

# Electromechanics of Carbon Nanotubes

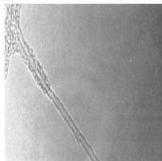
Zhao WANG

UTINAM Institute  
University of Franche-Comté, France

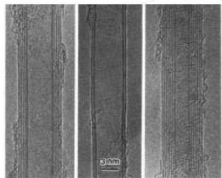
2008

# Carbon Nanotubes (CNTs)

Single-walled CNT (SWCNT)



Multi-walled CNTs (MWCNT)

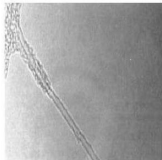


S. Iijima: *Nature* **354**, 56 (1991)

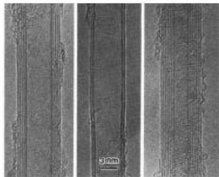
diamètre < 10nm

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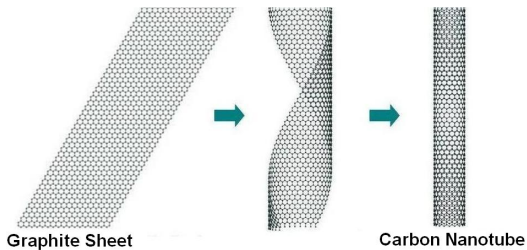
Single-walled CNT (SWCNT)



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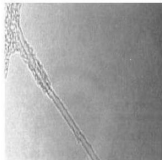


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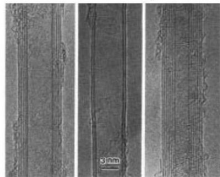


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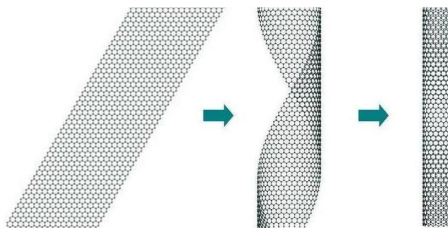
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Graphite sheet

Carbon nanotube

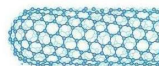
Chiralité



Armchair



Zigzag



Chiral

1/3 Metallic

2/3 Semiconducting

# Overview on applications

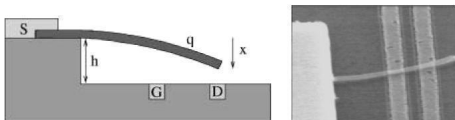
## Unique properties:

- Strongest and stiffest materials on earth, Young's modulus  $\approx 1$  TPa
- Very high thermal conductivity, 4000 W/m.K
- Very high current density  $10^9$  A/cm<sup>2</sup> - Ballistic electron transport - Superconductivity at low temperature
- Darkest ever - a carpet of nanotube - 99.9% light adsorption
- Large surface area - large aspect ratio

## Promising applications:

NEMS, field emission, FETs, multifunctional composites, (bio-)sensors, supercapacitors, medical devices, drugs and ...

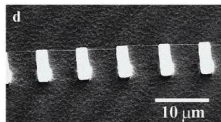
# Nanoelectromechanical systems (NEMS)



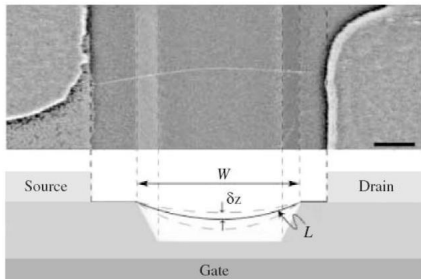
CNT nanorelay device

J. Kinaret et al., *Appl. Phys. Lett.* 82, 1287 (2002). S. Lee et al., *Nano Lett.* 4, 2027 (2004).

logical devices, nano-capacitor, biological reaction control and artificial muscle.



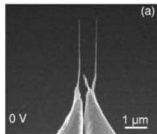
HONGJIE DAI *Acc. Chem. Res.* 2002, 35, 1035



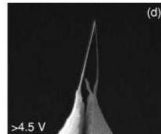
a suspended device

V. Sazonova et al., *Nature* 431, 284 (2004).

biomedical sensors, ultrasensitive mass or charge detectors



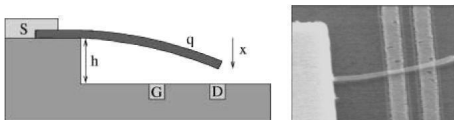
nanotube nanowire device and a Si cantilever base



S. Akita et al., *Appl. Phys. Lett.* 79, 1691 (2001).

memory

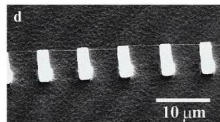
# Nanoelectromechanical systems (NEMS)



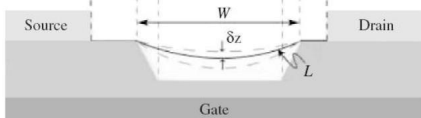
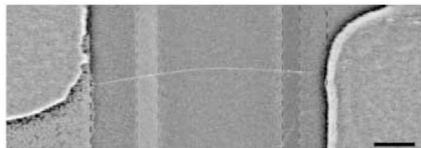
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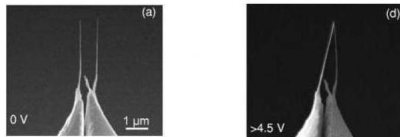
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nanotube nanowire and a Si cantilever base

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memory

*Purpose of our studies:* to understand the *electromechanical* properties of the carbon nanotubes (CNTs) for their future uses.

- 1 Mechanical properties
- 2 Electrostatic properties
- 3 Electromechanical properties
- 4 Selection of nanotubes using physisorption.



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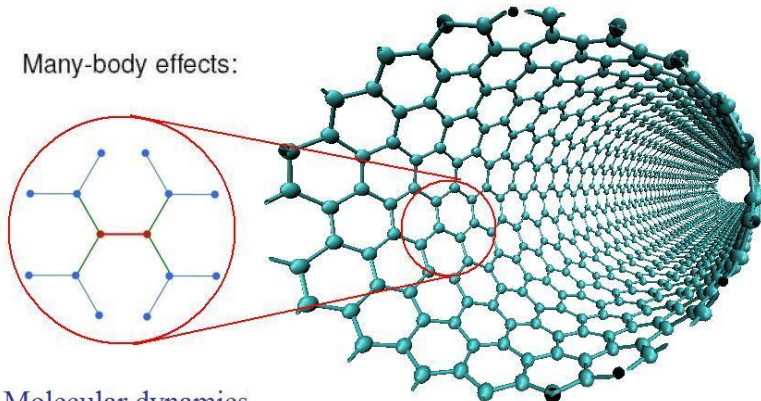
- 1 Mechanical properties
- 2 Electrostatic properties
- 3 Electromechanical properties
- 4 Selection of nanotubes using physisorption.

## 1. Mechanical properties of CNTs

# Theoretical method

Interatomic interaction: **AIREBO** potential function  
Stuart *et al*, *JCP* **112**, 6472 (2000).

Many-body effects:



Molecular dynamics  
Energy minimization

# Empirical potential

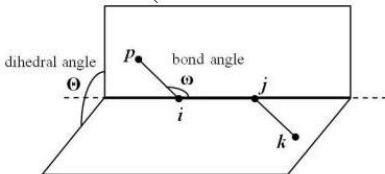
The interatomic potential  $U^P \rightarrow$  AIREBO

Stuart *et al*, *JCP* **112**, 6472 (2000).

interatomic repulsion and attraction terms. a parameterized Lennard-Jones 12-6.

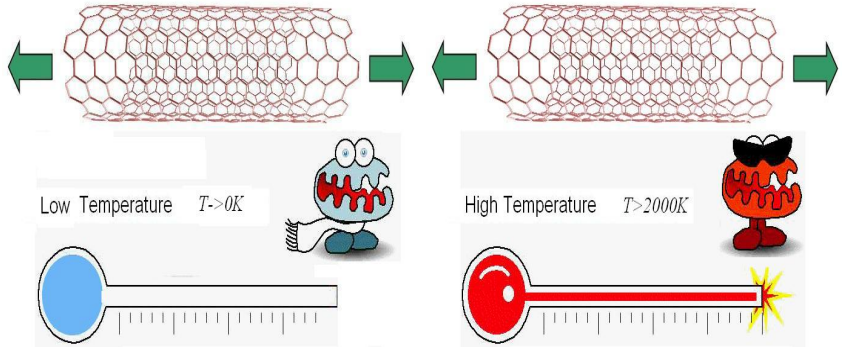
$$U^P = \frac{1}{2} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \left[ \underbrace{\varphi^R(r_{i,j}) - b_{i,j} \varphi^A(r_{i,j})}_{\text{bond order function.}} + \underbrace{\varphi^{LJ}(r_{i,j})}_{\text{a parameterized Lennard-Jones 12-6.}} + \sum_{\substack{k=1 \\ k \neq i,j}}^N \sum_{\substack{\ell=1 \\ \ell \neq i,j,k}}^N \varphi_{kij\ell}^{\text{tor}} \right]$$

single bond torsional interactions.



Parameters fitted to a database of small hydrocarbon, graphite and diamond lattices.  
*JCP* **112**, 6472 (2000).

# Tensile deformation via Molecular Dynamics



# Non-linear elasticity under tensile loading

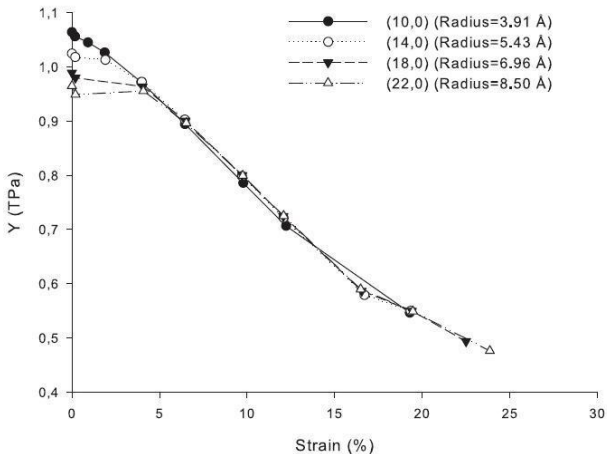


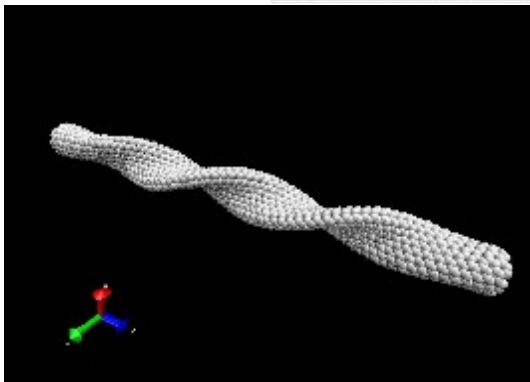
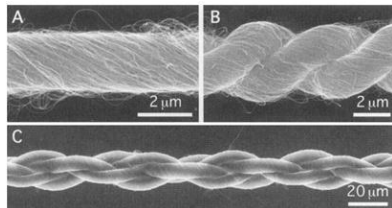
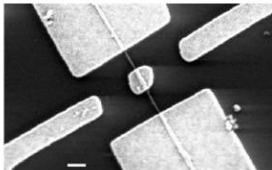
FIG. 4: Effective Young's modulus of one group of zigzag SWCNTs under tensile loading versus axial strain.

Ref: Z. WANG *et al.*, (2008), *F.N.C.N.*, accepted

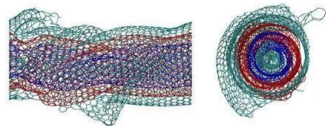
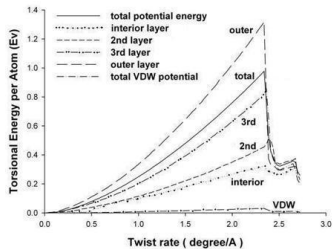
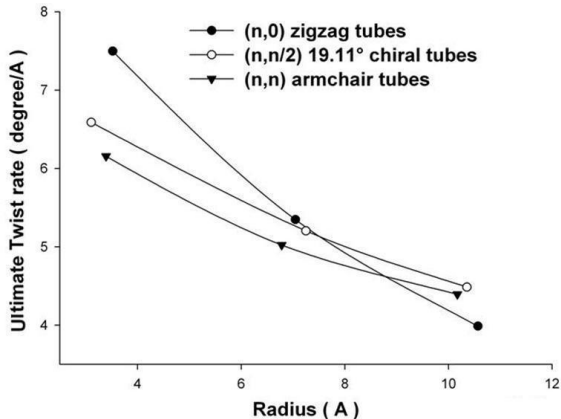


# Torsion of CNTs via Molecular Dynamics Simulations

A Rotational nanoactuator



# Ultimate Twist Rate



Ref: Z. WANG *et al.*, submitted to *Comput. Mat. Sci.*

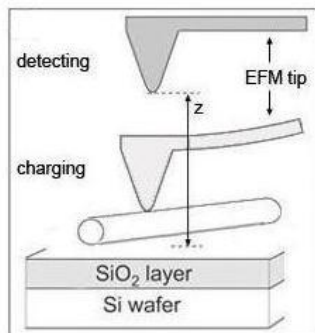
## 2. Electrostatic properties of CNTs

*Experimental Collaborators:*

M. Zdrojek, Warsaw University of Technology, Poland

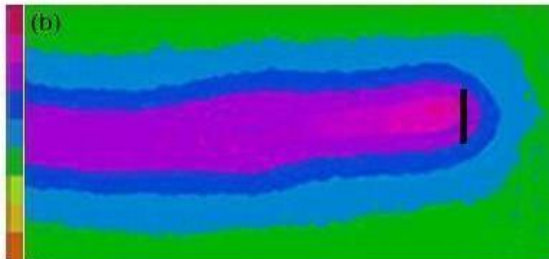
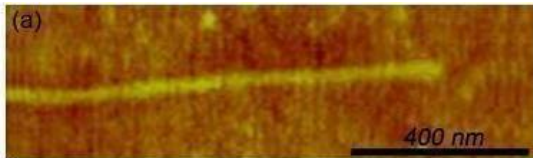
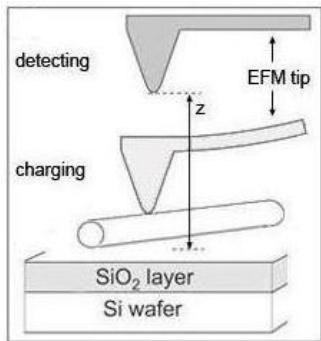
T. Mélin , ISEN, IEMN, Villeneuve d'Ascq, France

# Charge injection experiment



Electric force microscopy charge injection and detection experiments

# Charge injection experiment



# For each carbon atom

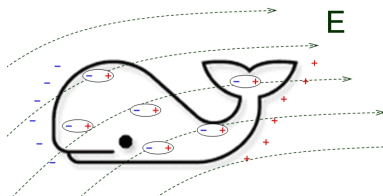
- Atomic electric polarization:



- Charge-dipole model:

# For each carbon atom

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- Charge-dipole model:

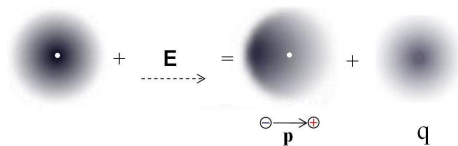
# For each carbon atom

- Atomic electric polarization:
- Charge-dipole model:



# For each carbon atom

- Atomic electric polarization:
- Charge-dipole model:



# Formulation of electrostatic energy

$U^{elec}$ : For a systems with N atoms:

Charge-dipole model:

$$U^{elec} = \sum_{i=1}^N q_i(\chi_i + V_i) - \sum_{i=1}^N \mathbf{p}_i \cdot \mathbf{E}_i + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N q_i T_{q-q}^{i,j} q_j \\ - \sum_{i=1}^N \sum_{j=1}^N \mathbf{p}_i \cdot \mathbf{T}_{p-q}^{i,j} q_j - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \mathbf{p}_i \cdot \mathbf{T}_{p-p}^{i,j} \cdot \mathbf{p}_j$$

$\chi_i$  stands for the electron affinity of atom  $i$

$V_i$  is the external potential

# Formulation of electrostatic energy

$U^{elec}$ : For a systems with N atoms:

$$\begin{aligned}
 U^{elec} = & \sum_{i=1}^N q_i(\chi_i + V_i) - \sum_{i=1}^N \mathbf{p}_i \cdot \mathbf{E}_i + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N q_i T_{q-q}^{i,j} q_j \\
 & - \sum_{i=1}^N \sum_{j=1}^N \mathbf{p}_i \cdot \mathbf{T}_{p-q}^{i,j} q_j - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \mathbf{p}_i \cdot \mathbf{T}_{p-p}^{i,j} \cdot \mathbf{p}_j
 \end{aligned}$$

$\boxed{\mathbf{q} - \mathbf{E}}$ 
 $\boxed{\mathbf{p} - \mathbf{E}}$ 
 $\boxed{\mathbf{q} - \mathbf{q}}$

$\boxed{\mathbf{p} - \mathbf{q}}$ 
 $\boxed{\mathbf{p} - \mathbf{p}}$

# Final formula for Charge-dipole model:

The equilibrium state of the dipole and charge distribution should correspond to the minimum value of  $U^{elec}$ .  $\Rightarrow$

$$\forall i = 1, \dots, N \quad \frac{\partial U^{elec}}{\partial p_{i,x}} = \frac{\partial U^{elec}}{\partial p_{i,y}} = \frac{\partial U^{elec}}{\partial p_{i,z}} = \frac{\partial U^{elec}}{\partial q_i} = 0$$

Last step:

Solution of Linear Algebraic Equations : LAPACK

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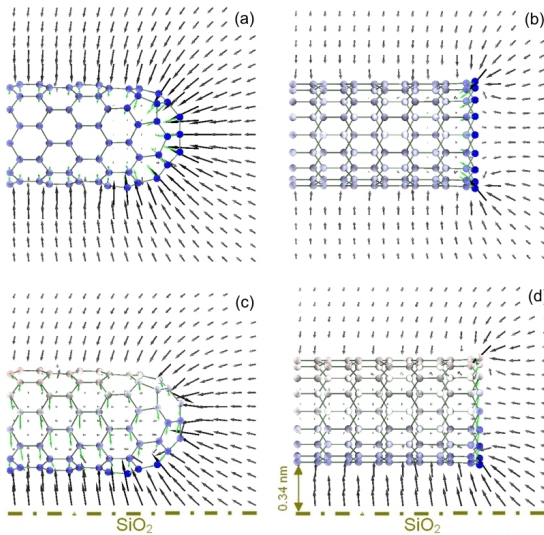
## Final Formula

$$\begin{cases} \sum_{j=1}^N \mathbf{T}_{p-p}^{i,j} \mathbf{p}_j + \sum_{j=1}^N \mathbf{T}_{p-q}^{i,j} q_j = -\mathbf{E}_i \\ \sum_{j=1}^N \mathbf{T}_{p-q}^{i,j} \cdot \mathbf{p}_j + \sum_{j=1}^N T_{q-q}^{i,j} q_j = -(\chi_i + V_i) \end{cases}$$

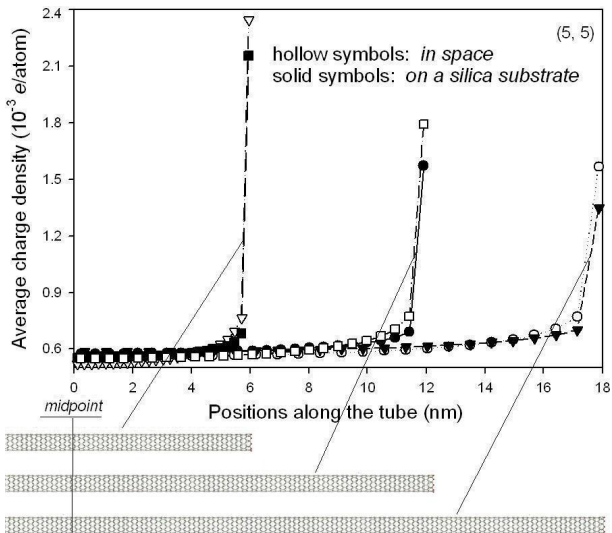
Last step:

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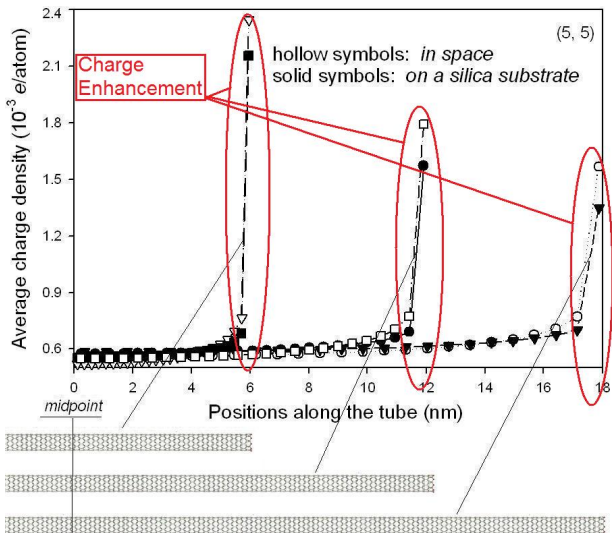
# Charge distribution



# Charge enhancement

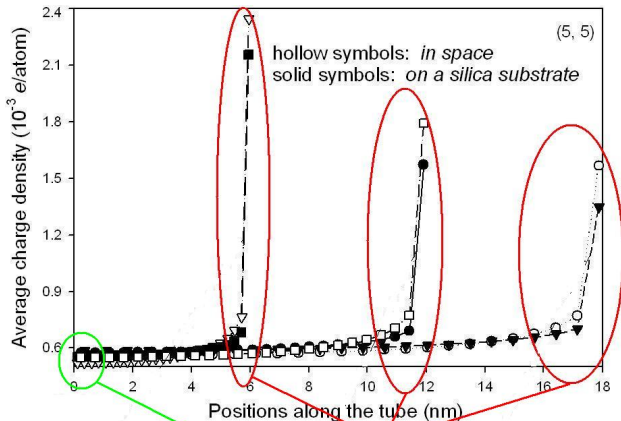


# Charge enhancement



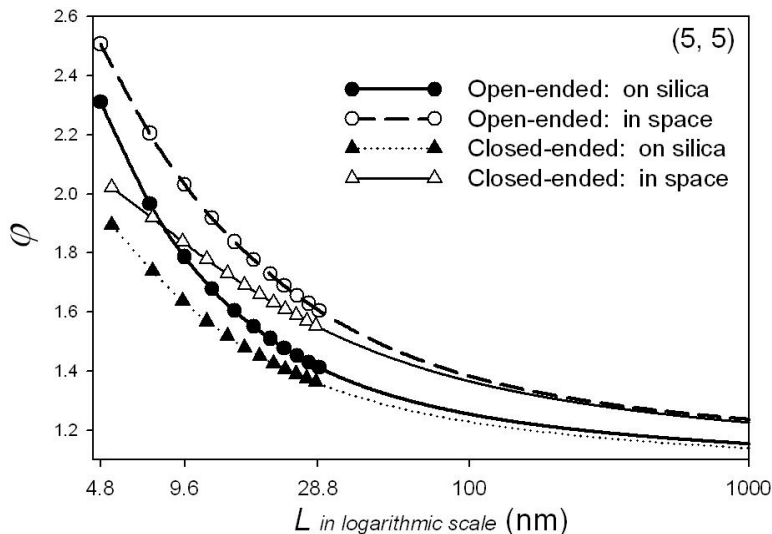


# Charge enhancement

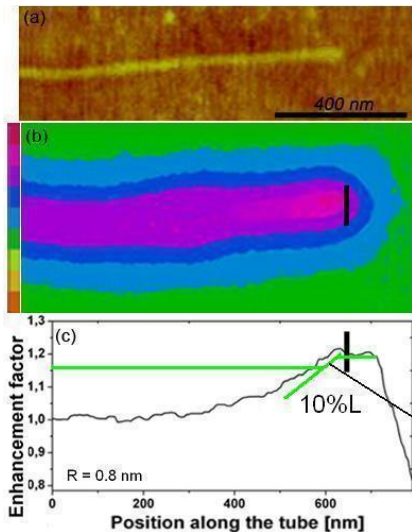


$$\text{enhancement ratio: } \varphi = \frac{\sigma_{\text{end}}}{\sigma_{\text{middle}}}$$

# Charge distribution

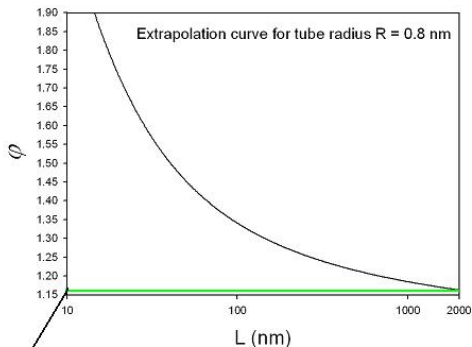
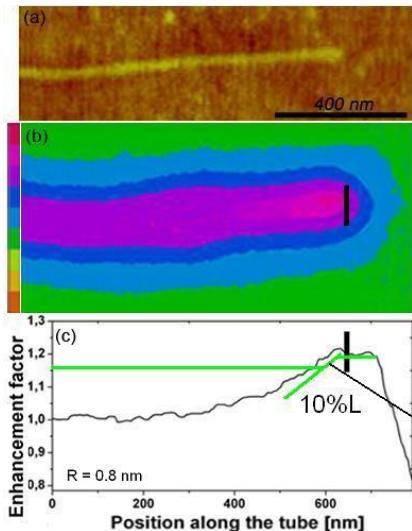


# Experimental verification



*EFM* Measurement  $\varphi = 1.17$

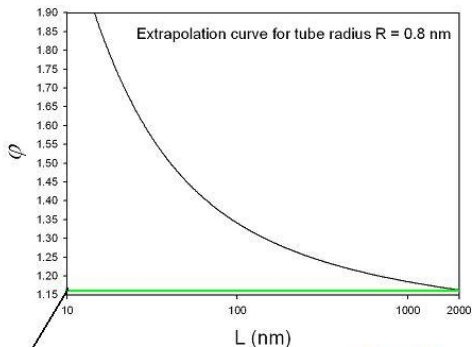
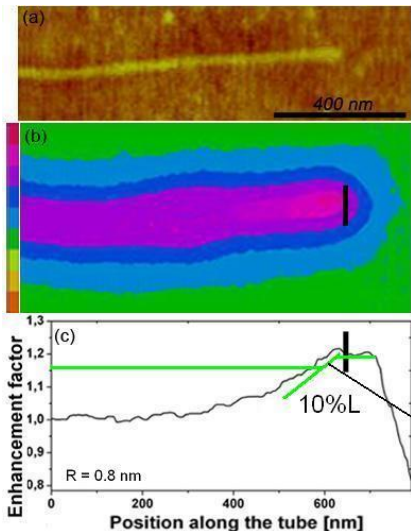
# Experimental verification



Numerical Extrapolation  $\phi = 1.165$

EFM Measurement  $\phi = 1.17$

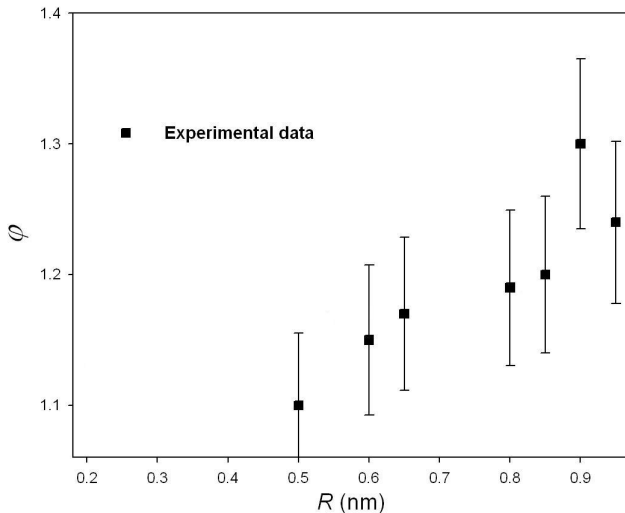
# Experimental verification



Numerical Extrapolation  $\phi = 1.165$

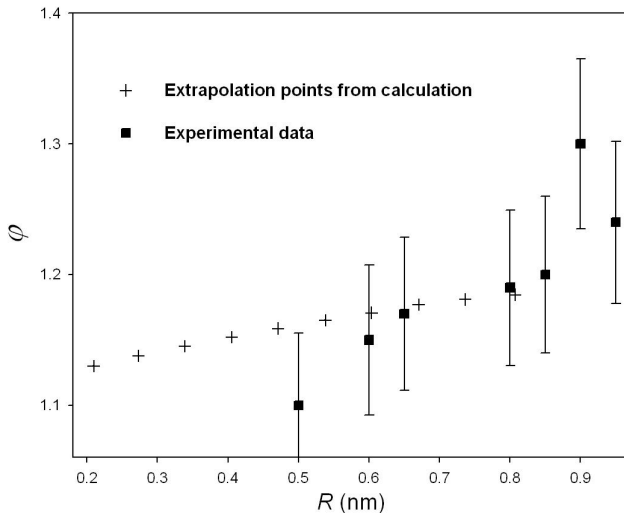
EFM Measurement  $\phi = 1.17$

# Enhancement ratio vs. tube Radius R



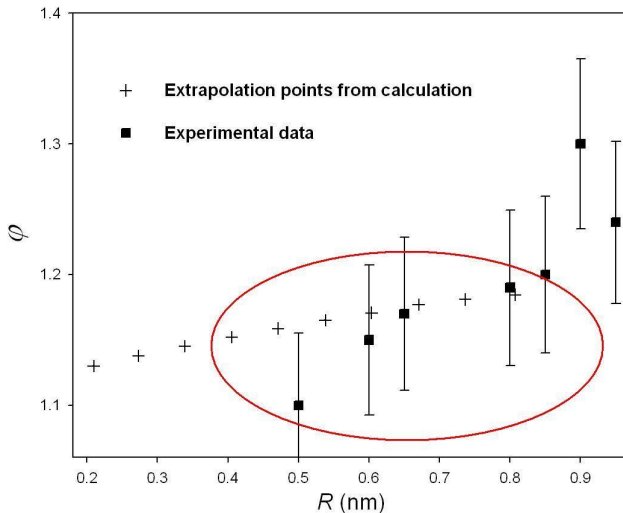
Ref: Z. WANG *et al.*, Phys. Rev. B 78, 085425 (2008)

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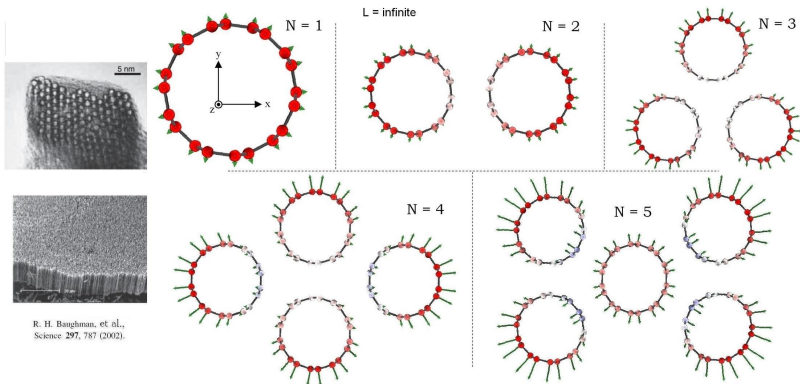
# Enhancement ratio vs. tube Radius R



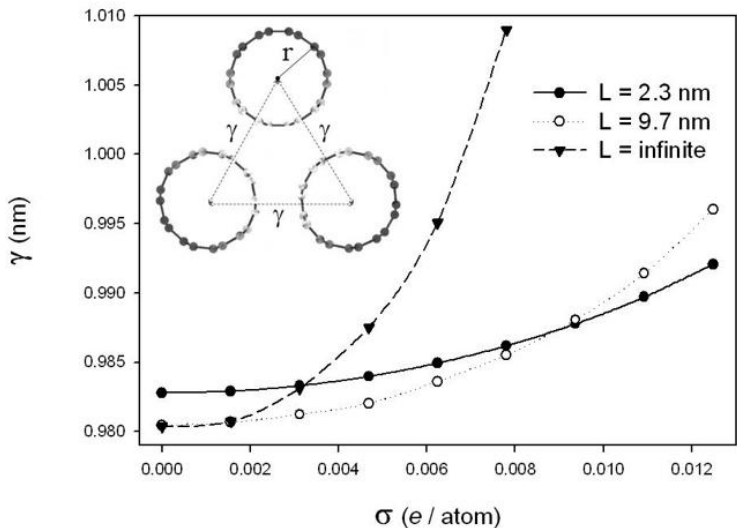
Ref: Z. WANG *et al.*, Phys. Rev. B 78, 085425 (2008)



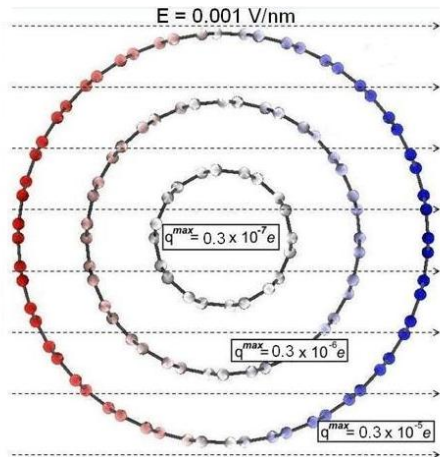
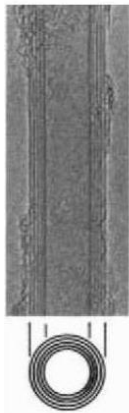
# Nanotube bundles



# Nanotube bundles



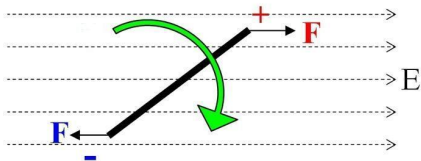
# MWCNTs in an external field



## 3. Electromechanical properties of CNTs

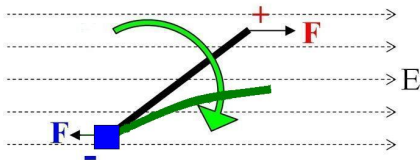
# Electric-field induced deformation

When an electric field  
is applied to a CNT:



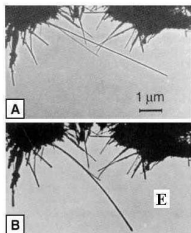
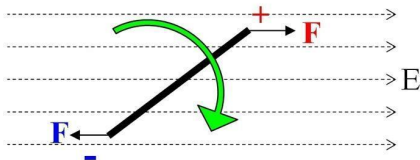
# Electric-field induced deformation

When an electric field  
is applied to a CNT:

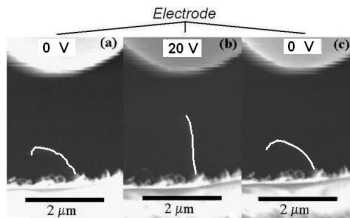


# Electric-field induced deformation

When an electric field is applied to a CNT:



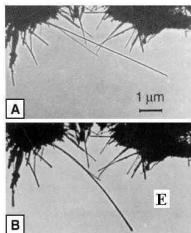
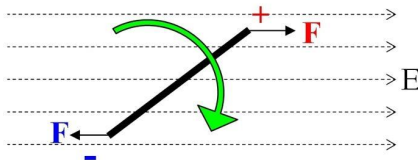
P. Poncharal *et al.*, *Science* **283**, 1513 (1999).



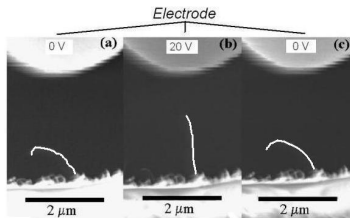
Y. Wei *et al.*, *Appl. Phys. Lett.* **79**, 4527 (2001).

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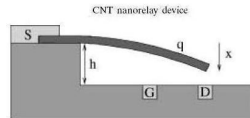


P. Poncharal *et al.*, *Science* **283**, 1513 (1999).

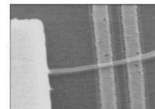


Y. Wei *et al.*, *Appl. Phys. Lett.* **79**, 4527 (2001).

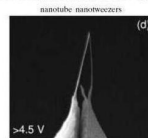
## NEMS



J. Kinaret *et al.*, *Appl. Phys. Lett.* **82**, 1287 (2002).



S. Lee *et al.*, *Nano Lett.* **4**, 2027 (2004).



S. Akita *et al.*, *Appl. Phys. Lett.* **79**, 1691 (2001).



- Total potential energy of system:

$$U^{tot} = U^{elec} + U^{ia}$$

- $U^{elec}$ : *Electric-field induced energy.*

Semiconducting CNTs  $\rightarrow$  regularized **Dipole-only** model.

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Metallic CNTs  $\rightarrow$  regularized **Charge-Dipole** model.

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Adaptive interatomic reactive empirical bond order (**AIREBO**) potential.

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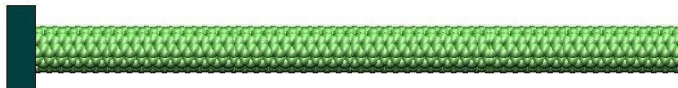
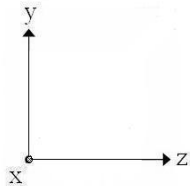
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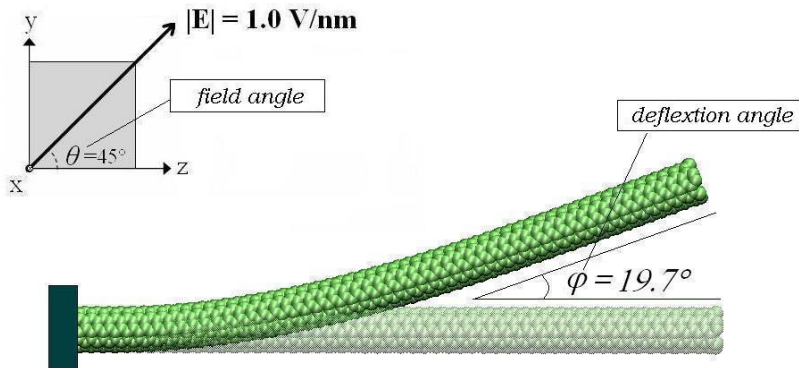
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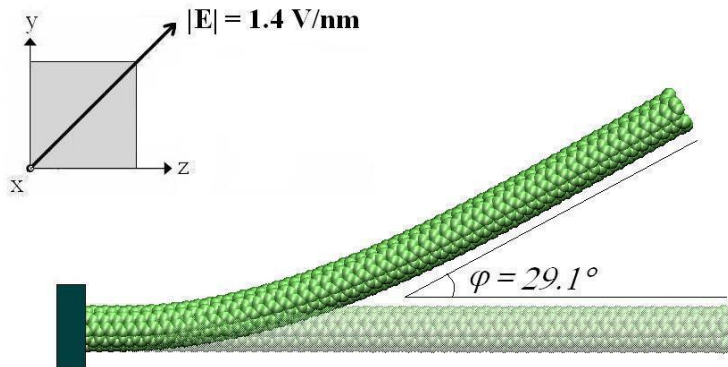
# Molecular simulations



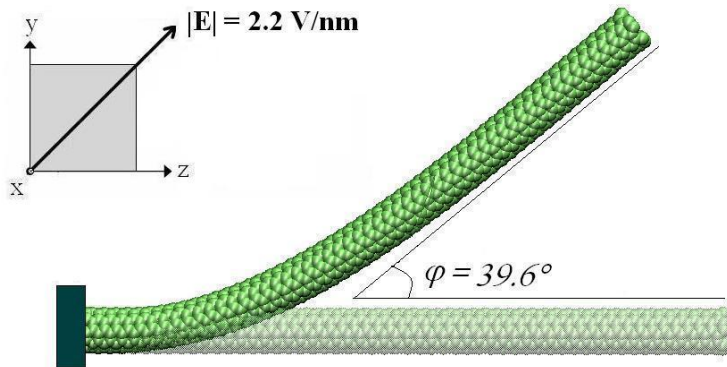
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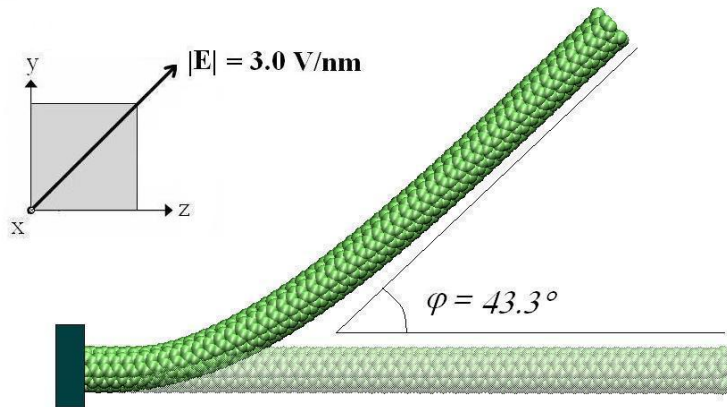


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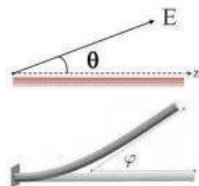
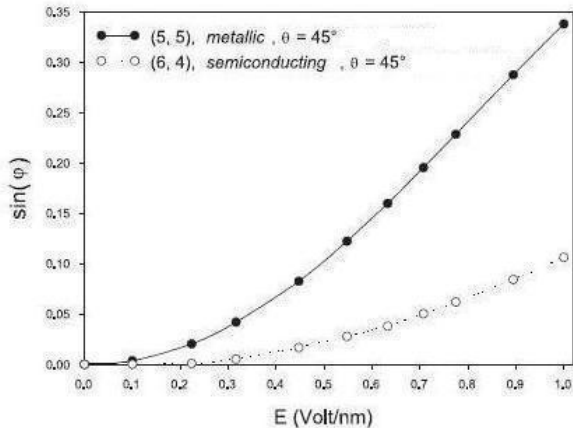




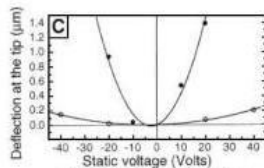
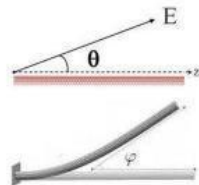
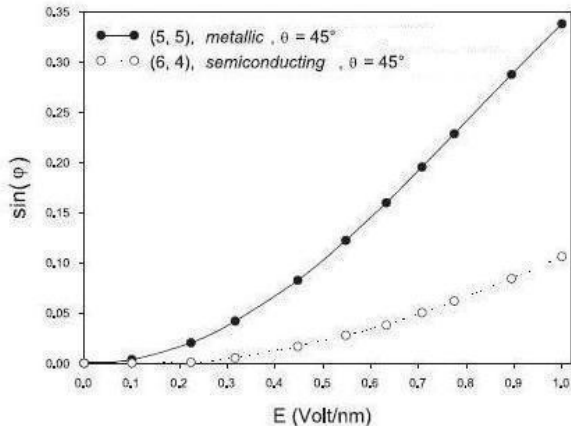
# Molecular simulations



# Influence of field strength E

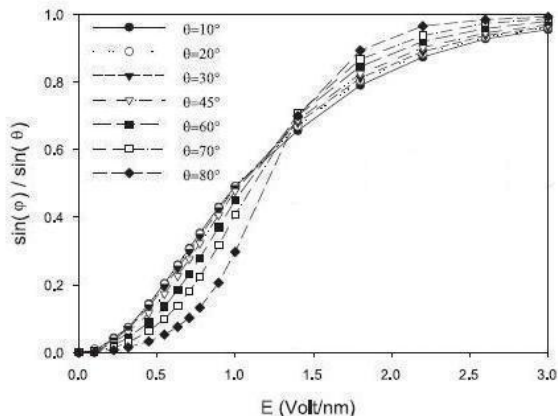


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Poncharal *et al.*,  
Science **283**, 1513 (1999).

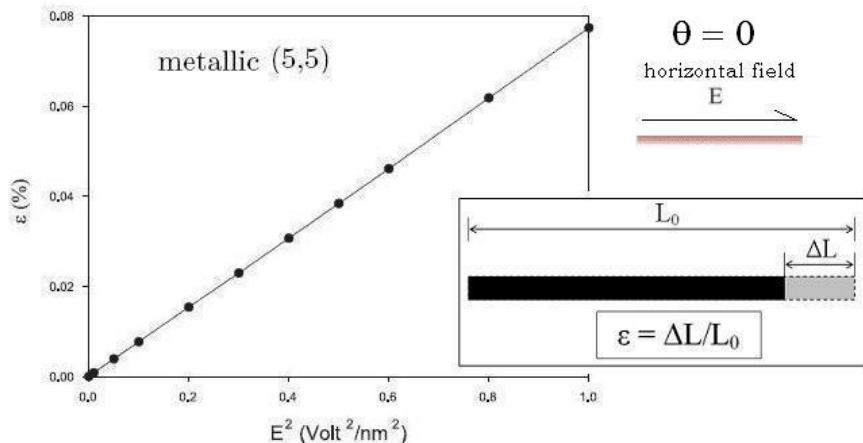
# Influence of field direction



$\sin(\varphi)/\sin(\theta)$  versus  $E$

for a metallic tube (5,5),  $L \approx 13.16$  nm.

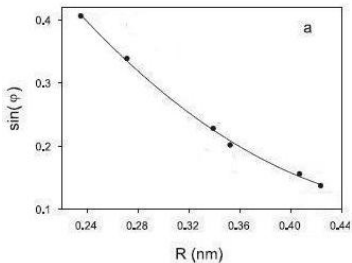
# Electrostriction



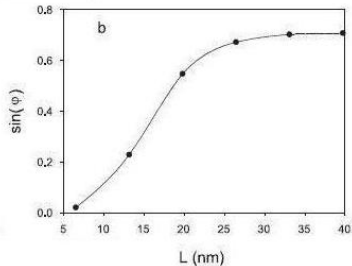
Axial strain  $\epsilon$  (%) versus  $E^2$  for a metallic tube (5,5) ( $L \approx 13.16$  nm)  
applied electric fields : parallel to the tube axis

# Effects of tube geometry

$$E = 0.775 \text{ V/nm}, \theta = 45^\circ$$



$\sin(\varphi)$  versus  $R$   
 $L \approx 13.2 \text{ nm}$

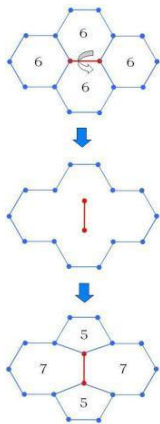


$\sin(\varphi)$  versus  $L$   
 $R \approx 0.3 \text{ nm}$

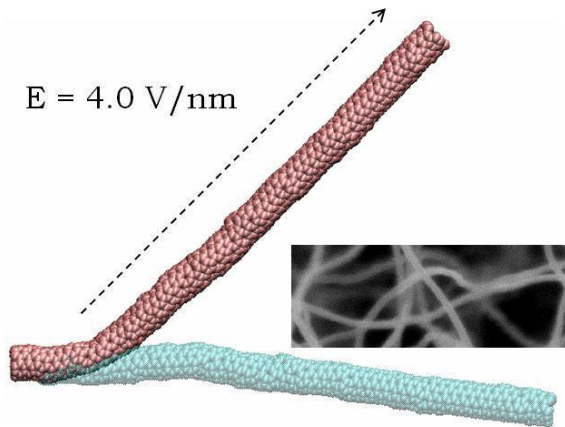
Ref: Z. WANG *et al.*, Phys. Rev. B 75, 205414 (2007)

76, 195434 (2007)

# Effects of defects



Stone-Wales defect



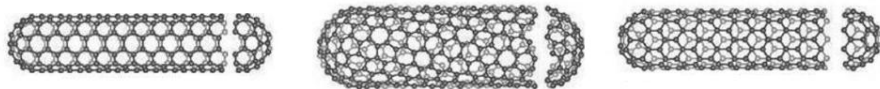
## 4. Selection of nanotubes - physisorption

*Experimental Collaborators:*

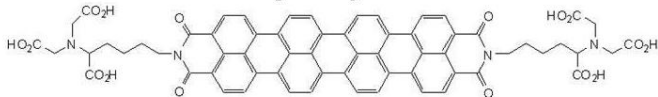
S. Meunier, University of Strasbourg, France.



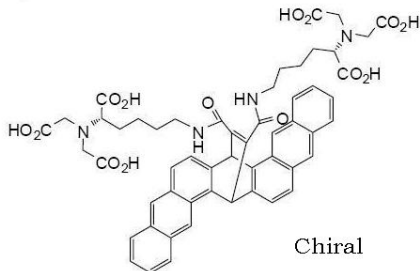
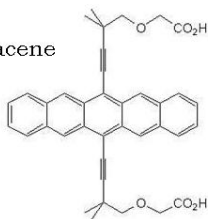
# Molecules used in experiment



quaterrylene



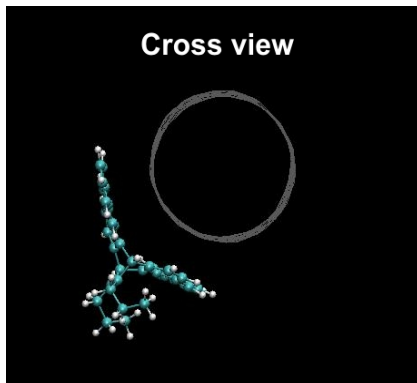
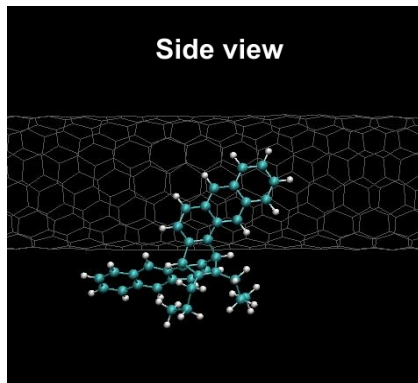
pentacene



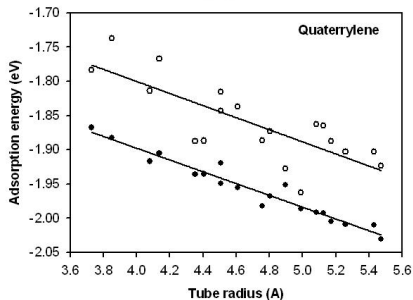
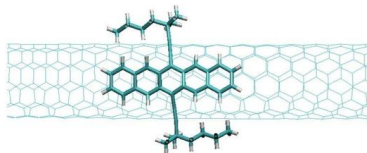
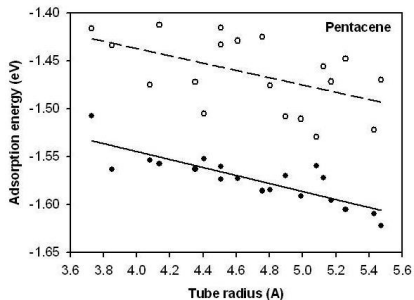
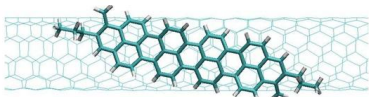
Chiral

# Simulation

Adsorption of chiral molecules on nanotube surface at room temperature.



# Results



# Conclusions et Perspectives

- 1 Elasticité non-linéaire de nanotubes (CNTs) - Modèle AIREBO - déformation axiale sous forte contraintes
  - 2 Torsion de CNTs - taux de torsion ultime - énergie de déformation
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- Collaborateurs: T. Mélin, M. Zdrojek, S. Meunier, S. Stuart, P. Hoang et R. Langlet.
- Membres du Jury: A. Bosseboeuf, J. Dijon et F. Torrens.
- Tout le monde au Labo.
- Tous les amis et les invités.
- Xuan - Ma Chérie



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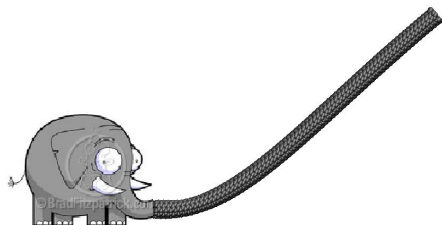
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***Merci à Tous!***

for further calculation details:

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