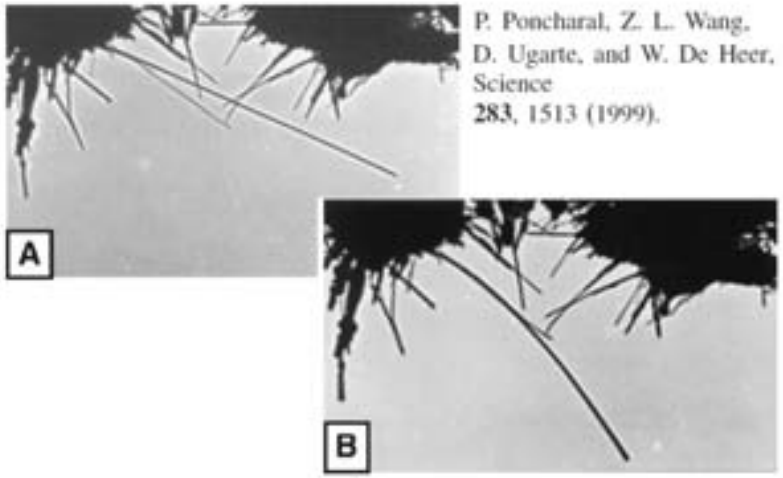
Deformation of nanotubes by an electric field

Zhao Wang

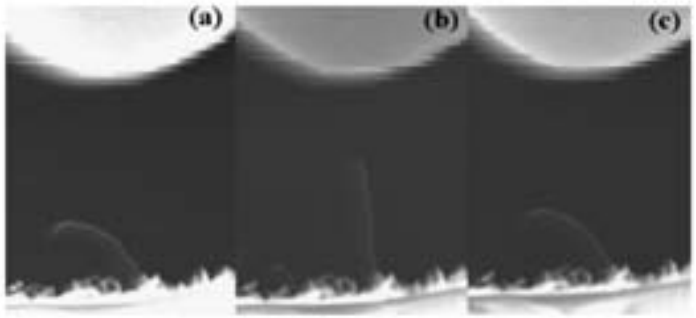
EMPA - Swiss Federal Laboratories for Materials Testing and Research, Thun, Switzerland.

TNT2009

Introduction -> electrostatic deformation



P. Poncharal, Z. L. Wang, D. Ugarte, and W. De Heer, Science **283**, 1513 (1999).



Y. Wei, C. Xie, K. A. Dean, and B. F. Coll, Appl. Phys. Lett. **79**, 4527 (2001).

Quantification - molecular simulations

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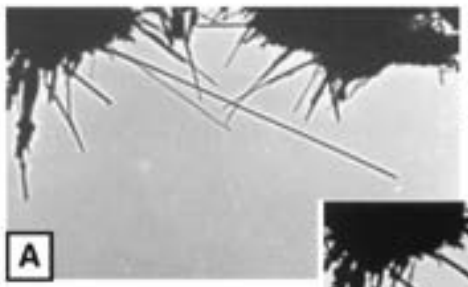
Introduction -> electrostatic deformation



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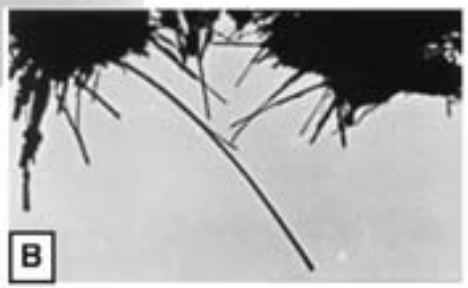
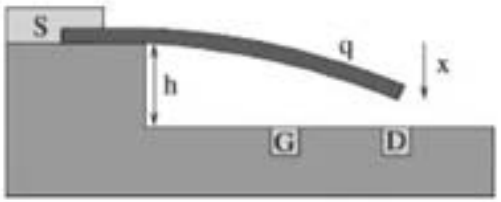
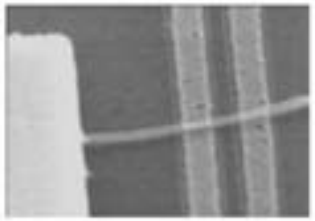
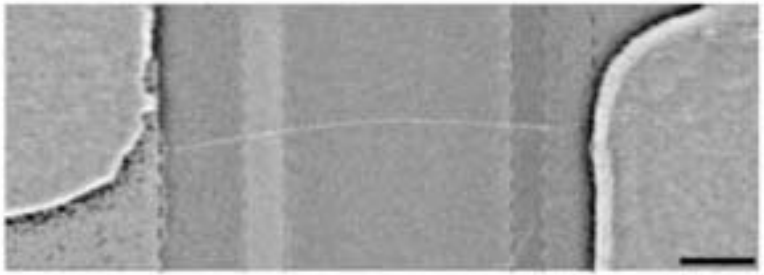




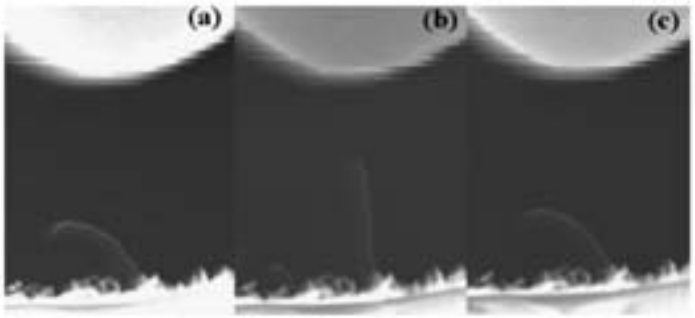


CNT nanorelay device

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



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



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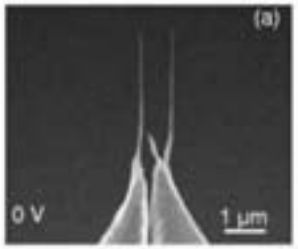

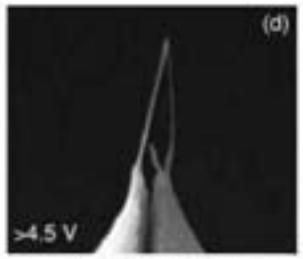

nanotube nanotweezers and a Si cantilever base S. Akita et al., *Appl. Phys. Lett.* 79, 1691 (2001).

Quantification - molecular simulations

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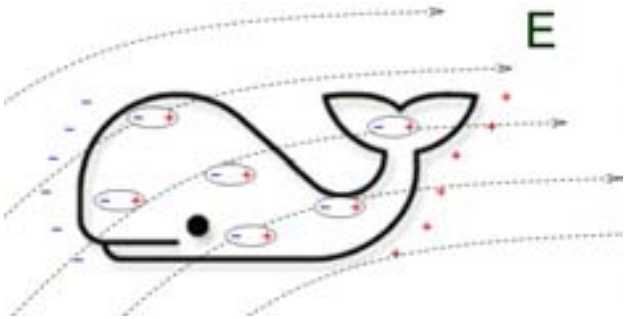
Outline

1. Computational methods: Simulations.



2. Results: Cantilevered and Doubly clamped CNTs.

3. Brief Introduction to: Recent works on Graphene Nanoribbons.

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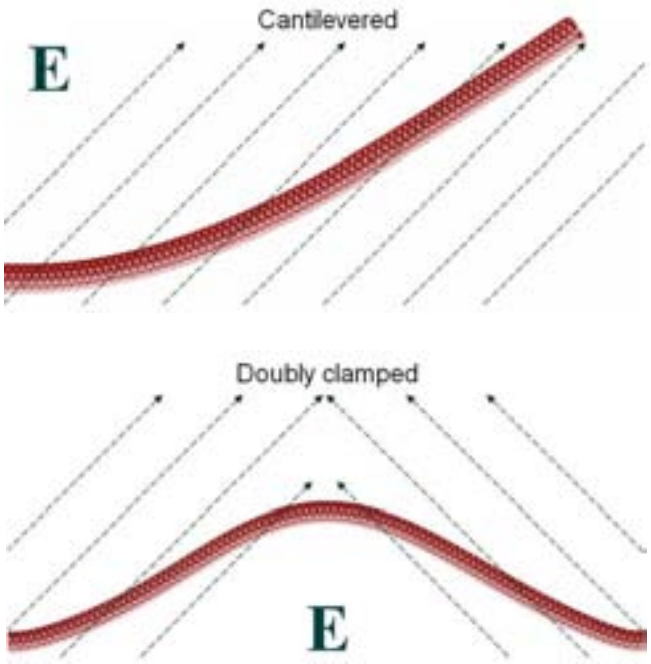

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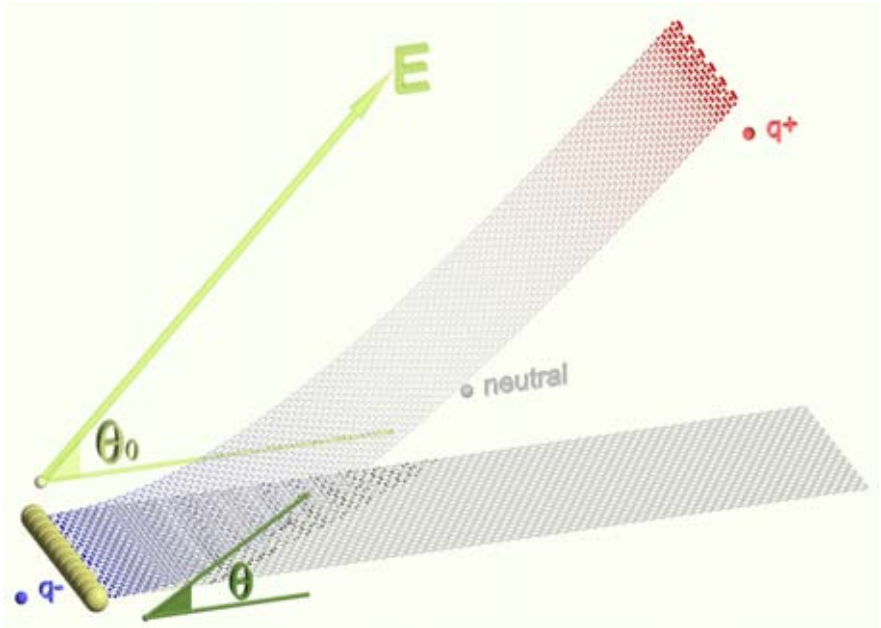

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Quantification - molecular simulations

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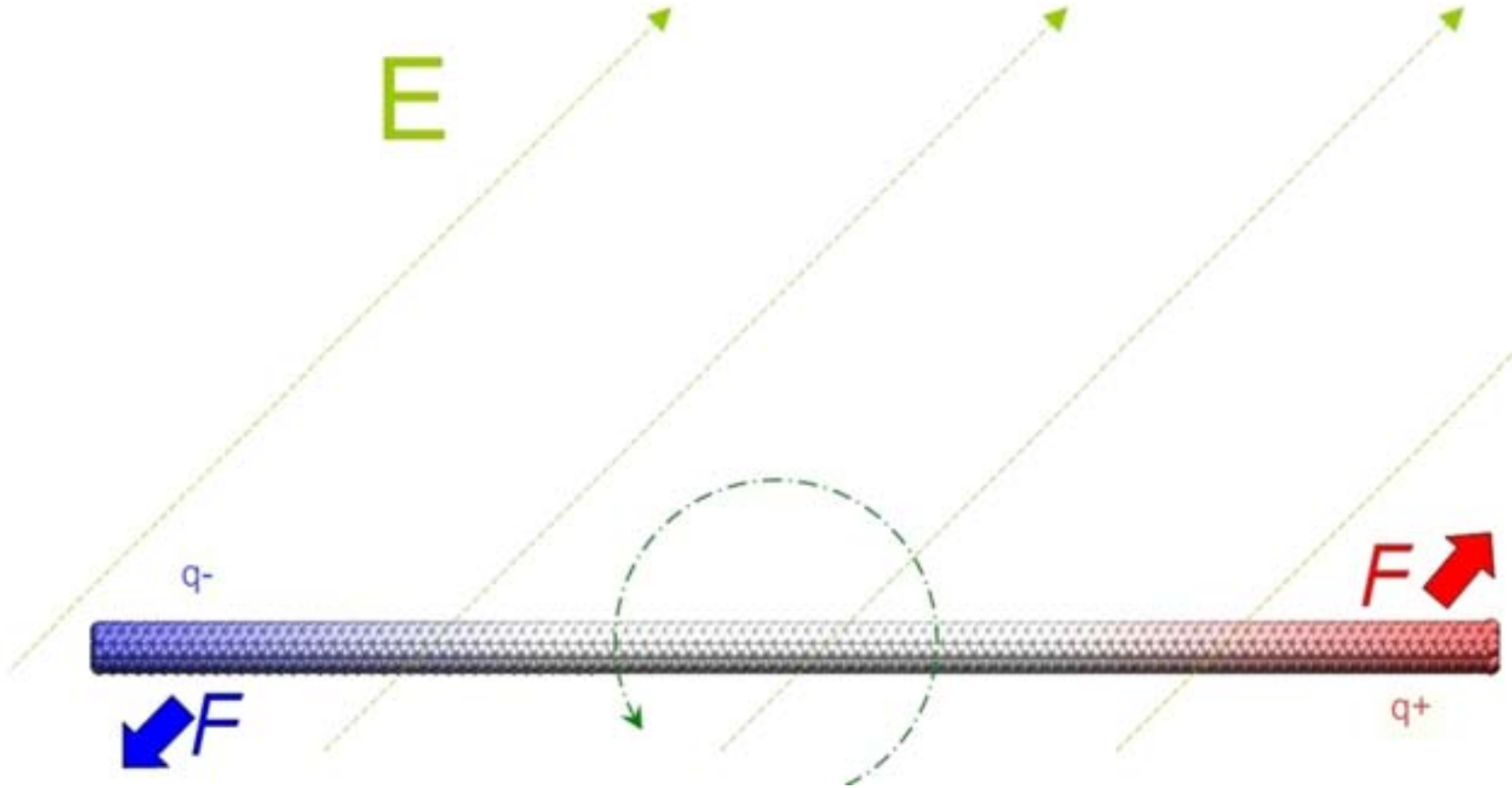

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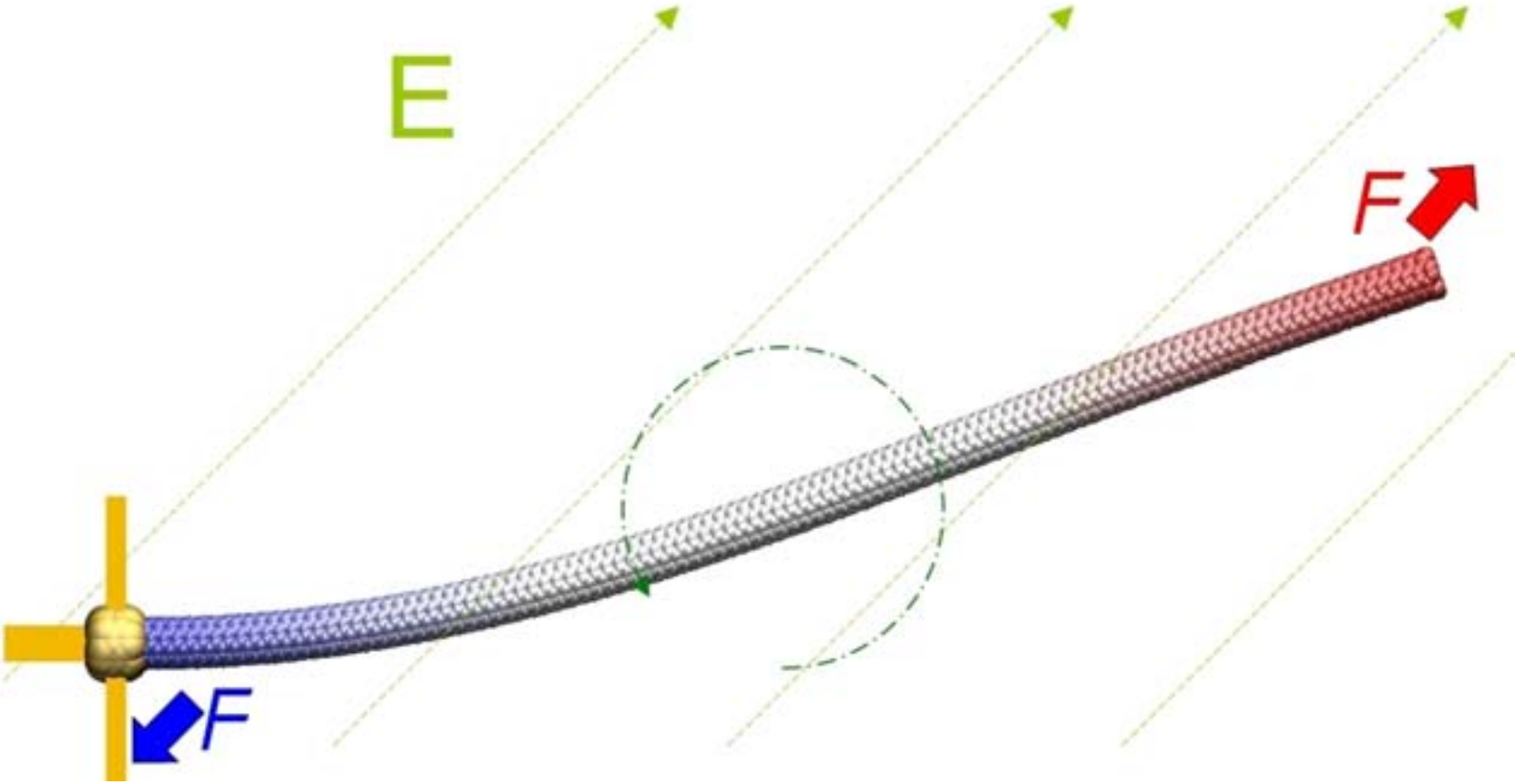

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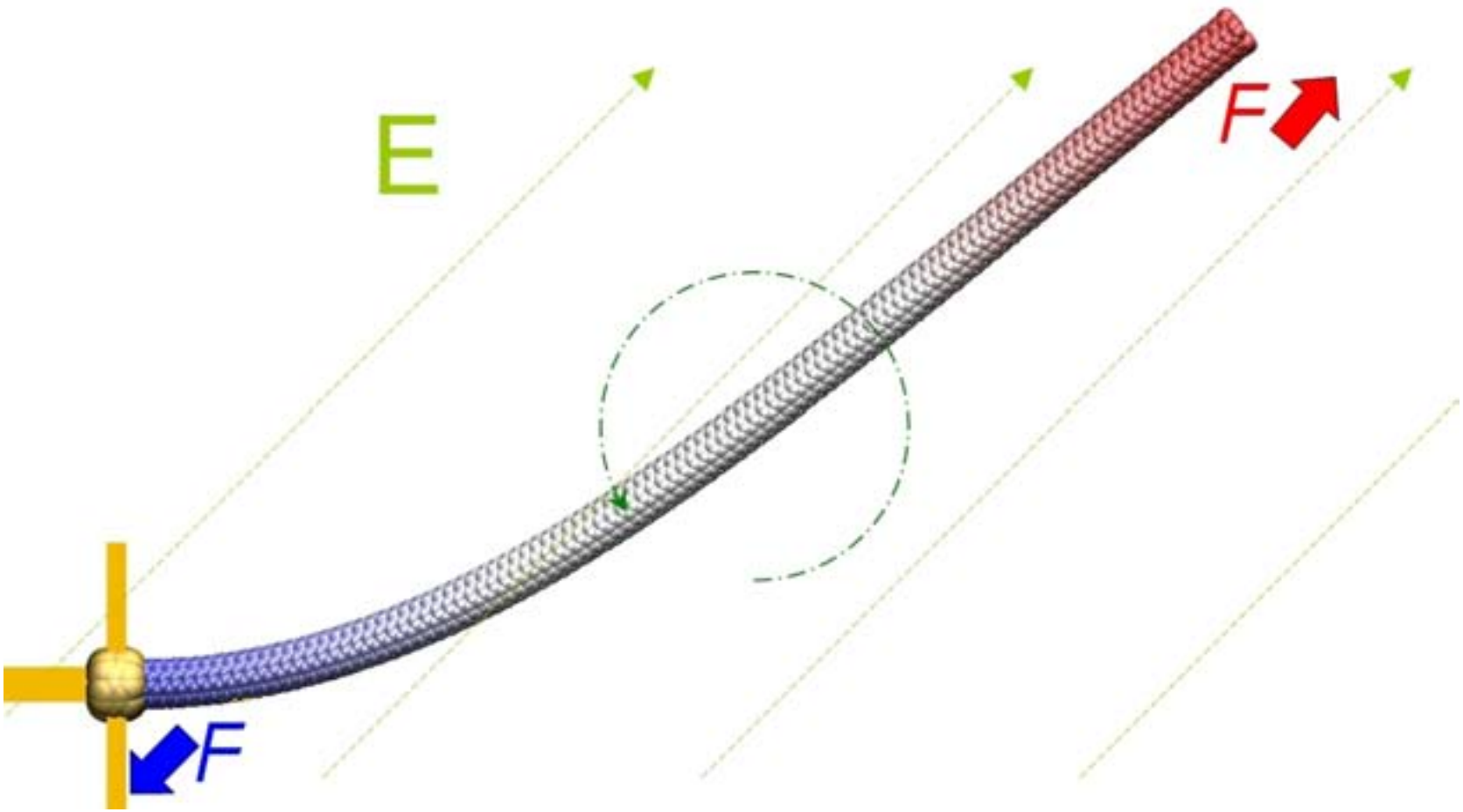

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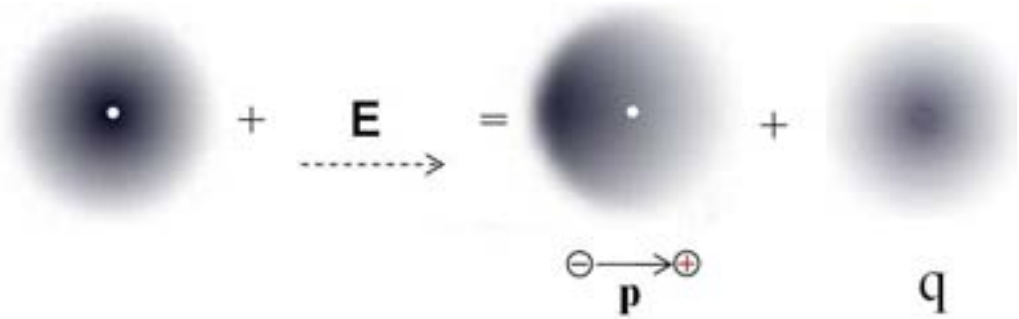
Computational method

- Deformation - Minimizing total potential energy U_{tot}:

$$U_{tot} = U_{elec} + U_{bond}$$

- U_{elec}: Atomistic charge-dipole model.



Ref: PRB 78, 085425 (2008).

79, 155407 (2009).

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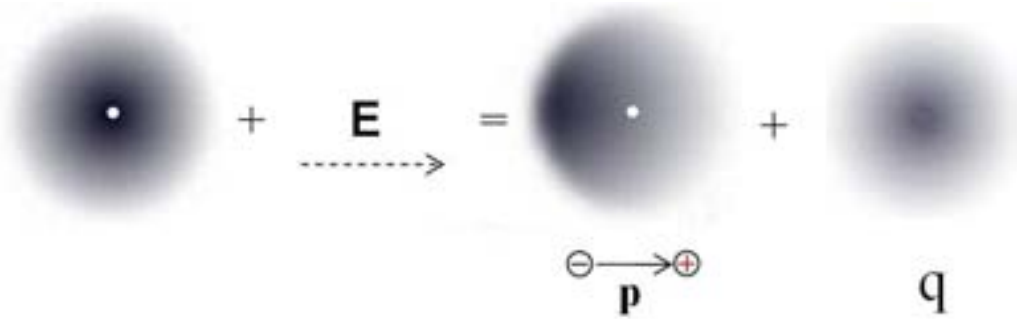

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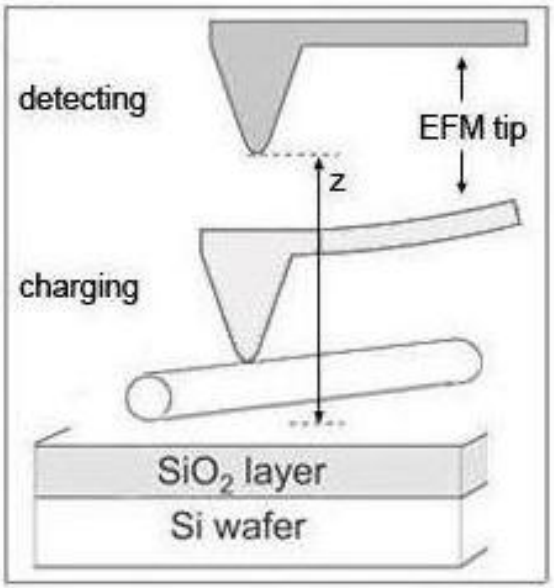
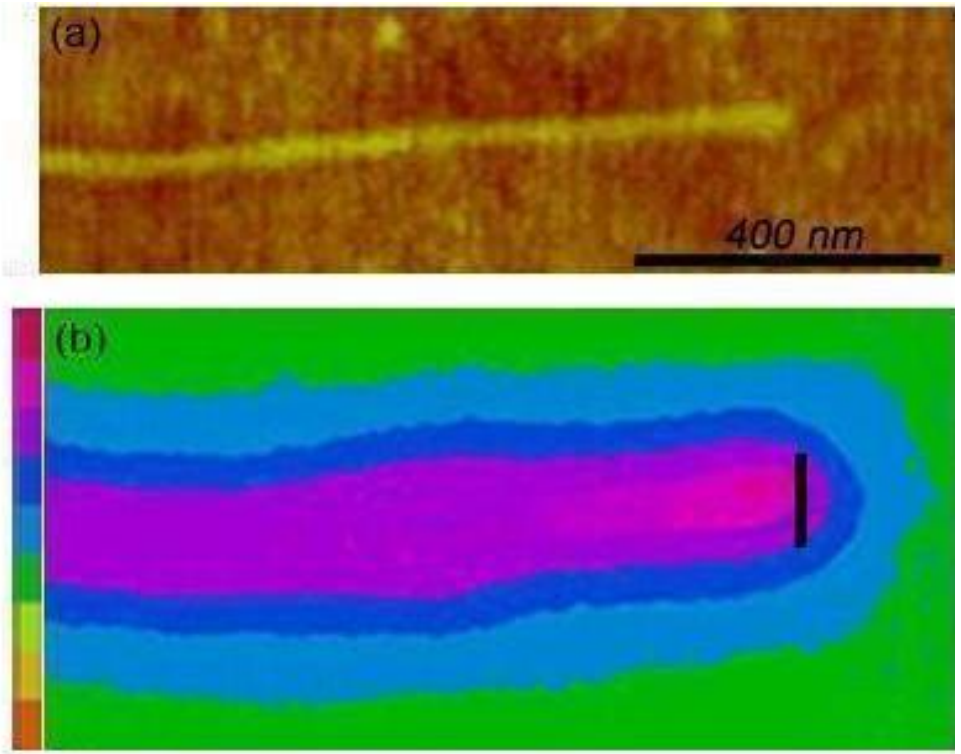
Charge-dipole model: Experimental verification

Charge injection experiments:





M. Zdrojek and T. Mélin, ISEN, IEMN, France.

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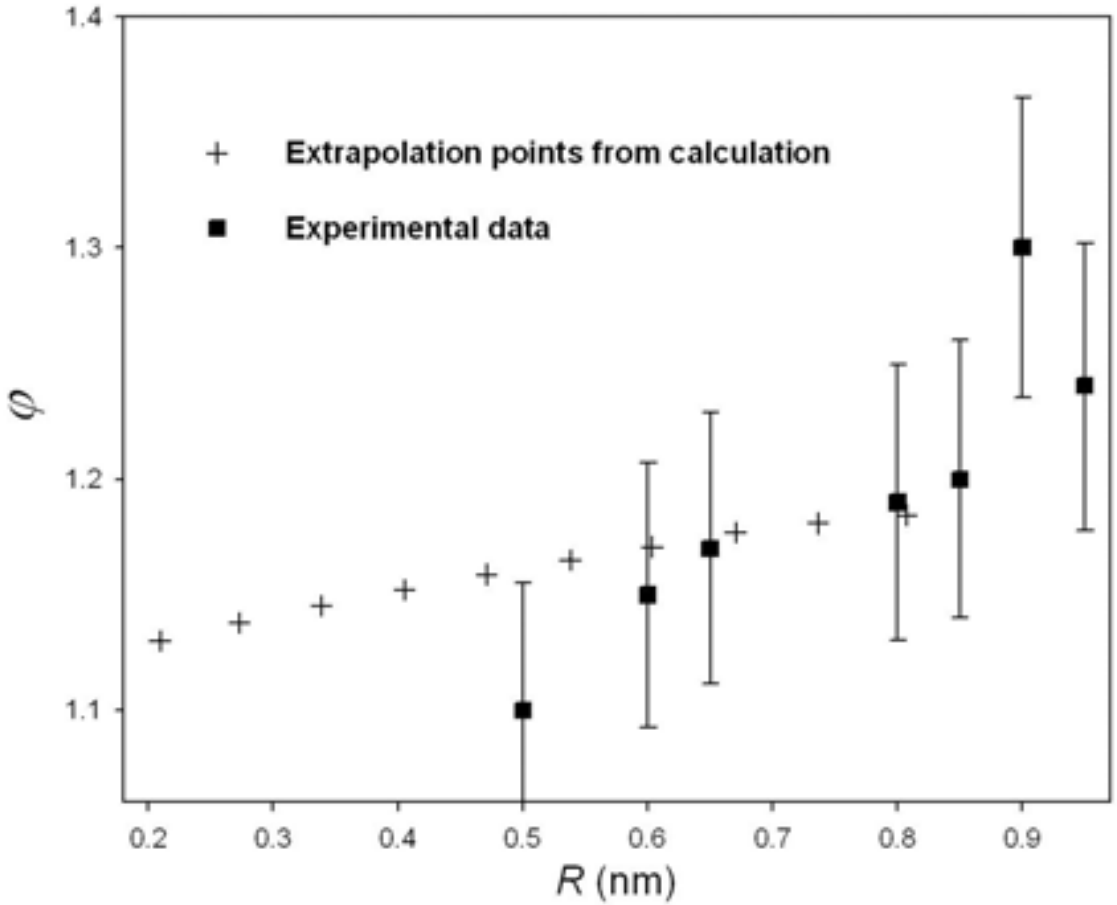
Charge-dipole model: Experimental verification

Enhancement ratio vs. tube Radius R



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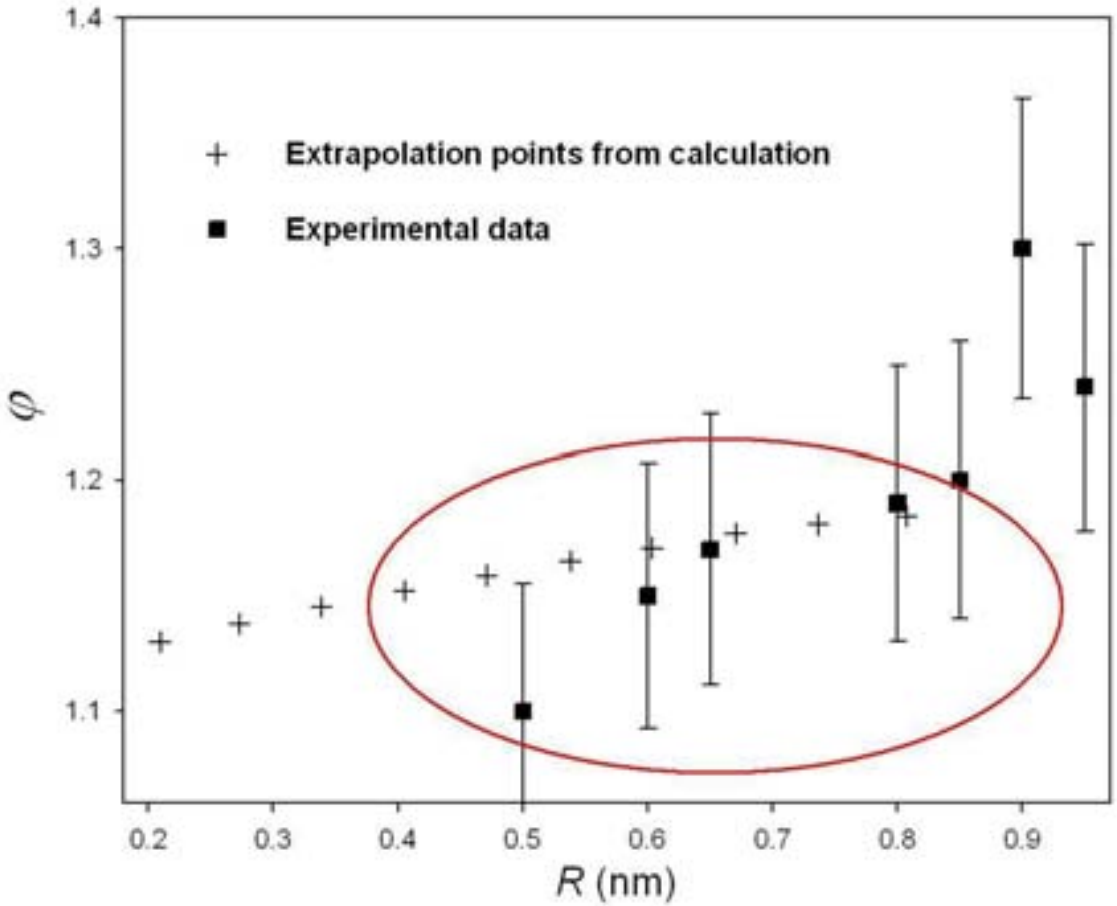

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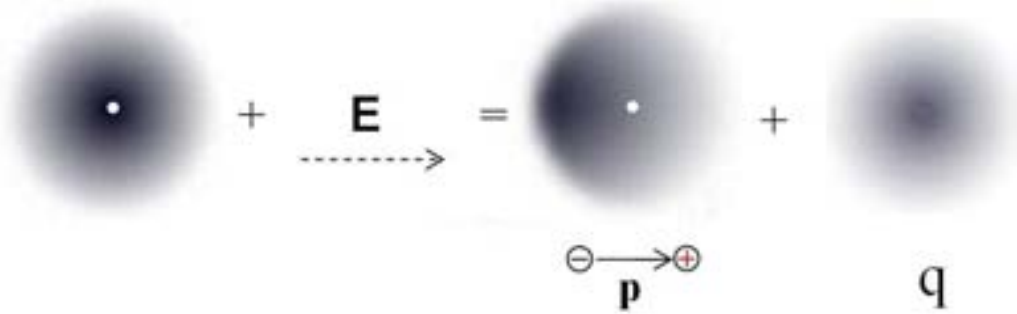

Ref: PRB 78, 085425 (2008).

79, 155407 (2009).

- U_{bond}: Empirical many-body potential - AIREBO.

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

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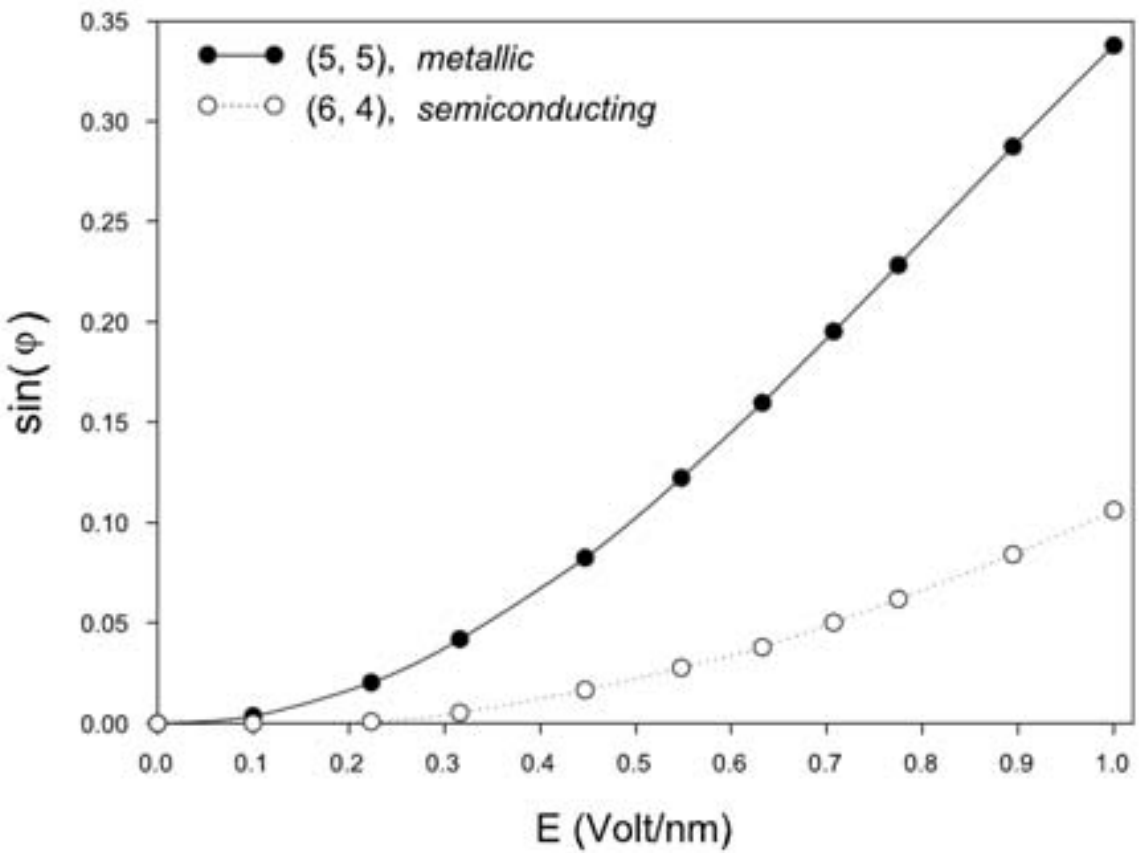
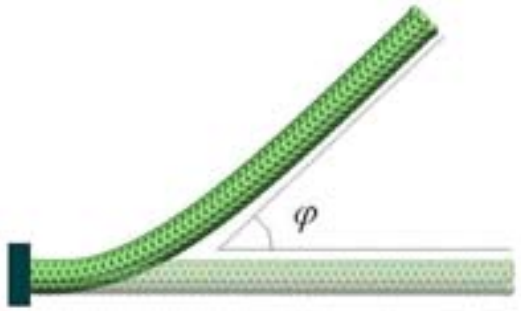
Cantilevered NT: Influence of field strength E





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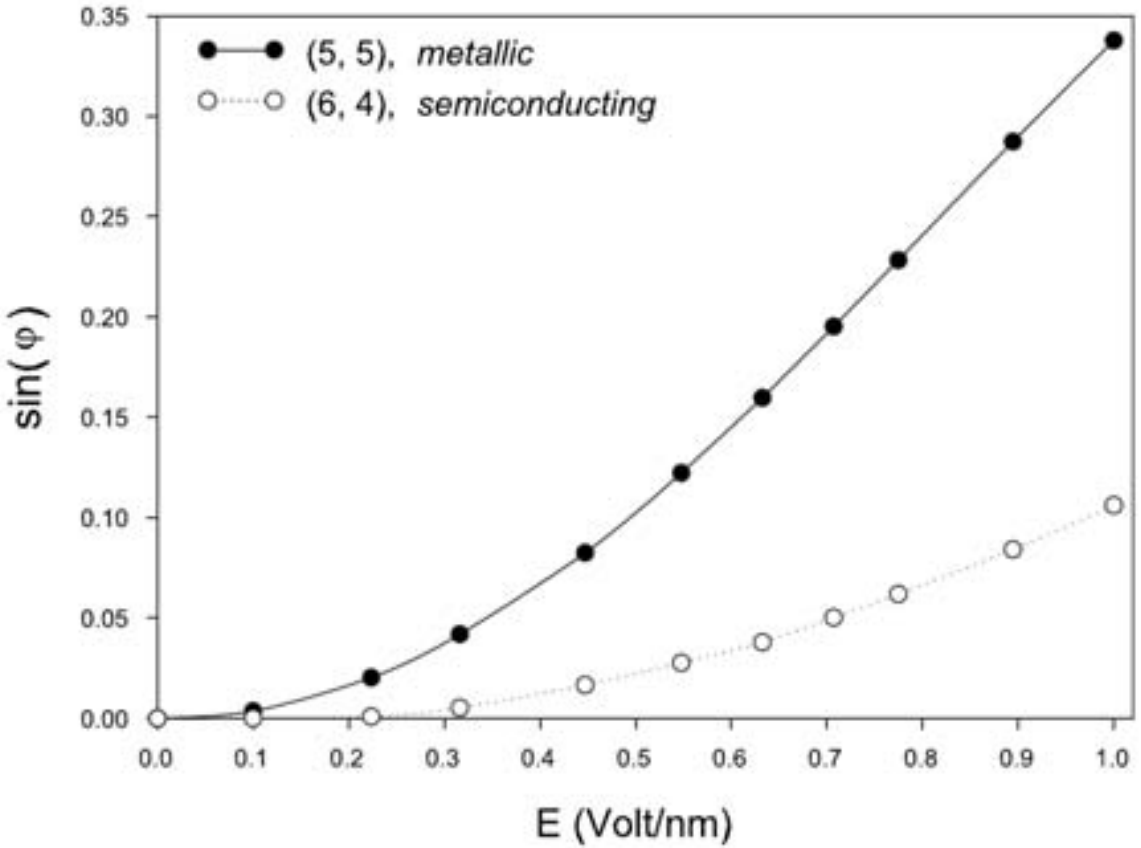

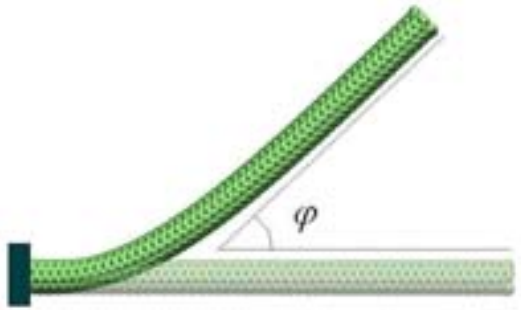

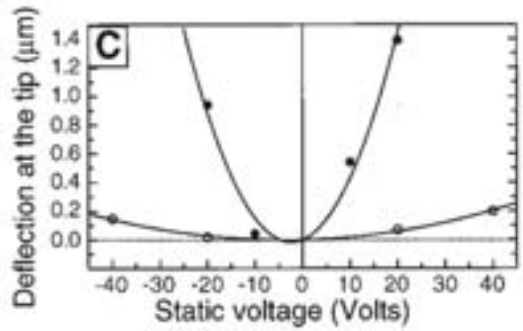

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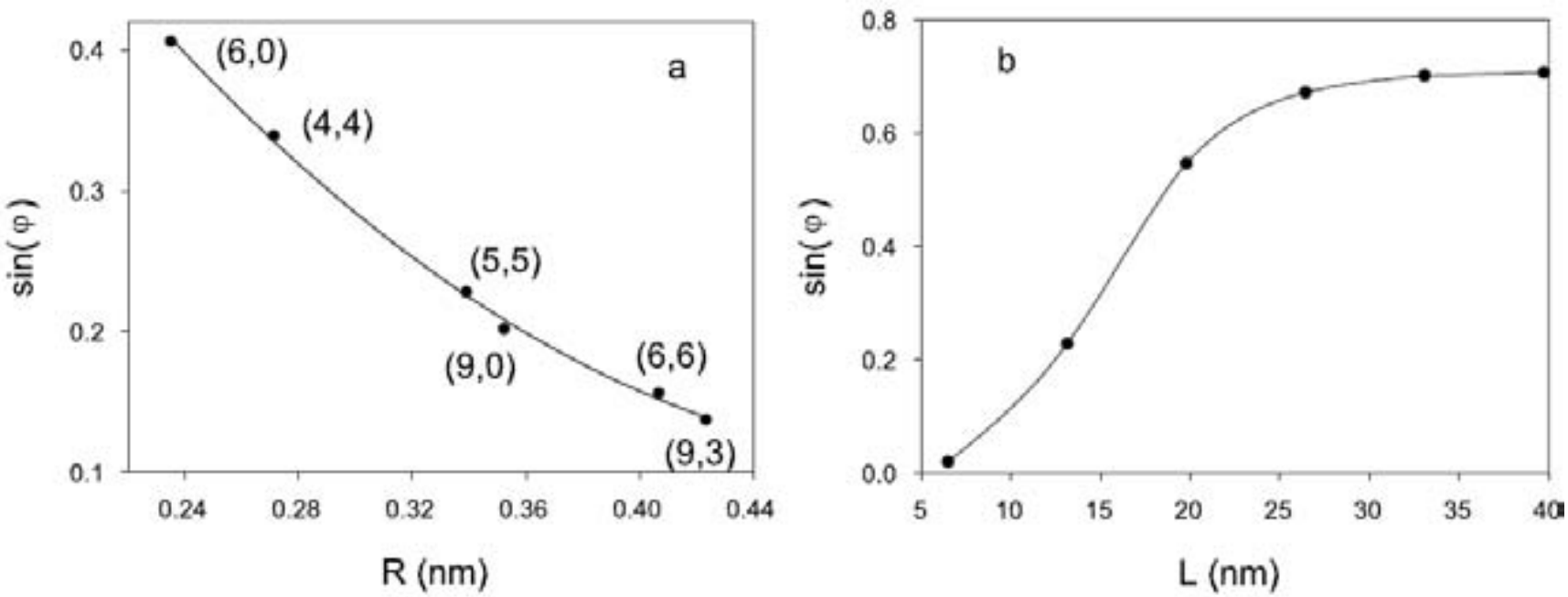
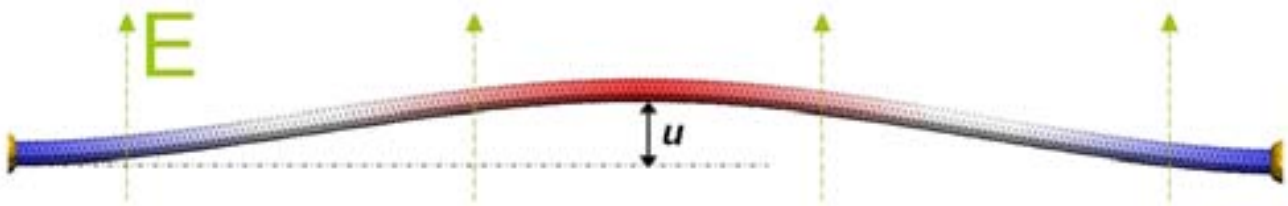
Cantilevered NT: Effects of tube geometry



Ref: PRB 75, 205414 (2007).
76, 195434 (2007).

SWCNT > MWCNT

Suspended NT: Influence of field strength E



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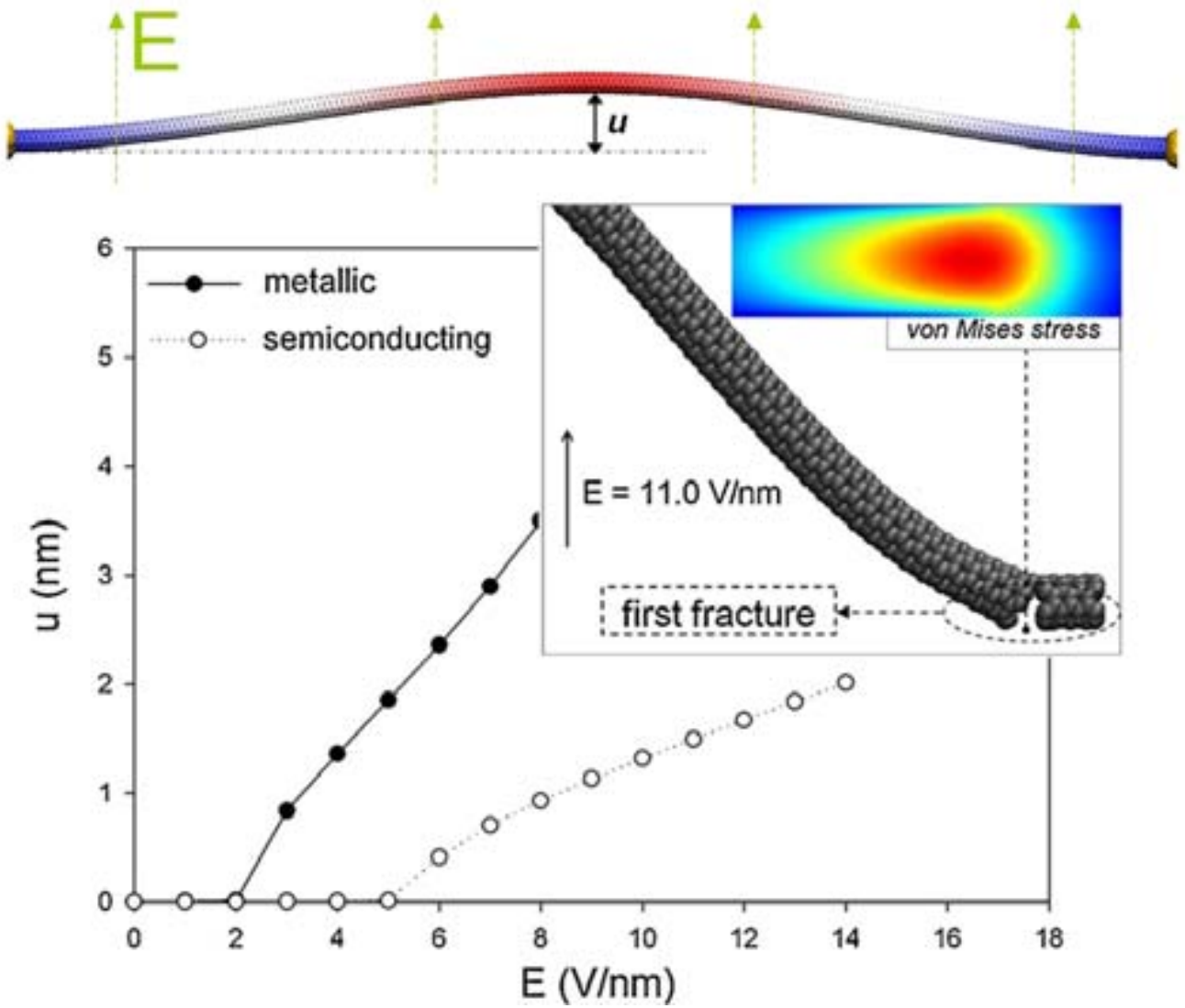

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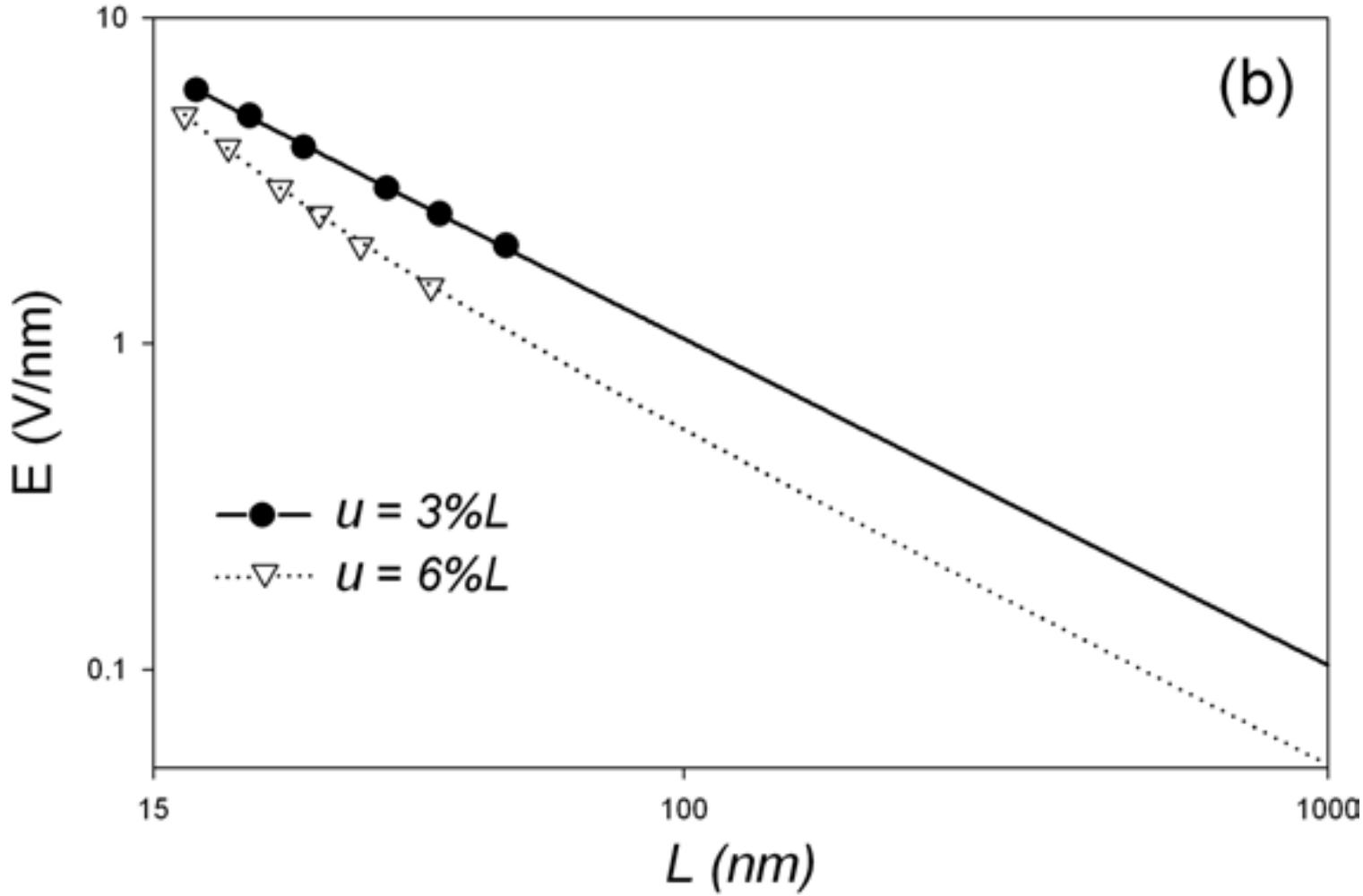

Ref: PRL 102, 215501 (2009).

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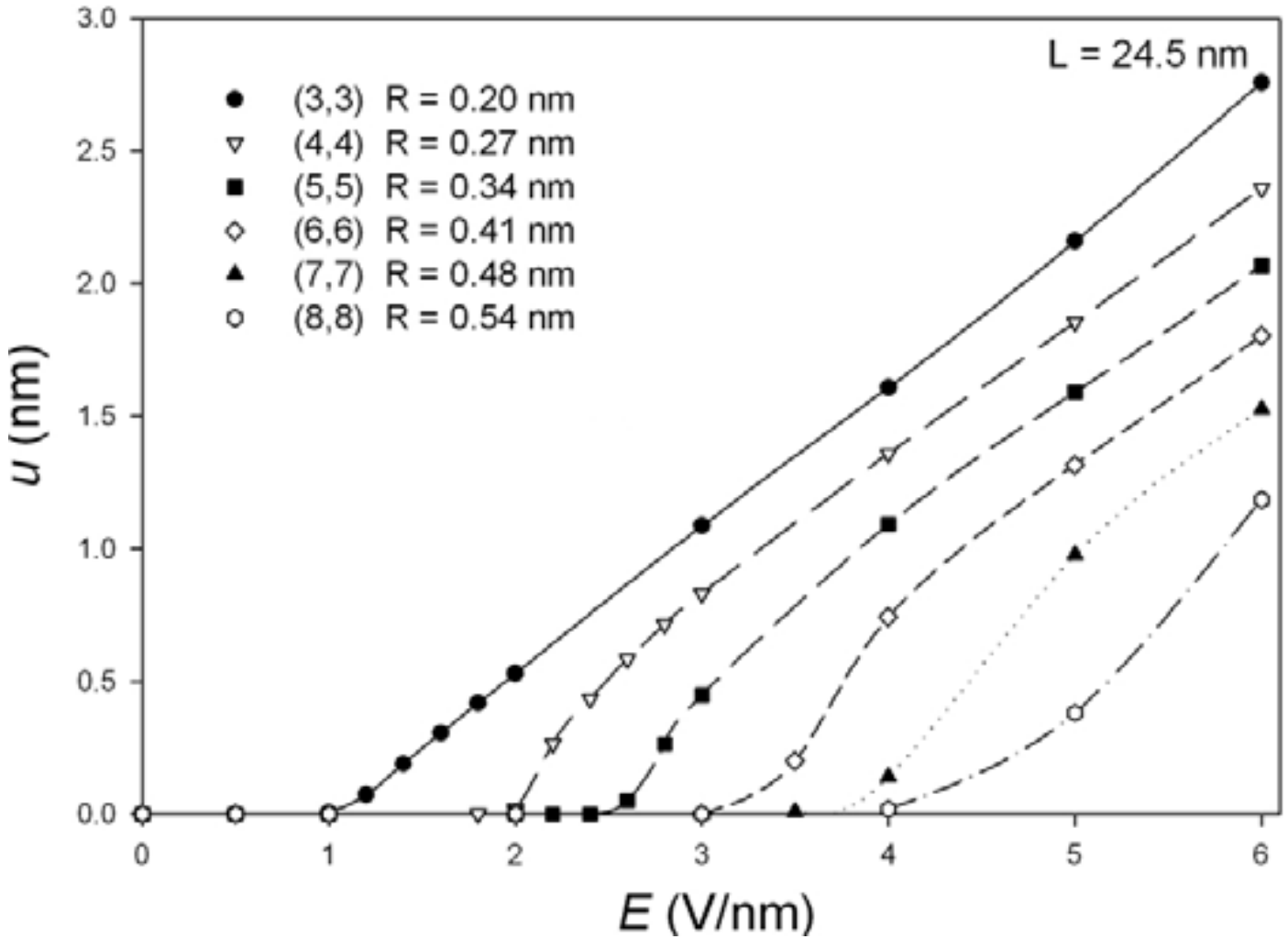
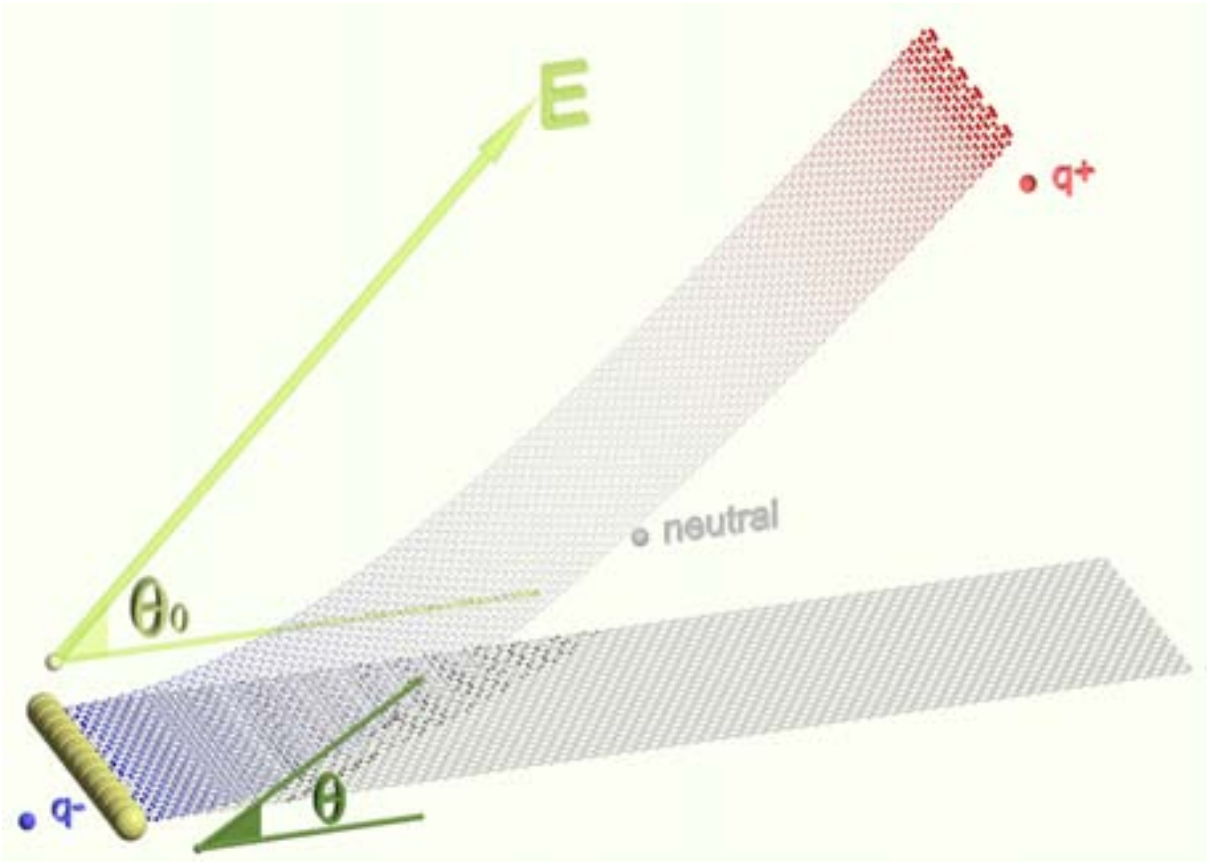


Ref: PRL 102, 215501 (2009).

Cantilevered Graphene: Alignment



Ref: Carbon 47, 3050 (2009).

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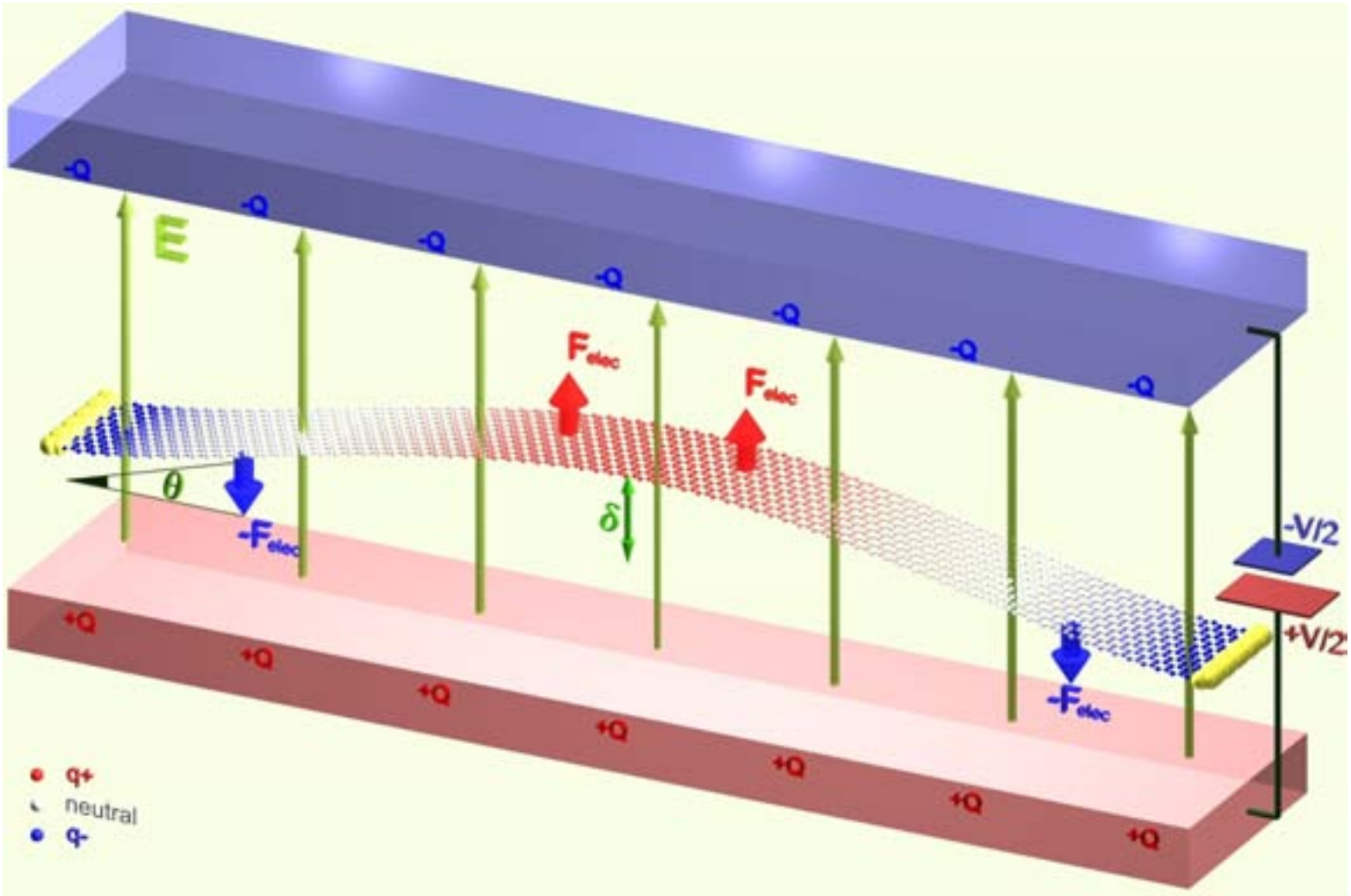
Suspended Graphene: Deformation



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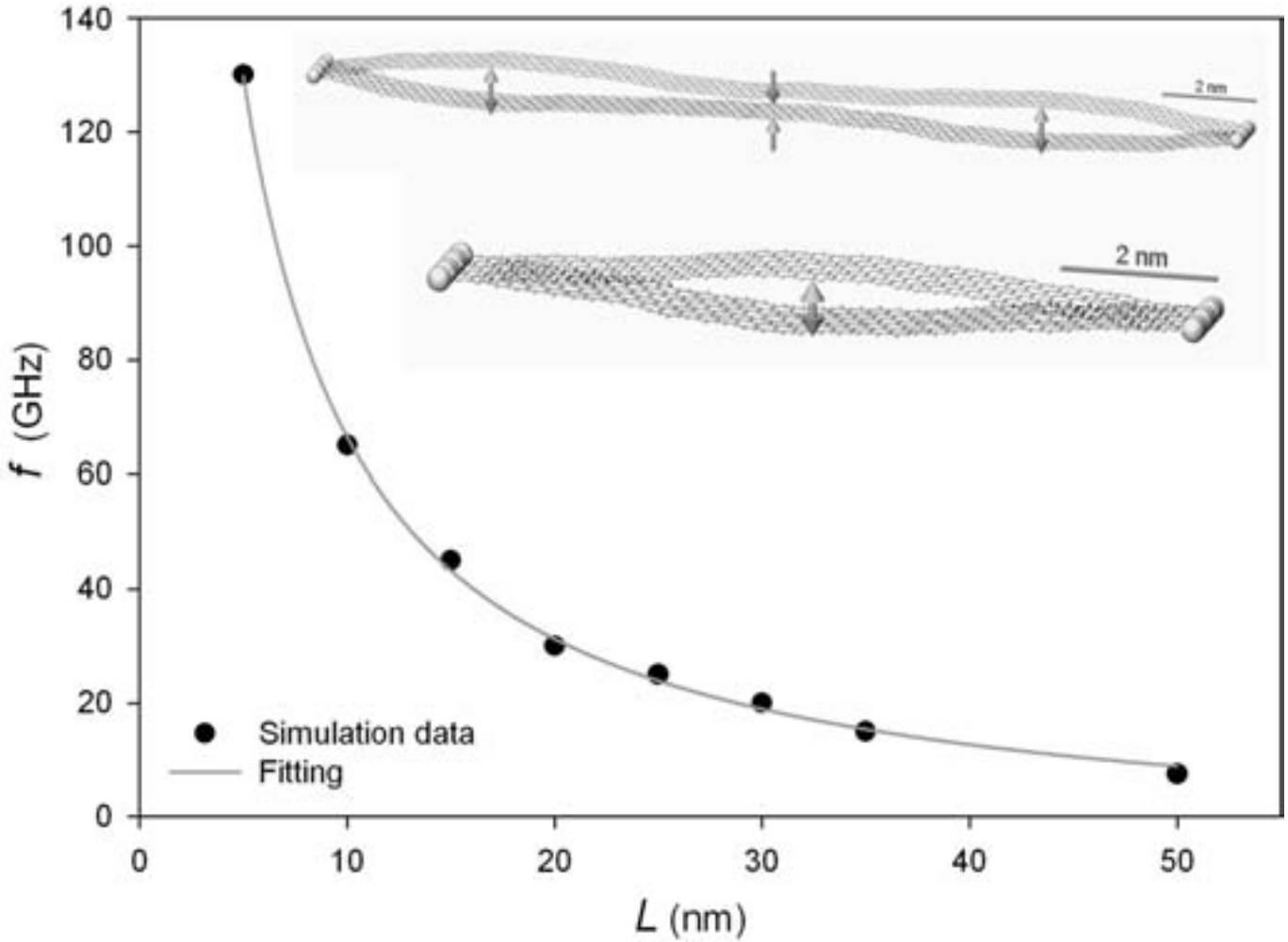
Suspended Graphene: Vibration



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Main points

- Metallic nanotubes -> more mechanically sensitive to an external electric field than the semiconducting ones.
- Single-walled tubes -> more electrostatic deformation than the multi-walled ones.
- Deformation -> increases with length but decreases with radius.
- Graphene nanoribbons -> easier to be bent.

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Co-workers

Exp	L. Philippe, J. Michler	EMPA, Thun, Switzerland.
Theo	M. Devel, R. Langlet	University of Franche-Comté, Besançon, France.
Theo	R. W. Scharstein	University of Alabama, Tuscaloosa, AL, USA.
Theo	D. A. Stewart	Cornell Nanoscale Facility (CNF), Ithaca, NY, USA.
Exp	M. Zdrojek	Institut Catala de Nanotecnologia, Bellaterra, Spain.
Exp	T. Mélin	ISEN, IEMN, Villeneuve d'Ascq, France.
Theo	S. J. Stuart	Clemson University, South Carolina, USA.

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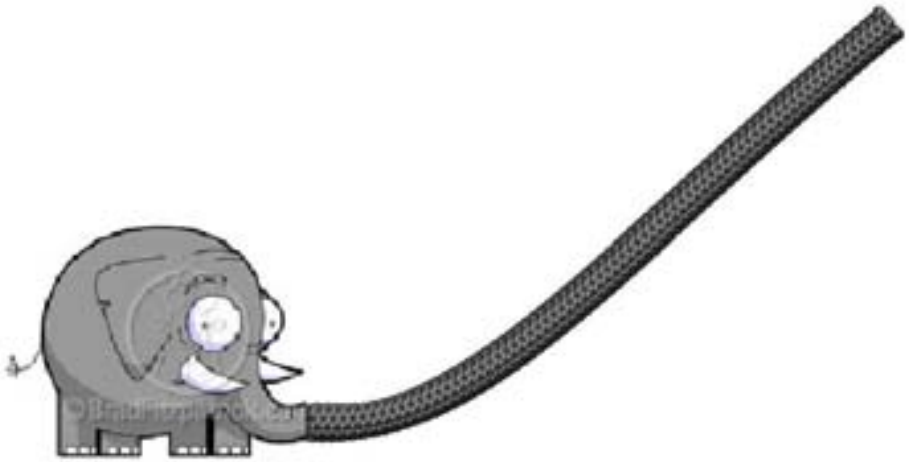
Thanks



Thank you for your attention!

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