mechanisms active in the source region in the OFF-state regime and promoting inelastic tunneling of carriers from the valence to the conduction band.

Considering the mean-free-paths reported for  $\text{MoS}_2$  [461],  $I_{ON}$  would mainly be impacted in the devices bearing channel lengths beyond  $20\ \text{nm}$ , and a compromise would therefore be necessary to maximize the performance of the standard TFETs.

In the case of both the DBE and UC-TFETs however,  $I_{ON}$  is at its peak when the channel is kept extremely short; as a result, peak ON current is not expected to be meaningfully impacted by phonon scattering.

As a final highlight of the promising potential of in-plane TMD heterojunctions for use in ultra-low power operation TFETs, the highest performances observed for all devices (at  $V_{DS} = V_{DD} = 0.3$  V and with channel lengths ranging from 5 nm to 27 nm) are shown in Table 3.

|                                     |          | $L_{ch}$<br>(nm) | $SS$<br>(mV/dec) | $I_{ON}$<br>( $\mu\text{A}/\mu\text{m}$ ) | $ON/OFF$            | Impact of<br>$L_{ch}$ increase  |
|-------------------------------------|----------|------------------|------------------|---|---------------------|---|
| MoTe <sub>2</sub> -MoS <sub>2</sub> | standard | 5.025            | 73               | 0.153                                     | $1.53 \times 10^4$  |    |
|                                     |          | 13.4             | 10               | 923                                       | $9.23 \times 10^7$  |   |
|                                     |          | 26.8             | 5                | 970                                       | $9.7 \times 10^7$   |   |
|                                     | DBE      | 5.025            | 3                | 1119                                      | $1.119 \times 10^8$ |    |
|                                     |          | 13.4             | 2                | 1115                                      | $1.115 \times 10^8$ |   |
|                                     |          | 26.8             | 4                | 1105                                      | $1.105 \times 10^8$ |   |
|                                     | UC       | 5.025            | 3                | 907                                       | $9.07 \times 10^7$  |  |
|                                     |          | 13.4             | 3                | 693                                       | $6.93 \times 10^7$  |   |
|                                     |          | 26.8             | 2                | 397                                       | $3.97 \times 10^7$  |   |
| WTe <sub>2</sub> -MoS <sub>2</sub>  | standard | 5.025            | 60               | 97  | $9.7 \times 10^6$   |  |
|                                     |          | 13.4             | 25               | 1344                                      | $1.344 \times 10^8$ |   |
|                                     |          | 26.8             | 4                | 1918                                      | $1.918 \times 10^8$ |   |
|                                     | DBE      | 5.025            | 4                | 2550                                      | $2.550 \times 10^8$ |  |
|                                     |          | 13.4             | 3                | 2512                                      | $2.512 \times 10^8$ |   |
|                                     |          | 26.8             | 3                | 2531                                      | $2.532 \times 10^8$ |   |
|                                     | UC       | 5.025            | 3                | 2516                                      | $2.516 \times 10^8$ |  |
|                                     |          | 13.4             | 2                | 1239                                      | $1.239 \times 10^8$ |   |
|                                     |          | 26.8             | 2                | 586                                       | $5.86 \times 10^7$  |   |

Table 3. Highest performance ( $SS$ ,  $I_{ON}$  and  $ON/OFF$ ) observed for all TFETs studied in this thesis, at  $V_{DS} = V_{DD} = 0.3$  V and channel lengths ranging from 5 nm to 27 nm.

# Appendix A – TB parameters

|                  | <b>MoS<sub>2</sub></b> |                |                |                | <b>MoSe<sub>2</sub></b> |                |                |                | <b>WS<sub>2</sub></b> |                |                |                |
|------------------|------------------------|----------------|----------------|----------------|-------------------------|----------------|----------------|----------------|-----------------------|----------------|----------------|----------------|
|                  | $H_{AA}^{(0)}$         | $H_{BB}^{(0)}$ | $H_{CC}^{(0)}$ | $H_{DD}^{(0)}$ | $H_{AA}^{(0)}$          | $H_{BB}^{(0)}$ | $H_{CC}^{(0)}$ | $H_{DD}^{(0)}$ | $H_{AA}^{(0)}$        | $H_{BB}^{(0)}$ | $H_{CC}^{(0)}$ | $H_{DD}^{(0)}$ |
| $\epsilon_0$     | ----                   | -6.720         | -6.082         | -8.839         | ----                    | -5.986         | -5.559         | -8.231         | ----                  | -6.838         | -5.734         | -9.078         |
| $\epsilon_1$     | -4.873                 | -7.235         | -5.856         | -7.850         | -4.547                  | -6.502         | -5.314         | -7.110         | -4.327                | -7.250         | -5.498         | -8.033         |
| $\alpha_0^{(0)}$ | ----                   | 1.623          | -1.021         | -0.858         | ----                    | 1.396          | -1.090         | -0.742         | ----                  | 1.743          | -1.212         | 0.158          |
| $\alpha_1^{(0)}$ | -2.498                 | -1.500         | -1.817         | -3.317         | -2.498                  | -1.440         | -2.023         | -3.316         | -2.631                | -1.854         | -1.916         | -4.290         |
| $\beta_0^{(0)}$  | -0.890                 | -0.094         | -0.370         | -1.142         | -0.890                  | -0.121         | -0.296         | -1.146         | -0.986                | 0.089          | -0.292         | -1.390         |
| $\beta_1^{(0)}$  | ----                   | 0.273          | -0.043         | 0.720          | ----                    | 0.270          | 0.004          | 0.829          | ----                  | 0.487          | 0.036          | 1.586          |

|                  | <b>WSe<sub>2</sub></b> |                |                |                | <b>MoTe<sub>2</sub></b> |                |                |                | <b>WTe<sub>2</sub></b> |                |                |                |
|------------------|------------------------|----------------|----------------|----------------|-------------------------|----------------|----------------|----------------|------------------------|----------------|----------------|----------------|
|                  | $H_{AA}^{(0)}$         | $H_{BB}^{(0)}$ | $H_{CC}^{(0)}$ | $H_{DD}^{(0)}$ | $H_{AA}^{(0)}$          | $H_{BB}^{(0)}$ | $H_{CC}^{(0)}$ | $H_{DD}^{(0)}$ | $H_{AA}^{(0)}$         | $H_{BB}^{(0)}$ | $H_{CC}^{(0)}$ | $H_{DD}^{(0)}$ |
| $\epsilon_0$     | ----                   | -6.066         | -5.267         | -8.466         | ----                    | -5.264         | -5.250         | -7.601         | ----                   | -5.305         | -5.052         | -7.786         |
| $\epsilon_1$     | -4.069                 | -6.494         | -5.001         | -7.277         | -4.339                  | -5.807         | -4.945         | -6.390         | -3.969                 | -5.789         | -4.716         | -6.566         |
| $\alpha_0^{(0)}$ | ----                   | 1.385          | -1.012         | -0.050         | ----                    | -1.685         | -0.835         | -0.182         | ----                   | 1.695          | -0.819         | 0.696          |
| $\alpha_1^{(0)}$ | -2.357                 | -1.724         | -1.967         | -4.138         | -1.820                  | -1.235         | -2.061         | -3.463         | -1.795                 | -1.536         | -2.022         | -4.519         |
| $\beta_0^{(0)}$  | -0.902                 | 0.059          | -0.220         | -1.337         | -0.829                  | -0.250         | -0.232         | -1.267         | -0.935                 | -0.078         | -0.126         | -1.482         |
| $\beta_1^{(0)}$  | ----                   | 0.482          | -0.022         | 1.507          | ----                    | 0.333          | 0.063          | 0.954          | ----                   | 0.556          | 0.043          | 1.576          |

Table 4. TB parameters necessary to build the  $H_{JJ}^{(0)}$  Hamiltonians for all six TMDs

|                  | MoS <sub>2</sub> |                |                | MoSe <sub>2</sub> |                |                | WS <sub>2</sub> |                |                |
|------------------|------------------|----------------|----------------|-------------------|----------------|----------------|-----------------|----------------|----------------|
|                  | $H_{BA}^{(1)}$   | $H_{DC}^{(1)}$ | $H_{DC}^{(3)}$ | $H_{BA}^{(1)}$    | $H_{DC}^{(1)}$ | $H_{DC}^{(3)}$ | $H_{BA}^{(1)}$  | $H_{DC}^{(1)}$ | $H_{DC}^{(3)}$ |
| $t_0^{(n)}$      | -0.789           | 1.411          | 0.014          | -0.695            | 1.268          | 0.017          | -0.884          | 1.558          | 0.010          |
| $t_1^{(n)}$      | 2.158            | 0.652          | -0.245         | 1.941             | 0.554          | -0.215         | 2.302           | 0.664          | -0.273         |
| $t_2^{(n)}$      | ----             | -0.940         | -0.150         | ----              | -0.874         | -0.155         | ----            | -0.993         | -0.154         |
| $t_3^{(n)}$      | -1.379           | -0.954         | -0.221         | -1.326            | -0.858         | -0.223         | -1.436          | -0.943         | -0.265         |
| $t_4^{(n)}$      | ----             | -0.883         | -0.069         | ----              | -0.772         | -0.069         | ----            | -1.005         | -0.066         |
| $\alpha_0^{(n)}$ | 0.545            | -0.486         | 0.173          | 0.408             | -0.407         | 0.175          | 0.585           | -0.609         | 0.537          |
| $\alpha_1^{(n)}$ | -0.605           | 0.843          | 0.204          | -0.417            | 0.825          | 0.185          | -0.482          | 1.045          | 0.185          |
| $\alpha_2^{(n)}$ | ----             | 2.178          | 0.567          | ----              | 1.928          | 0.554          | ----            | 2.827          | 0.623          |
| $\alpha_3^{(n)}$ | 1.845            | 0.446          | 0.744          | 1.718             | 0.272          | 0.760          | 1.826           | 0.071          | 1.055          |
| $\alpha_4^{(n)}$ | ----             | -0.208         | 0.035          | ----              | -0.298         | 0.062          | ----            | -0.241         | -0.090         |
| $\beta_0^{(n)}$  | -1.076           | 1.724          | -0.178         | -0.897            | 1.530          | -0.164         | -1.128          | 2.402          | -0.345         |
| $\beta_1^{(n)}$  | 0.401            | -0.353         | -1.069         | 0.264             | -0.367         | -0.995         | 0.140           | -0.900         | -1.110         |
| $\beta_2^{(n)}$  | ----             | -2.204         | -0.070         | ----              | -1.995         | -0.093         | ----            | -2.293         | -0.125         |
| $\beta_3^{(n)}$  | -2.100           | -0.682         | -0.267         | -1.874            | -0.510         | -0.292         | -1.990          | -0.306         | -0.120         |
| $\beta_4^{(n)}$  | ----             | -0.850         | -0.281         | ----              | -0.727         | -0.290         | ----            | -1.184         | -0.536         |
| $\beta_5^{(n)}$  | 0.859            | 0.899          | -0.690         | 0.770             | 0.761          | -0.664         | 0.915           | 0.902          | -1.093         |
| $\beta_6^{(n)}$  | ----             | -0.542         | -0.382         | ----              | -0.475         | -0.391         | ----            | -0.193         | -0.644         |
| $\beta_7^{(n)}$  | -0.377           | -2.093         | -0.340         | -0.469            | -1.841         | -0.299         | -0.634          | -2.934         | -0.535         |
| $\beta_8^{(n)}$  | -0.836           | 1.101          | 0.015          | -0.717            | 1.005          | 0.007          | -0.944          | 1.427          | -0.127         |

Table 5. TB parameters necessary to build the  $H_{IJ}^{(n)}$  Hamiltonians for MoS<sub>2</sub>, MoSe<sub>2</sub> and WS<sub>2</sub>

|                  | <b>WSe<sub>2</sub></b> |                |                | <b>MoTe<sub>2</sub></b> |                |                | <b>WTe<sub>2</sub></b> |                |                |
|------------------|------------------------|----------------|----------------|-------------------------|----------------|----------------|------------------------|----------------|----------------|
|                  | $H_{BA}^{(1)}$         | $H_{DC}^{(1)}$ | $H_{DC}^{(3)}$ | $H_{BA}^{(1)}$          | $H_{DC}^{(1)}$ | $H_{DC}^{(3)}$ | $H_{BA}^{(1)}$         | $H_{DC}^{(1)}$ | $H_{DC}^{(3)}$ |
| $t_0^{(n)}$      | -0.773                 | 1.399          | 0.017          | -0.557                  | 1.117          | 0.038          | -0.617                 | 1.221          | 0.053          |
| $t_1^{(n)}$      | 2.079                  | 0.567          | -0.242         | 1.690                   | 0.461          | -0.194         | 1.813                  | 0.480          | -0.218         |
| $t_2^{(n)}$      | ----                   | -0.905         | -0.161         | ----                    | -0.798         | -0.144         | ----                   | -0.798         | -0.142         |
| $t_3^{(n)}$      | -1.401                 | -0.853         | -0.263         | -1.197                  | -0.678         | -0.204         | -1.263                 | -0.673         | -0.225         |
| $t_4^{(n)}$      | ----                   | -0.896         | -0.068         | ----                    | -0.652         | -0.050         | ----                   | -0.772         | -0.045         |
| $\alpha_0^{(n)}$ | 0.406                  | -0.493         | 0.468          | 0.260                   | -0.364         | 0.217          | 0.286                  | -0.545         | 0.629          |
| $\alpha_1^{(n)}$ | -0.322                 | 0.917          | 0.202          | -0.275                  | 0.813          | 0.199          | -0.202                 | 0.903          | 0.276          |
| $\alpha_2^{(n)}$ | ----                   | 2.409          | 0.653          | ----                    | 1.850          | 0.545          | ----                   | 2.643          | 0.654          |
| $\alpha_3^{(n)}$ | 1.764                  | 0.022          | 1.050          | 1.309                   | -0.017         | 0.791          | 1.309                  | -0.393         | 1.123          |
| $\alpha_4^{(n)}$ | ----                   | -0.238         | -0.021         | ----                    | -0.438         | 0.021          | ----                   | -0.456         | -0.107         |
| $\beta_0^{(n)}$  | -0.929                 | 1.973          | -0.321         | -0.644                  | 1.435          | -0.125         | -0.665                 | 1.828          | -0.278         |
| $\beta_1^{(n)}$  | -0.029                 | -0.877         | -1.094         | 0.106                   | -0.372         | -0.985         | -0.121                 | -0.818         | -1.079         |
| $\beta_2^{(n)}$  | ----                   | -2.153         | -0.114         | ----                    | -1.711         | -0.113         | ----                   | -1.812         | -0.180         |
| $\beta_3^{(n)}$  | -1.879                 | -0.276         | -0.241         | -1.534                  | -0.337         | -0.219         | -1.4841                | -0.048         | -0.160         |
| $\beta_4^{(n)}$  | ----                   | -0.897         | -0.476         | ----                    | -0.668         | -0.297         | ----                   | -0.824         | -0.544         |
| $\beta_5^{(n)}$  | 0.798                  | 0.761          | -1.022         | 0.482                   | 0.633          | -0.663         | 0.461                  | 0.593          | -0.997         |
| $\beta_6^{(n)}$  | ----                   | -0.300         | -0.651         | ----                    | -0.403         | -0.425         | ----                   | -0.150         | -0.726         |
| $\beta_7^{(n)}$  | -0.690                 | -2.447         | -0.423         | -0.728                  | -1.753         | -0.330         | -1.001                 | -2.304         | -0.430         |
| $\beta_8^{(n)}$  | -0.793                 | 1.082          | -0.058         | -0.588                  | -0.877         | 0.018          | -0.577                 | 0.941          | 0.012          |

Table 6. TB parameters necessary to build the  $H_{IJ}^{(n)}$  Hamiltonians for WSe<sub>2</sub>, MoTe<sub>2</sub> and WTe<sub>2</sub>

|                  | MoS <sub>2</sub> |                |                |                | MoSe <sub>2</sub> |                |                |                | WS <sub>2</sub> |                |                |                |
|------------------|------------------|----------------|----------------|----------------|-------------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
|                  | $H_{AA}^{(2)}$   | $H_{BB}^{(2)}$ | $H_{CC}^{(2)}$ | $H_{DD}^{(2)}$ | $H_{AA}^{(2)}$    | $H_{BB}^{(2)}$ | $H_{CC}^{(2)}$ | $H_{DD}^{(2)}$ | $H_{AA}^{(2)}$  | $H_{BB}^{(2)}$ | $H_{CC}^{(2)}$ | $H_{DD}^{(2)}$ |
| $t_0^{(2)}$      | -0.206           | 0.865          | 0.275          | 0.912          | -0.146            | 0.964          | 0.251          | 0.991          | -0.198          | 0.873          | 0.355          | 0.965          |
| $t_1^{(2)}$      | 0.031            | -0.187         | -0.558         | 0.006          | 0.017             | -0.172         | -0.473         | -0.004         | 0.027           | -0.218         | -0.691         | 0.014          |
| $t_2^{(2)}$      | ----             | -0.174         | -0.298         | -0.192         | ----              | -0.211         | -0.264         | -0.217         | ----            | -0.175         | -0.371         | -0.212         |
| $t_3^{(2)}$      | -0.257           | -0.070         | -0.249         | -0.038         | -0.810            | -0.068         | -0.201         | -0.039         | -0.310          | -0.099         | -0.304         | -0.101         |
| $t_4^{(2)}$      | ----             | 0.100          | 0.114          | -0.106         | ----              | 0.076          | 0.096          | -0.121         | ----            | 0.110          | 0.145          | -0.163         |
| $t_5^{(2)}$      | ----             | -0.068         | 0.410          | 0.008          | ----              | -0.074         | 0.352          | 0.005          | ----            | -0.082         | 0.488          | -0.031         |
| $\alpha_0^{(2)}$ | -0.258           | -1.841         | -1.027         | -1.425         | -0.309            | -1.979         | -0.951         | -1.586         | -0.453          | -1.844         | -1.232         | -1.122         |
| $\alpha_1^{(2)}$ | -0.202           | -0.027         | 1.544          | -0.057         | -0.125            | -0.103         | 1.333          | -0.072         | -0.213          | -0.067         | 1.947          | -0.162         |
| $\alpha_2^{(2)}$ | ----             | 0.444          | 1.032          | 0.644          | ----              | 0.536          | 0.885          | 0.668          | ----            | 0.434          | 1.123          | 0.674          |
| $\alpha_3^{(2)}$ | 0.705            | -0.045         | 0.206          | -0.170         | 0.514             | -0.059         | 0.195          | -0.162         | 0.834           | -0.042         | 0.462          | -0.314         |
| $\alpha_4^{(2)}$ | ----             | -0.210         | 0.285          | -0.199         | ----              | -0.123         | 0.236          | -0.202         | ----            | -0.208         | 0.365          | -0.333         |
| $\alpha_5^{(2)}$ | ----             | 0.141          | -0.738         | 0.065          | ----              | 0.142          | -0.596         | 0.050          | ----            | 0.177          | -0.654         | 0.105          |
| $\beta_0^{(2)}$  | -0.676           | -2.203         | -0.910         | -2.013         | -0.588            | -2.378         | -0.793         | -2.180         | -0.942          | -2.254         | -1.068         | -1.920         |
| $\beta_1^{(2)}$  | -0.192           | 0.768          | 1.337          | 0.828          | -0.118            | 0.827          | 1.108          | 0.884          | -0.175          | 0.772          | 1.240          | 1.039          |
| $\beta_2^{(2)}$  | ----             | 0.350          | 0.376          | 0.540          | ----              | 0.445          | 0.333          | 0.576          | ----            | 0.283          | 0.522          | -0.580         |
| $\beta_3^{(2)}$  | 0.555            | -0.065         | -0.003         | 0.143          | 0.416             | -0.016         | 0.008          | 0.155          | 0.649           | -0.054         | -0.083         | 0.345          |
| $\beta_4^{(2)}$  | ----             | -0.208         | 0.188          | -0.056         | ----              | -0.146         | 0.126          | -0.026         | ----            | -0.198         | 0.179          | 0.062          |
| $\beta_5^{(2)}$  | ----             | 0.096          | -0.779         | 0.082          | ----              | 0.112          | -0.667         | 0.073          | ----            | 0.127          | -0.863         | 0.130          |
| $\beta_6^{(2)}$  | -0.095           | 0.482          | -0.634         | 0.744          | -0.063            | 0.567          | -0.565         | 0.777          | -0.076          | 0.467          | -0.960         | 0.858          |
| $\beta_7^{(2)}$  | ----             | -0.146         | 0.288          | 0.051          | ----              | -0.128         | 0.255          | 0.066          | ----            | -0.128         | 0.484          | 0.146          |
| $\beta_8^{(2)}$  | ----             | -0.089         | -0.152         | -0.099         | ----              | -0.092         | -0.110         | -0.127         | ----            | -0.117         | -0.046         | -0.236         |

Table 7. TB parameters necessary to build the  $H_{JJ}^{(2)}$  Hamiltonians for MoS<sub>2</sub>, MoSe<sub>2</sub> and WS<sub>2</sub>

|                  | <b>WSe<sub>2</sub></b> |                |                |                | <b>MoTe<sub>2</sub></b> |                |                |                | <b>WTe<sub>2</sub></b> |                |                |                |
|------------------|------------------------|----------------|----------------|----------------|-------------------------|----------------|----------------|----------------|------------------------|----------------|----------------|----------------|
|                  | $H_{AA}^{(2)}$         | $H_{BB}^{(2)}$ | $H_{CC}^{(2)}$ | $H_{DD}^{(2)}$ | $H_{AA}^{(2)}$          | $H_{BB}^{(2)}$ | $H_{CC}^{(2)}$ | $H_{DD}^{(2)}$ | $H_{AA}^{(2)}$         | $H_{BB}^{(2)}$ | $H_{CC}^{(2)}$ | $H_{DD}^{(2)}$ |
| $t_0^{(2)}$      | -0.137                 | 0.977          | 0.320          | 1.047          | -0.156                  | -1.071         | 0.205          | 1.063          | -0.158                 | 1.079          | 0.255          | 1.112          |
| $t_1^{(2)}$      | 0.013                  | -0.198         | -0.584         | 0.003          | 0.018                   | -0.111         | -0.372         | 0.038          | 0.015                  | -0.130         | -0.447         | 0.049          |
| $t_2^{(2)}$      | ----                   | -0.217         | -0.333         | -0.241         | ----                    | -0.251         | -0.214         | -0.232         | ----                   | -0.258         | -0.270         | -0.252         |
| $t_3^{(2)}$      | -0.232                 | -0.092         | -0.245         | -0.102         | -0.167                  | -0.056         | -0.163         | -0.044         | -0.198                 | -0.073         | -0.189         | -0.111         |
| $t_4^{(2)}$      | ----                   | 0.079          | 0.124          | -0.185         | ----                    | -0.045         | 0.071          | -0.092         | ----                   | -0.045         | 0.094          | -0.155         |
| $t_5^{(2)}$      | ----                   | -0.091         | 0.423          | -0.038         | ----                    | -0.077         | 0.283          | -0.007         | ----                   | -0.095         | 0.339          | -0.056         |
| $\alpha_0^{(2)}$ | -0.490                 | -1.986         | -1.127         | -1.357         | -0.262                  | -2.085         | -0.797         | -1.680         | -0.414                 | -2.068         | -0.897         | -1.367         |
| $\alpha_1^{(2)}$ | -0.117                 | -0.152         | 1.617          | -0.159         | -0.056                  | -0.320         | 1.102          | -0.251         | -0.034                 | -0.372         | 1.353          | -0.387         |
| $\alpha_2^{(2)}$ | ----                   | 0.557          | 1.013          | 0.718          | ----                    | 0.608          | 0.650          | 0.709          | ----                   | 0.621          | 0.665          | 0.777          |
| $\alpha_3^{(2)}$ | 0.589                  | -0.074         | 0.325          | -0.303         | 0.405                   | -0.069         | 0.204          | -0.195         | 0.458                  | -0.086         | 0.327          | -0.399         |
| $\alpha_4^{(2)}$ | ----                   | -0.105         | 0.291          | -0.287         | ----                    | -0.068         | 0.216          | -0.278         | ----                   | -0.049         | 0.264          | -0.392         |
| $\alpha_5^{(2)}$ | ----                   | 0.188          | -0.564         | 0.112          | ----                    | 0.148          | -0.402         | 0.067          | ----                   | 0.202          | -0.340         | 0.157          |
| $\beta_0^{(2)}$  | -0.809                 | -2.427         | -0.966         | -2.086         | -0.403                  | -2.633         | -0.606         | -2.405         | -0.556                 | -2.658         | -0.757         | -2.281         |
| $\beta_1^{(2)}$  | -0.090                 | 0.834          | 1.179          | 1.069          | -0.069                  | 0.976          | 0.870          | 1.037          | -0.005                 | 0.983          | 0.879          | 1.244          |
| $\beta_2^{(2)}$  | ----                   | 0.401          | 0.406          | 0.556          | ----                    | 0.564          | 0.243          | 0.609          | ----                   | 0.540          | 0.364          | 0.548          |
| $\beta_3^{(2)}$  | 0.480                  | 0.015          | -0.044         | 0.331          | 0.278                   | 0.013          | -0.015         | 0.176          | -0.319                 | 0.034          | -0.064         | 0.351          |
| $\beta_4^{(2)}$  | ----                   | -0.104         | 0.129          | 0.063          | ----                    | -0.027         | 0.129          | -0.099         | ----                   | 0.035          | 0.089          | -0.043         |
| $\beta_5^{(2)}$  | ----                   | 0.152          | -0.727         | 0.112          | ----                    | 0.118          | -0.524         | 0.077          | ----                   | 0.161          | -0.614         | 0.117          |
| $\beta_6^{(2)}$  | -0.037                 | 0.550          | -0.776         | 0.873          | -0.036                  | 0.677          | -0.436         | 0.850          | -0.013                 | 0.670          | -0.607         | 0.928          |
| $\beta_7^{(2)}$  | ----                   | -0.157         | 0.308          | 0.109          | ----                    | -0.112         | 0.174          | 0.108          | ----                   | -0.119         | 0.266          | 0.184          |
| $\beta_8^{(2)}$  | ----                   | -0.129         | -0.099         | -0.224         | ----                    | -0.101         | -0.071         | -0.141         | ----                   | -0.131         | -0.015         | -0.251         |

Table 8. TB parameters necessary to build the  $H_{JJ}^{(2)}$  Hamiltonians for WSe<sub>2</sub>, MoTe<sub>2</sub> and WTe<sub>2</sub>



# Appendix B – Band folding

In this Appendix, the band folding resulting in the doubling of the unit cell along the  $k_x$  direction will be highlighted for all six TMDs. The bandstructures of all six TMDs at  $k_y = 0$  and  $k_x$  ranging from  $-\frac{2\pi}{a}$  to  $\frac{2\pi}{a}$  are shown in Figure 121 and Figure 122.

The bands resulting from the base unit cell and the corresponding  $11 \times 11$  Hamiltonians are shown as red circles, while the bands obtained in the expanded unit cell and the corresponding  $22 \times 22$  Hamiltonians are shown as blue lines.

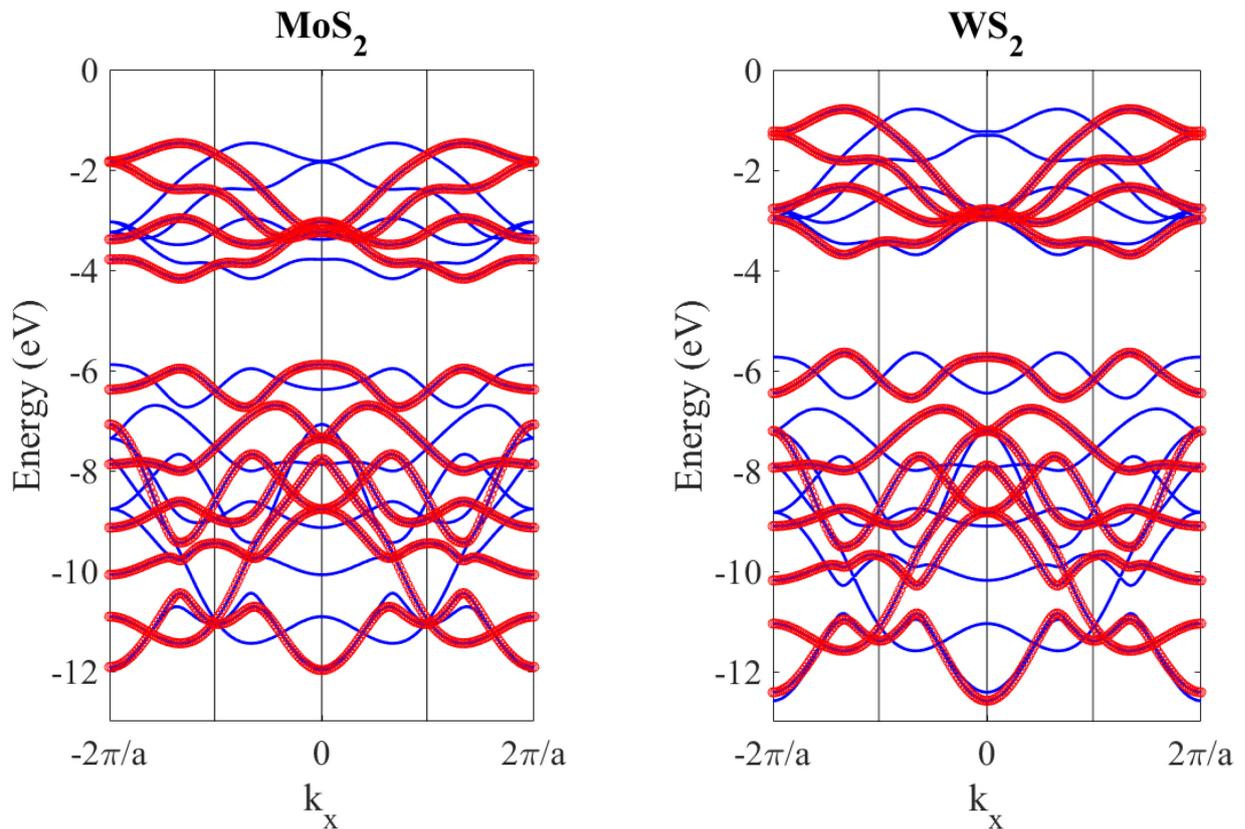


Figure 121. Bandstructure of  $\text{MoS}_2$  and  $\text{WS}_2$  at  $k_y = 0$  and  $k_x$  ranging from  $-\frac{2\pi}{a}$  to  $\frac{2\pi}{a}$  as obtained with the original  $11 \times 11$  Hamiltonians (red circles) and the  $22 \times 22$  Hamiltonians resulting from the expanded unit cell (blue lines), highlighting the band folding induced by the basis modification.

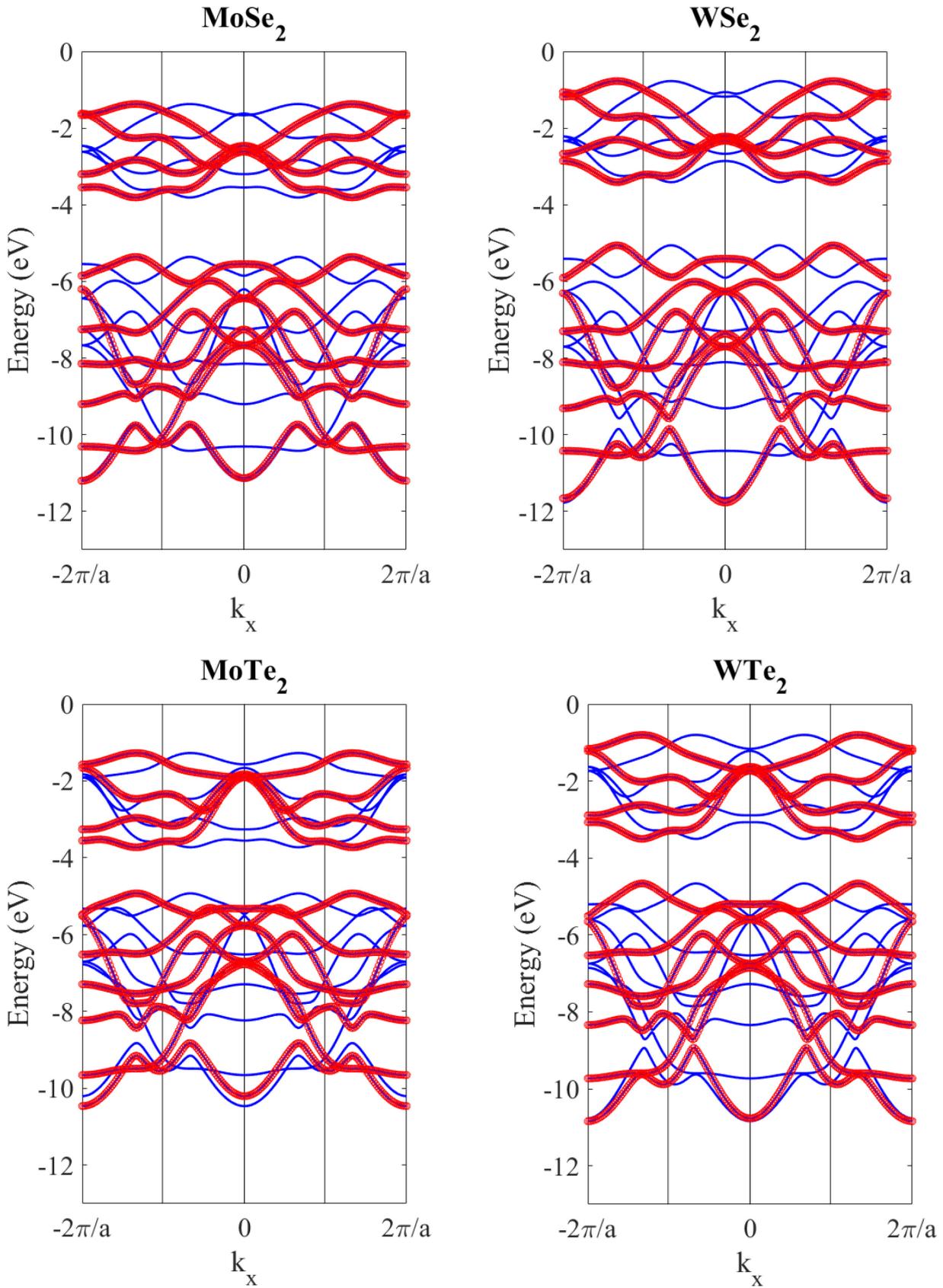


Figure 122. Bandstructure of MoSe<sub>2</sub>, WSe<sub>2</sub>, MoTe<sub>2</sub> and WTe<sub>2</sub> at  $k_y = 0$  and  $k_x$  ranging from  $-\frac{2\pi}{a}$  to  $\frac{2\pi}{a}$  as obtained with the original  $11 \times 11$  Hamiltonians (red circles) and the  $22 \times 22$  Hamiltonians resulting from the expanded unit cell (blue lines), highlighting the band folding induced by the basis modification.

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# List of publications and conferences

## Publications

**J. Choukroun**, M. Pala, S. Fang, E. Kaxiras, and P. Dollfus “*High performance  $WTe_2$ - $MoS_2$  in-plane heterojunction Tunnel Field Effect Transistors*”, 2018 48th European Solid-State Device Research Conference, [10.1109/ESSDERC.2018.8486869](https://doi.org/10.1109/ESSDERC.2018.8486869) *IEEE Proceedings* (2018)

**J. Choukroun**, M. Pala, S. Fang, E. Kaxiras, and P. Dollfus “*High performance Tunnel Field Effect Transistors based on in-plane transition metal dichalcogenide heterojunctions*”, [10.1088/1361-6528/aae7df](https://doi.org/10.1088/1361-6528/aae7df), to appear in *Nanotechnology* (2018)

**J. Choukroun**, M. Pala and P. Dollfus “*Ungated-channel architecture for high performance Tunnel Field Effect Transistors based on 2D material heterostructures*”, to be submitted

## International conferences

**J. Choukroun**, M. Pala, J. Saint-Martin, and P. Dollfus “*Atomistic simulation of electronic transport in planar graphene- $MoS_2$  heterostructure devices*”, GDR Graphene and co 2017 - Aussois, France (2017)

**J. Choukroun**, M. Pala, S. Fang, E. Kaxiras, and P. Dollfus “*High performance  $WTe_2$ - $MoS_2$  in-plane heterojunction Tunnel Field Effect Transistors*”, ESSDERC 2018 - Dresden, Germany (2018)

**J. Choukroun**, M. Pala, S. Fang, E. Kaxiras, and P. Dollfus “*Quantum simulation of high performance Tunnel Field Effect Transistors based on 2D material in-plane heterojunctions*”, 6th International Symposium on Graphene Devices, ISGD-6 - St Petersburg, Russia (2018)





**Titre :** Etude théorique d'hétérojonctions planaires de dichalcogénures de métaux de transition et de leurs applications dans le cadre de transistors ultra-basse consommation

**Mots clés :** TFET, transistor, matériaux 2D, TMD, simulation quantique

La miniaturisation des MOSFET a permis une forte diminution des transistors et des puces, ainsi qu'une augmentation exponentielle des capacités de calcul. Cette miniaturisation ne peut néanmoins continuer ainsi: de nos jours, un microprocesseur peut contenir des dizaines de milliards de transistors et la chaleur dégagée par ces composants peut fortement détériorer ses performances. De plus, du fait de leur principe même de fonctionnement, la tension d'alimentation des MOSFET ne peut être réduite sans en impacter les performances. De nouvelles architectures telles que le TFET -basé sur l'effet tunnel bande-à-bande et pouvant fonctionner à des tensions d'alimentation très basses- ainsi que de nouveaux matériaux pourraient donc apporter une alternative au MOSFET silicium. Les monocouches de dichalcogénures de métaux de transitions (TMDs) -des semi-conducteurs à bande interdite directe d'environ 1 à 2 eV- possèdent un fort potentiel pour l'électronique et la photonique. De plus, dans le cas de contraintes appropriées, ils peuvent conduire un alignement de bandes présentant un broken-gap; cette configuration permet de surpasser les limites habituelles du TFETs, à savoir de faibles courants dus à l'effet tunnel sur lequel ces dispositifs reposent.

Dans ce travail de thèse, des hétérojonctions planaires de TMD sont modélisées via une approche atomistique de liaisons fortes, et une configuration broken-gap est observée dans deux d'entre elles ( $\text{MoTe}_2/\text{MoS}_2$  et  $\text{WTe}_2/\text{MoS}_2$ ). Leur potentiel dans le cadre de transistors à effet tunnel (TFETs) est évalué au moyen de simulations de transport quantique basées sur un modèle TB atomistique ainsi que la théorie des fonctions de Green hors-équilibre. Des TFETs type-n basés sur ces hétérojonctions sont simulés et présentent des courants ON élevés ( $I_{ON} > 10^3 \mu\text{A}/\mu\text{m}$ ) ainsi que des pentes sous-seuil extrêmement raides ( $SS < 5 \text{ mV/dec}$ ) à des tensions d'alimentation très faibles ( $V_{DD} = 0.3 \text{ V}$ ). Plusieurs architectures novatrices basées sur ces TFETs et découlant de la nature 2D des matériaux utilisés sont également présentées, et permettent d'atteindre des performances encore plus élevées.

**Title :** Theoretical study of in-plane heterojunctions of transition metal dichalcogenides and their applications for low-power transistors.

**Keywords :** TFET, transistor, 2D materials, TMDs, quantum simulation

**Abstract :** Nowadays, microprocessors can contain tens of billions of transistors and as a result, heat dissipation and its impact on device performance has increasingly become a hindrance to further scaling. Due to their working mechanism, the power supply of MOSFETs cannot be reduced without deteriorating overall performance, and Si-MOSFETs scaling therefore seems to be reaching its end. New architectures such as the TFET, which can perform at low supply voltages thanks to its reliance on band-to-band tunneling, and new materials could solve this issue. Transition metal dichalcogenide monolayers (TMDs) are 2D semiconductors with direct band gaps ranging from 1 to 2 eV, and therefore hold potential in electronics and photonics. Moreover, when under appropriate strains, their band alignment can result in broken-gap configurations which can circumvent the traditionally low currents observed in TFETs due to the tunneling mechanism they rely upon.

In this work, in-plane TMD heterojunctions are investigated using an atomistic tight-binding approach, two of which lead to a broken-gap configuration (MoTe<sub>2</sub>/MoS<sub>2</sub> and WTe<sub>2</sub>/MoS<sub>2</sub>). The potential of these heterojunctions for use in tunnel field-effect transistors (TFETs) is evaluated via quantum transport computations based on an atomistic tight-binding model and the non-equilibrium Green's function theory.

N-type TFETs based on these in-plane TMD heterojunctions are shown to yield high ON currents ( $I_{ON} > 10^3 \mu\text{A}/\mu\text{m}$ ) and extremely low subthreshold swings ( $SS < 5 \text{ mV/dec}$ ) at low supply voltages ( $V_{DD} = 0.3 \text{ V}$ ). Innovative device architectures allowed by the 2D nature of these materials are also proposed, and shown to enhance performance even further.

