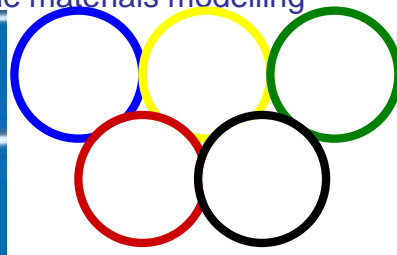


Indo-US Workshop on Nanotechnology: Issues in  
Interdisciplinary Research and Education  
Bangalore, Aug. 11-13 2004

A revolution is under way: manipulation of the material world  
at the **atomic** level – **ultimate** limit

Modelling materials properties, from the nanoscale to the  
macroscale – multiscale materials modelling



*ATHENS 2004*

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Harvard University

Examples of physical phenomena  
related to the behavior of complex systems

Brittle or ductile behavior of solids (**mechanical properties**)

Corrosion, catalysis, fatigue (**chemistry on and inside solids**)

All biological processes (**chemistry with enzymes in water**)

Phenomena related to electrons (**electronic and magnetic**)

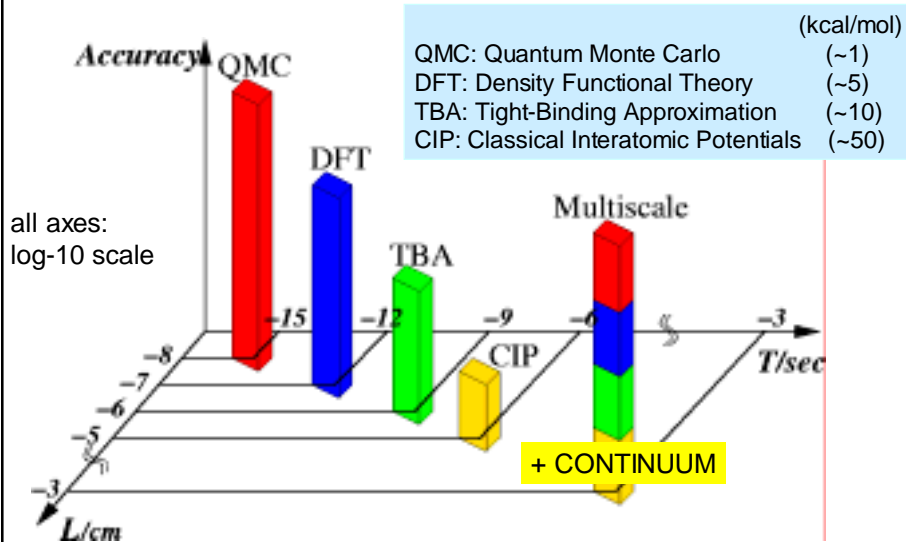
Ultimately, everything is related to microscopic, atomic-scale  
processes, but...

knowing how each and every atom (or electron) behaves  
is **impossible** and may even be **undesirable**

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## The quest for accuracy and realistic simulations leads to Multiscale Modeling Methods



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## Examples of what MMM can do

### Brittle or ductile behavior of solids (mechanical properties)

- Embrittlement of Molybdenum Disilicide (PN model + DFT)
- Nano-indentation of Silicon (QC method + TBA)
- Piezoelectric response of Lead Titanate (QC method + DFT)
- Dislocations in Aluminum and Silicon (SDPN model + DFT)
- Brittle fracture of Silicon (MAAD + TBA)**

### Corrosion, catalysis, fatigue (chemistry on and inside materials)

- Hydrogen-induced embrittlement of Aluminum (SDPN model + DFT)
- Ordering in Carbon-enriched Si surfaces (DFT + Potts model)
- Reactivity of Molybdenum-oxide surfaces (DFT + KMC)
- Role of geometry in catalytic efficiency of microchannels (LBE)
- Impurity-induced embrittlement of metal alloys (OF-DFT + EAM)**

### Biologically-related processes

- Conductivity of DNA nanowires (DFT + KG)**
- Rotary motion in ATP-ase (CHARMM)**

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The Computer Magazine for Scientists and Engineers

# COMPUTERS IN PHYSICS

NOVEMBER 2000

**Direct multiscale simulation of brittle fracture**

**microscopic:** dynamics w/quantum mechanical forces

**mesoscopic:** dynamics w/classical (empirical) forces

**macroscopic:** continuum elasticity, finite elements

Multiscale Ab-initio Atomistic Dynamics (MAAD -Silicon)

Abraham, Broughton, Bernstein, Kaxiras  
Europhys. Lett. **44**, 783 (1998),  
Phys.Rev. B **60**, 2391 (1999).

Materials Simulation Software Contest Awards

AMERICAN INSTITUTE OF PHYSICS

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## Essentials of the MAAD-Si simulation

(a) (b) (c)

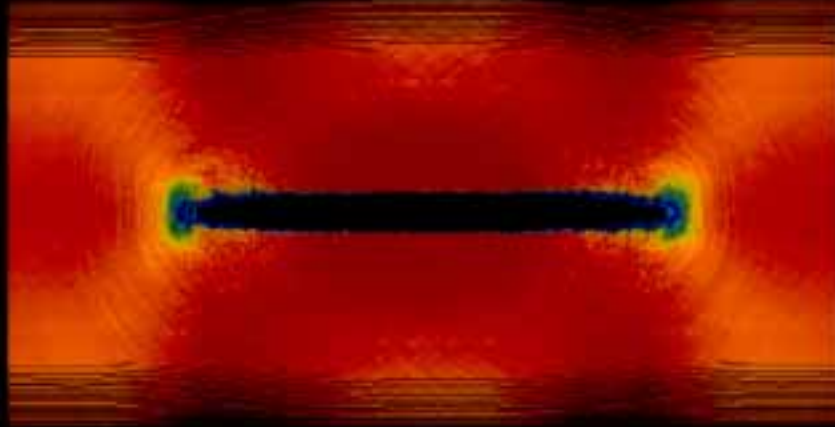
FE MD

TB MD

electrons  
"silicogens"

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Stress waves pass from MD to FE

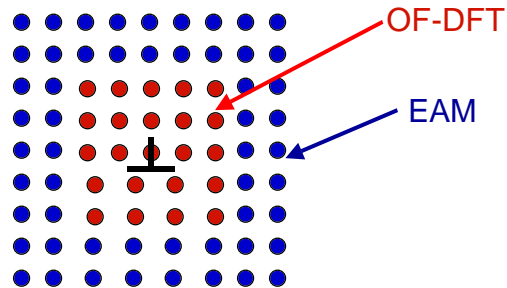


Seamless coupling across boundaries: no reflection of stress waves

Embrittlement of metal alloys by  
chemical impurities (hydrogen)

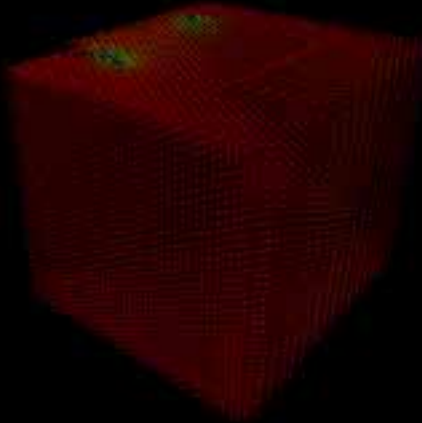


## Orbital-Free-DFT in Multiscale Simulations

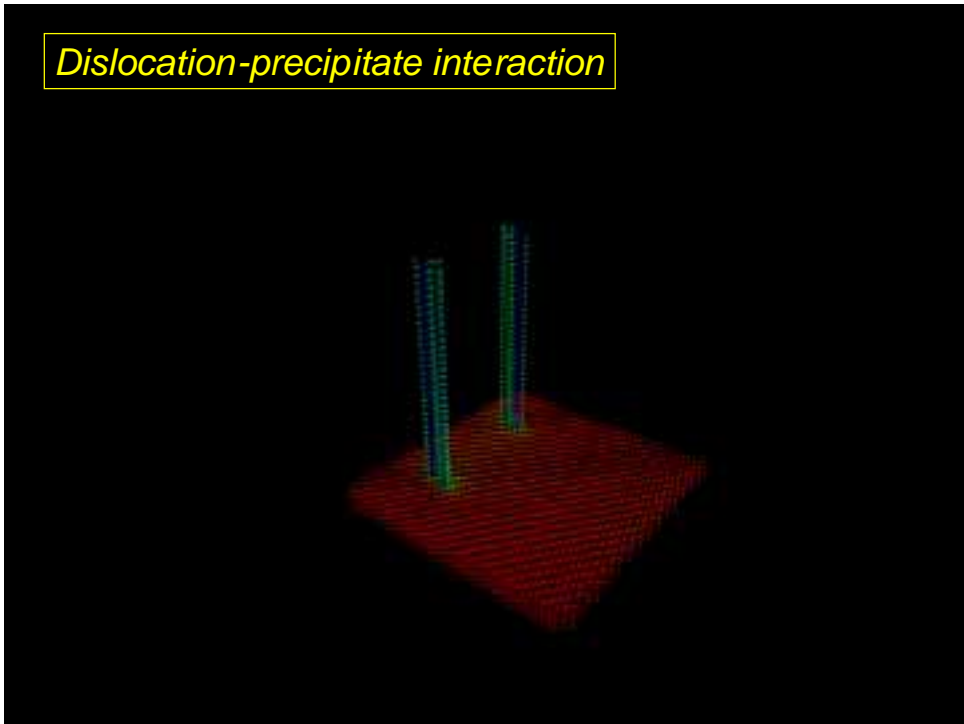


- Boundary conditions for  $\rho(\mathbf{r})$  only
- Coupling to classical atomistics:  
Embedded-Atom Method (EAM)
  - designed for simple metals
  - based on DFT arguments

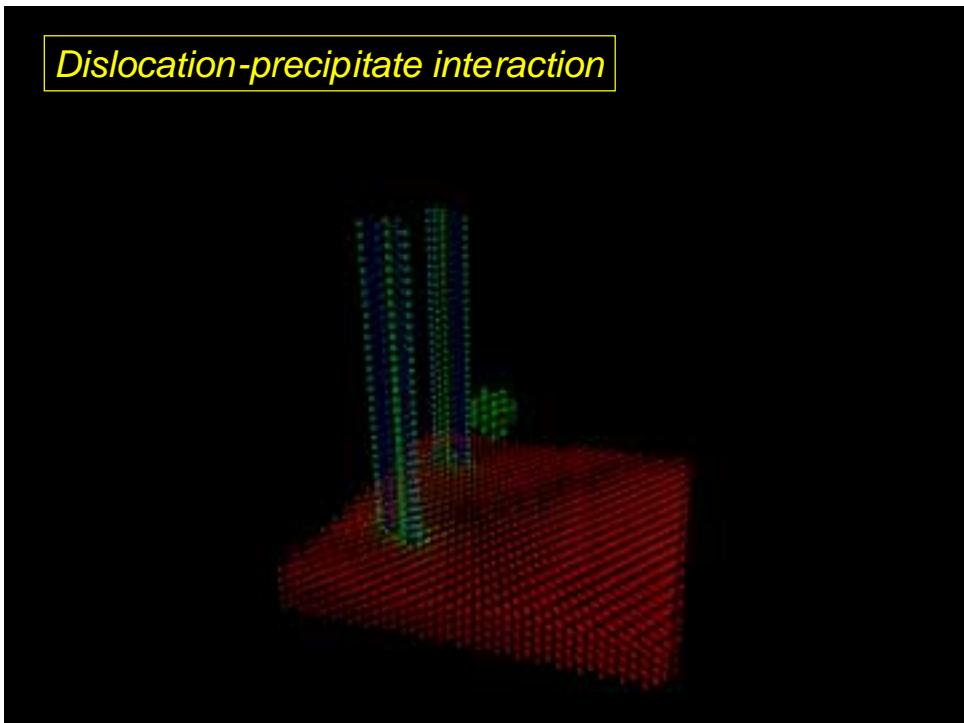
*Dislocation-precipitate interaction  
(60,000 atoms total, 300 atoms in OF-DFT region)*



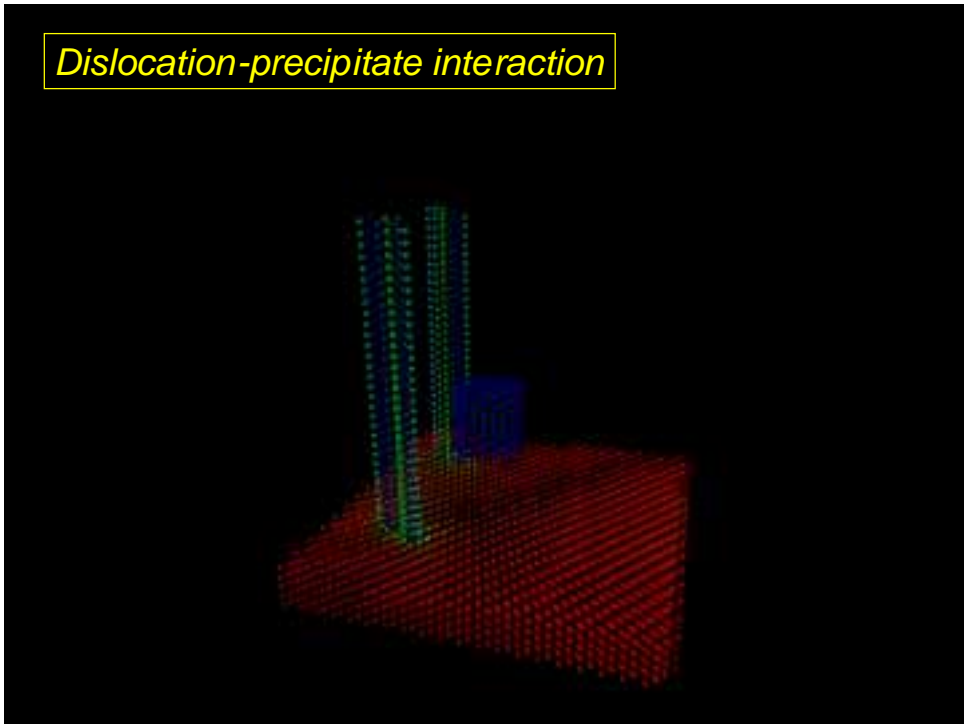
*Dislocation-precipitate interaction*



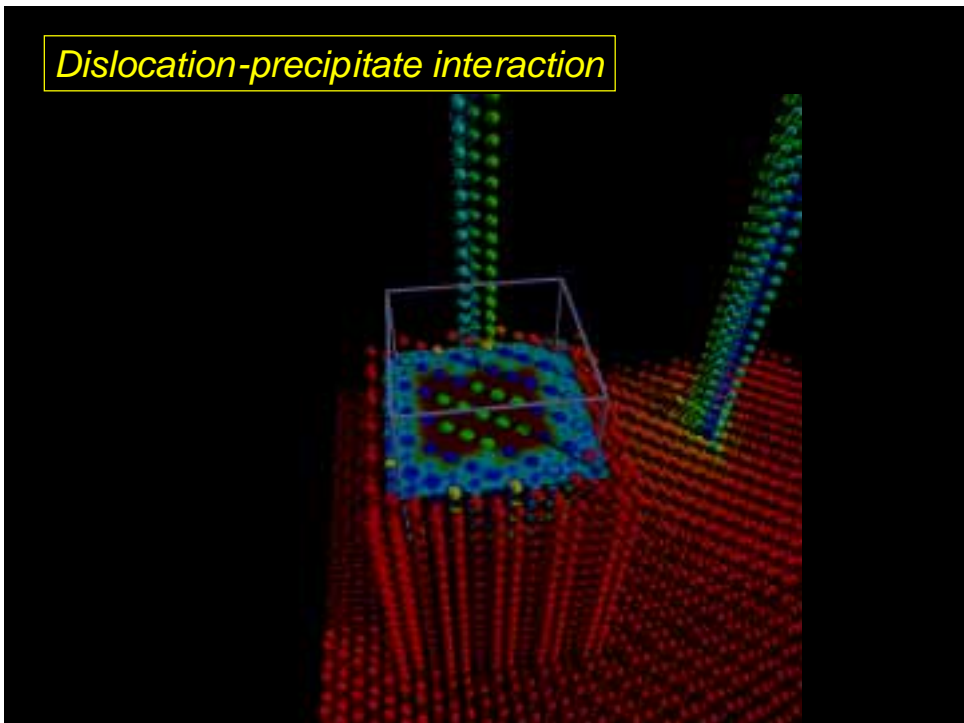
*Dislocation-precipitate interaction*



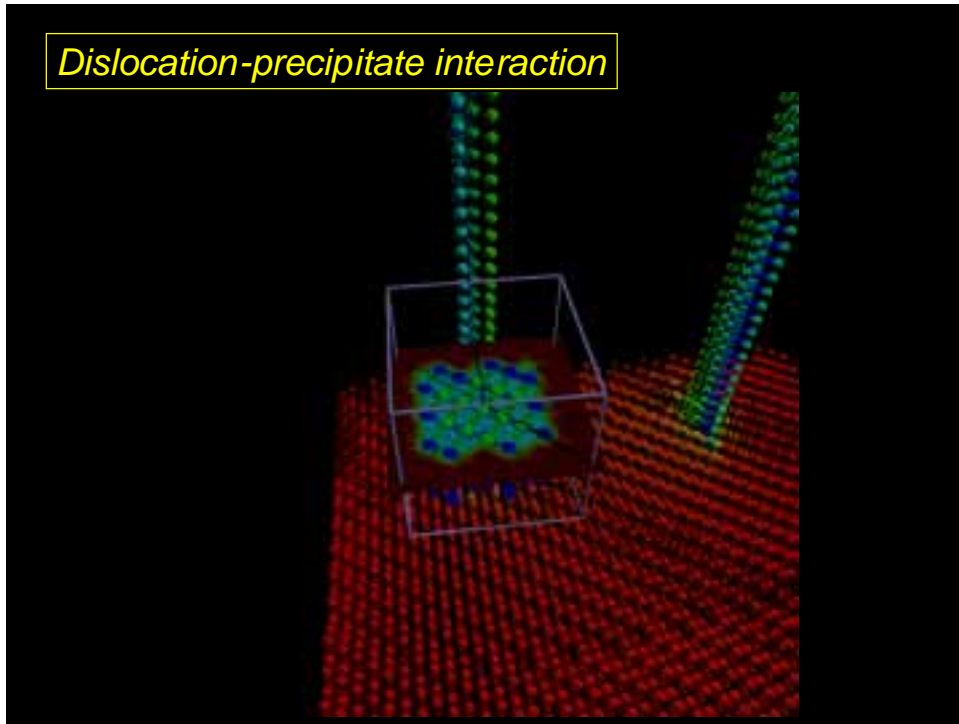
*Dislocation-precipitate interaction*



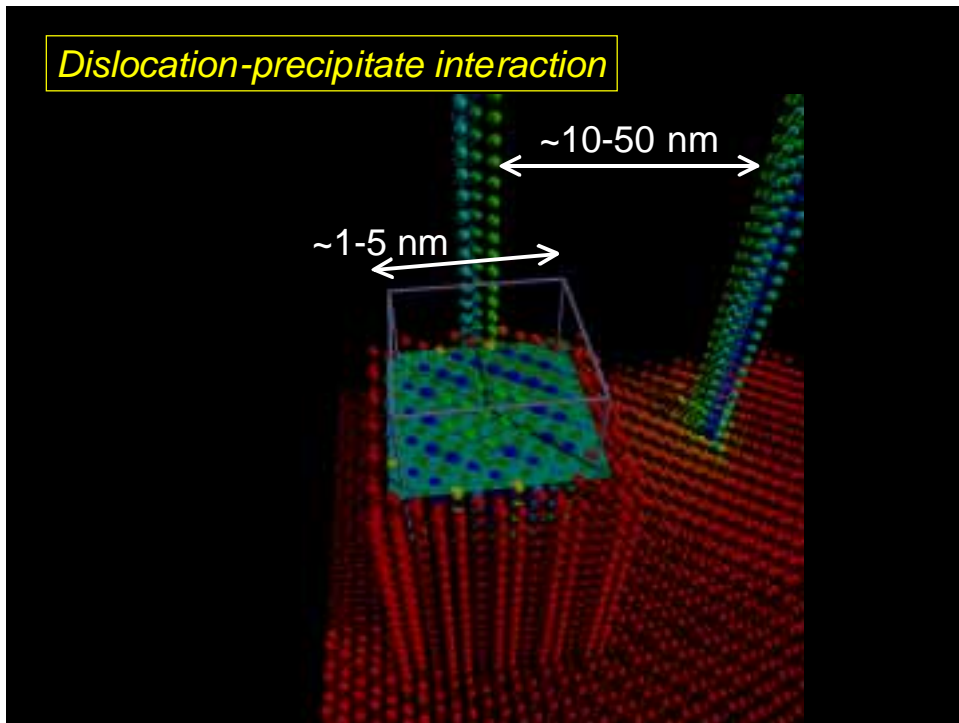
*Dislocation-precipitate interaction*



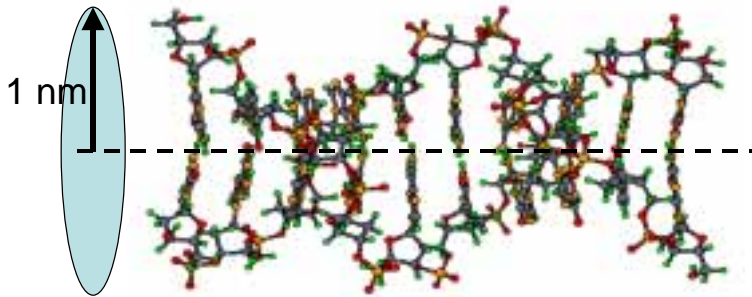
*Dislocation-precipitate interaction*



*Dislocation-precipitate interaction*



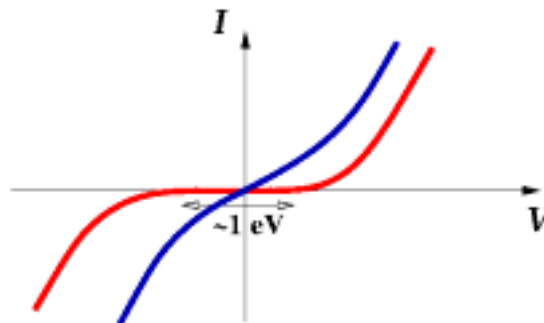
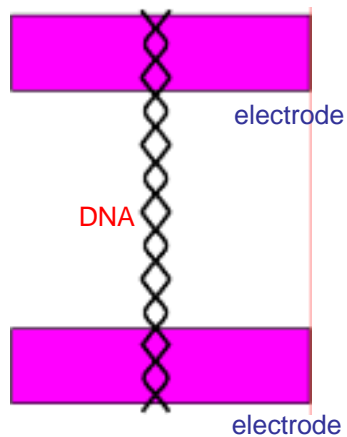
## Electronic Structure of overstretched DNA



Conductivity of DNA has been the subject of intense investigation

metallic – semiconducting – insulating behavior, all reported  
by experimental studies [Fink, *Cell. Mol. Life Sci.* **58** (2001)]

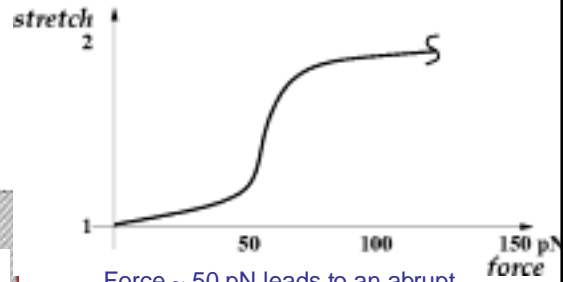
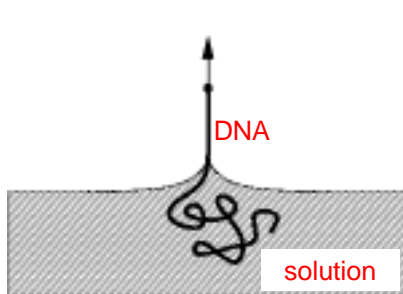
## Experimental measurement of DNA conductivity



Current  $I$  as function of voltage  $V$  can  
indicate behavior of **METAL** or  
**INSULATOR**

Porath, Bezryadin, De Vries, Dekker  
*Nature* **403**, 635 (2000)

## Relevance of stretched DNA forms\* in experiments



Force ~ 50 pN leads to an abrupt elongation by almost factor of 2  
Force > 100 pN leads to breaking

C. Bustamante and co-workers  
*Science* **258**, 1122 (1992); **271**, 795 (1996)

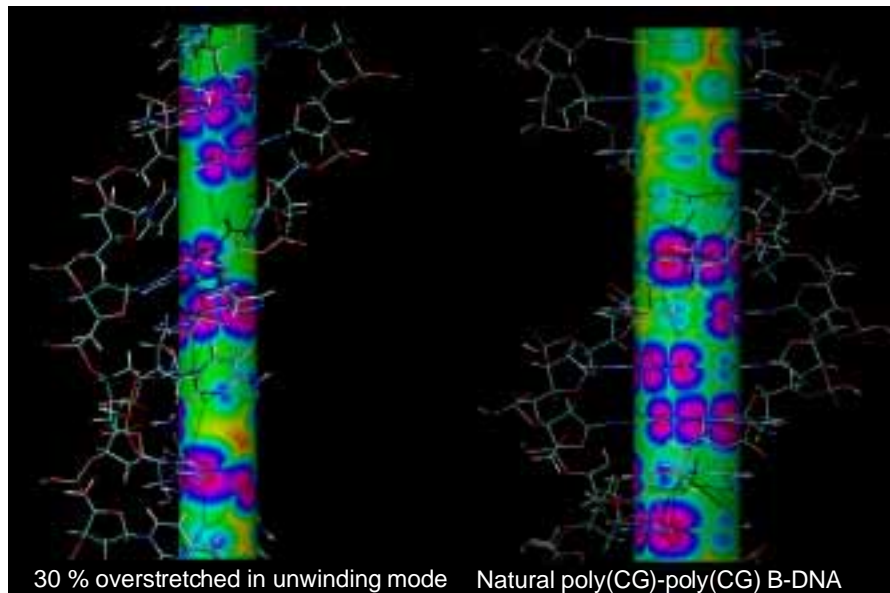
Multiscale issues: structure of stretched form (mesoscale) affects electronic states (microscopic)

\*Stretched structures from: A. Lebrun and R. Lavery,  
*Nucleic Acids Research* **24**, 2260 (1996)

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## Visualization of electronic states

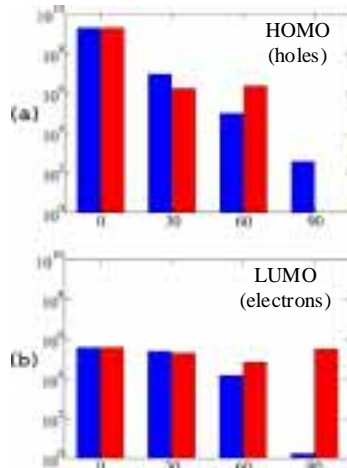


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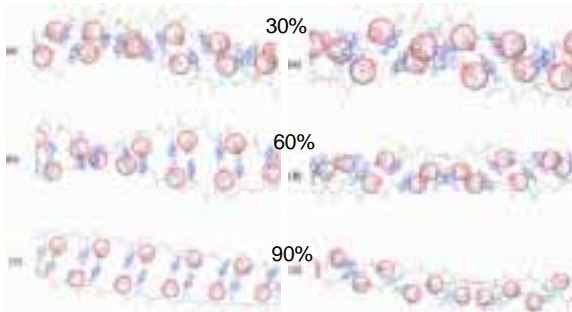
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## Hopping matrix elements of HOMO and LUMO bands

$$-\langle \quad | \quad | \quad \rangle$$



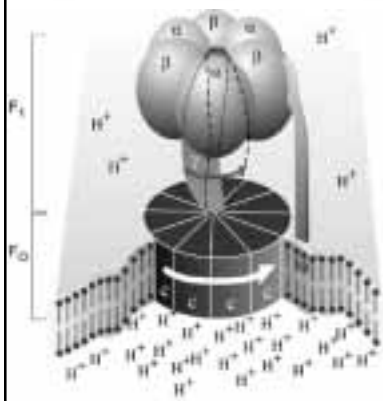
3'-3' stretching-mode      5'-5' stretching-mode



P. Maragakis, R. Barnett, E. Kaxiras,  
M. Elstner, Th. Frauenheim, Phys. Rev. B (2002)

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Nobel Prize  
(Chemistry):  
Mitchell (78)  
Boyer (97)  
Walker (97)



"ATP-ase biomolecular rotary motor containing a  
genetically engineered chemical switch"  
C.D. Montemagno & coworkers (UCLA) - 2002

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## Bottom up approach to ATP synthase

$F_1: \text{---}3\text{---}3\text{---}$

$F_o: ab_2c_{10-14}$

Fo: ion translocation / attachment-detachment	QM
Fo: subunit c conformational change	MD
Fo: subunits c & a rotational motion	MD
F1/Fo: electrochemical to mechanical energy	CF
F1: mechanical to chemical energy	??

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## Structure of Fo part

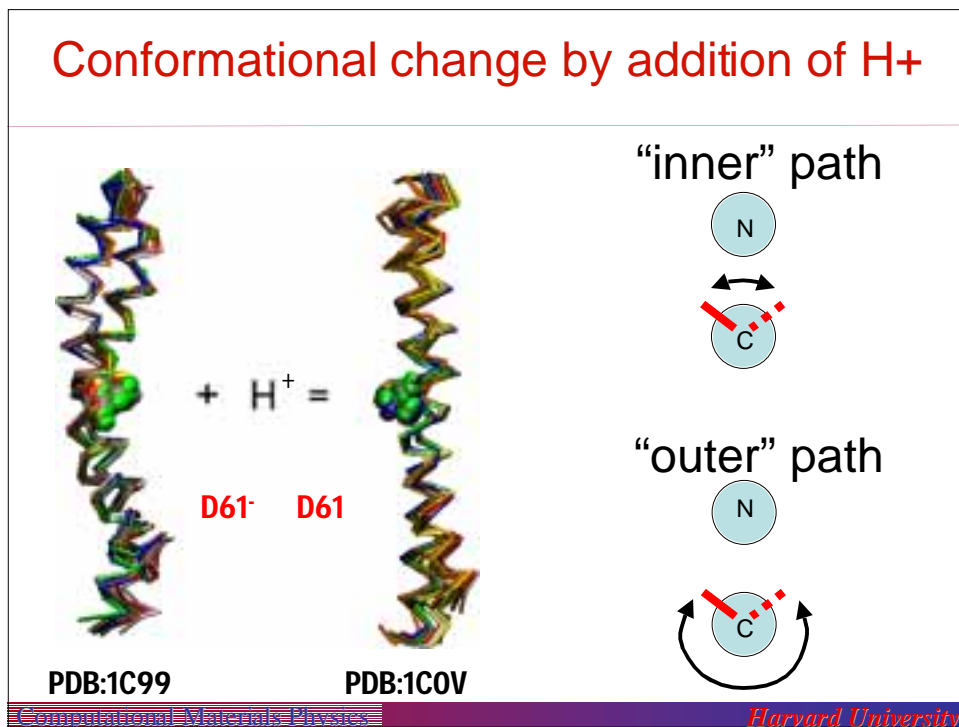
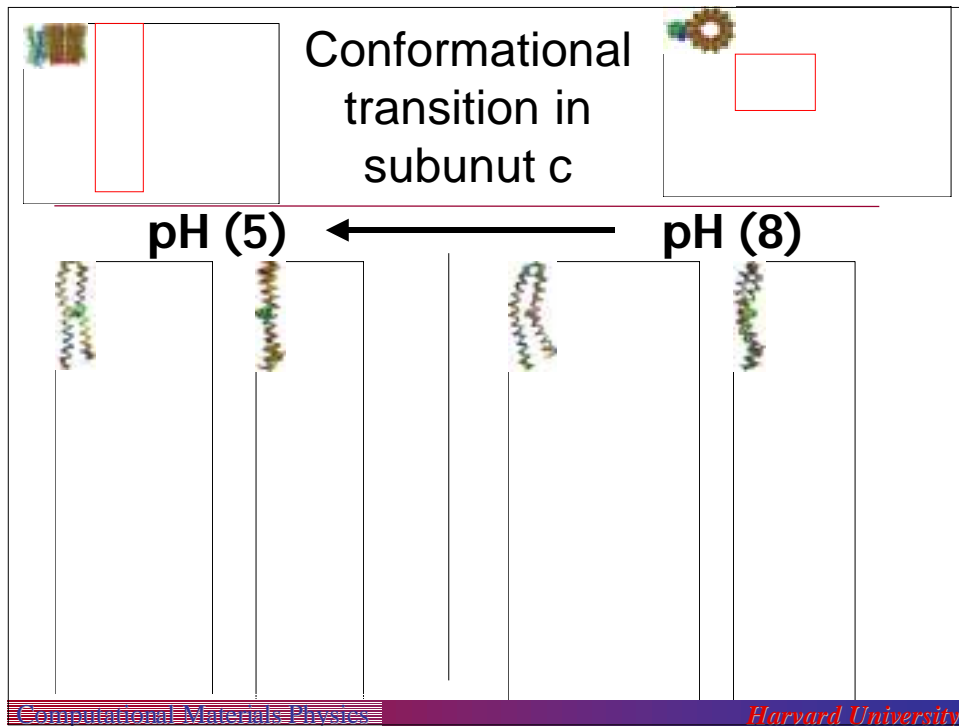
Stock et al., Science (1999)  
[first X-ray structure]

Rastogi and Girvin, Nature (1999)  
[first NMR studies of subunit c]

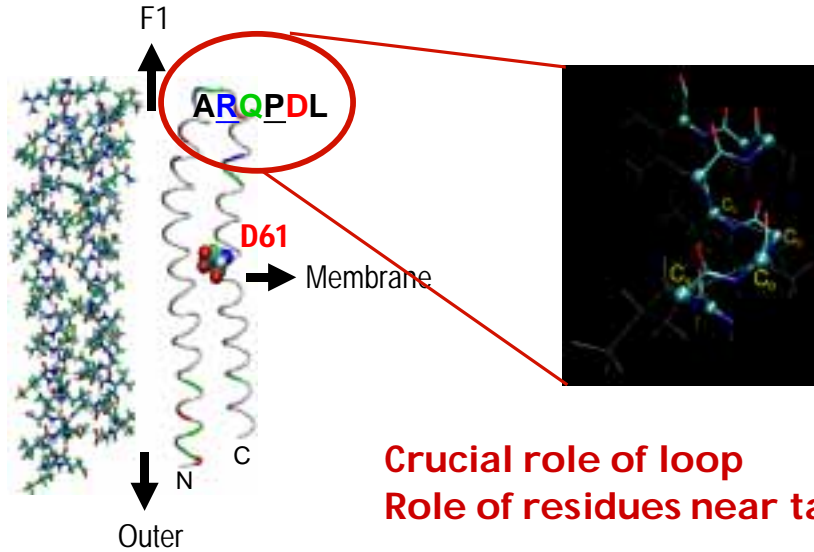
The smallest rotor:

- how is rotation accomplished?
- why choose this particular structure?

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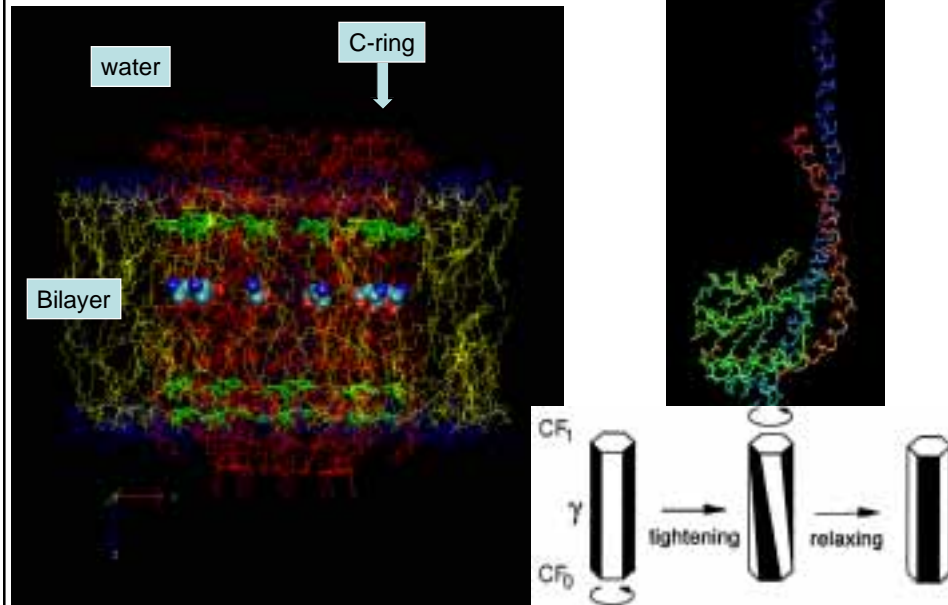


# Anatomy of subunit c at work



**Crucial role of loop**  
**Role of residues near tails**

# Future: c ring and mechanical energy transfer



## Multiscale Simulations of Complex Physical Systems

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Pantelis Kelires (U of Crete)  
Qiang Cui (Harvard)  
Martin Karplus (Harvard)  
Sauro Succi (U of Rome)  
Weitao Young (North Carolina)  
Weinan E (Princeton)  
Emily Carter (UCLA)

**Department of Physics and Division of Engineering and Applied Sciences**  
**Support: Harvard MRSEC (NSF), AFOSR (Brown MURI)**

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## Educational issues

**Interdisciplinarity** ↔ **Breadth of knowledge**

Specifics of a field: information / language barrier

Thorough grounding on basics, e.g.  
Quantum Mechanics (S. Tiwari)  
Thermodynamics (M. Rodwell)

Problems: taught by “experts”  
maintain student interest

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## Educational issues

Need for new standard “texts”:  
cut across scientific boundaries,  
modern & exciting examples,  
use of electronic media

Interdisciplinary courses:  
motivation – light at end of tunnel  
direct relation to current research

Applied Physics 298 – Physics & Chemistry of Materials  
Materials Research Science and Engineering Center (NSF)  
3 areas (introduction, examples), 28 lectures, 12 speakers