**School on Numerical Methods for Materials Science
Related to Renewable Energy Applications**

Model potential molecular dynamics simulations of nanostructured materials for photovoltaics

Alessandro Mattoni, Claudia Caddeo, M.Ilenia Saba

**Istituto Officina dei Materiali del CNR
Unità Cagliari SLACS**
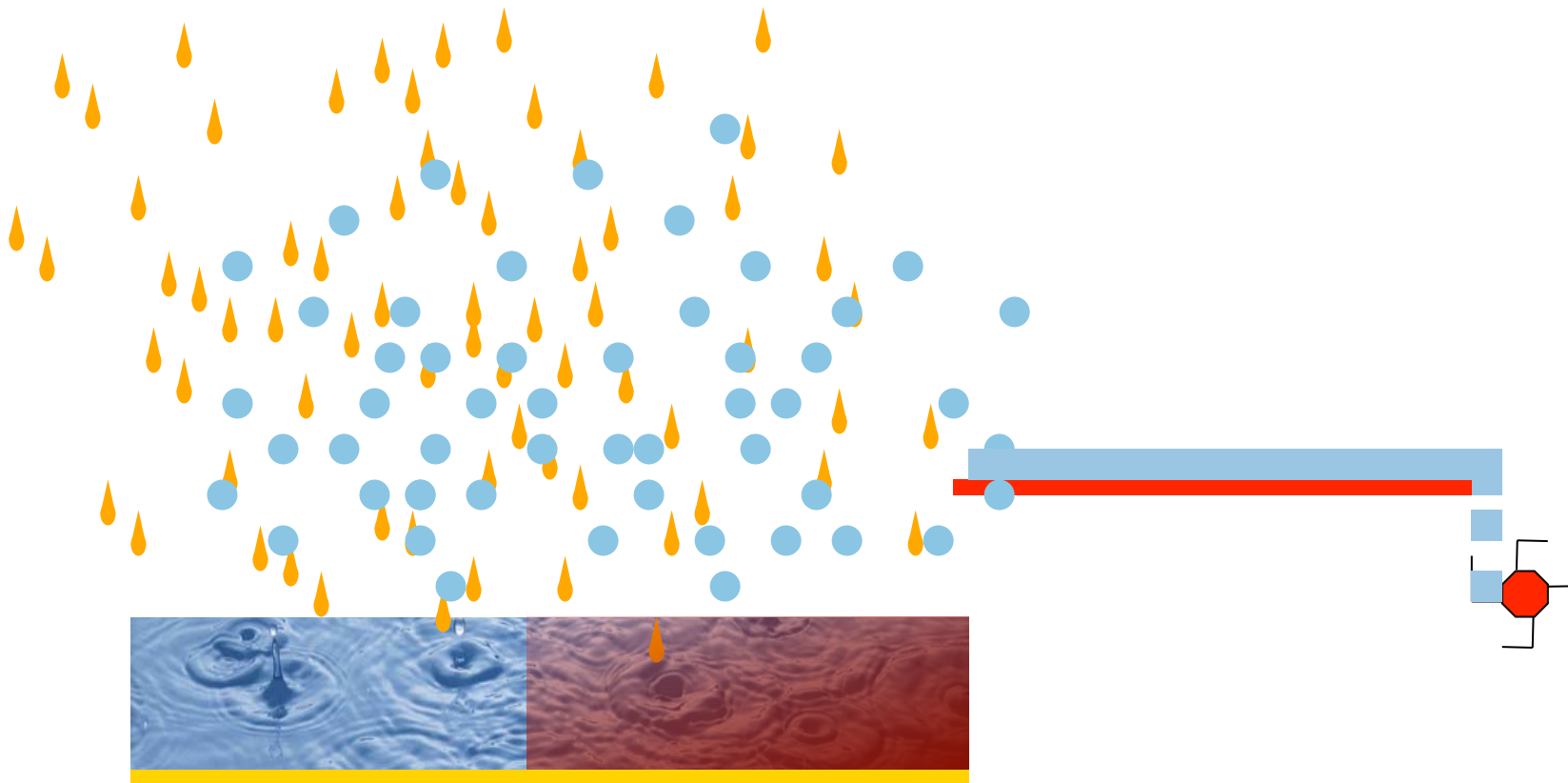
Univerity of Cagliari Dept of Physics

url: **http://www.dsf.unica.it/~mattoni**

email: **alessandro.mattoni@dsf.unica.it**

Trasport of fluid

Constant flux of fluid to the load

Absorption

Photon flux

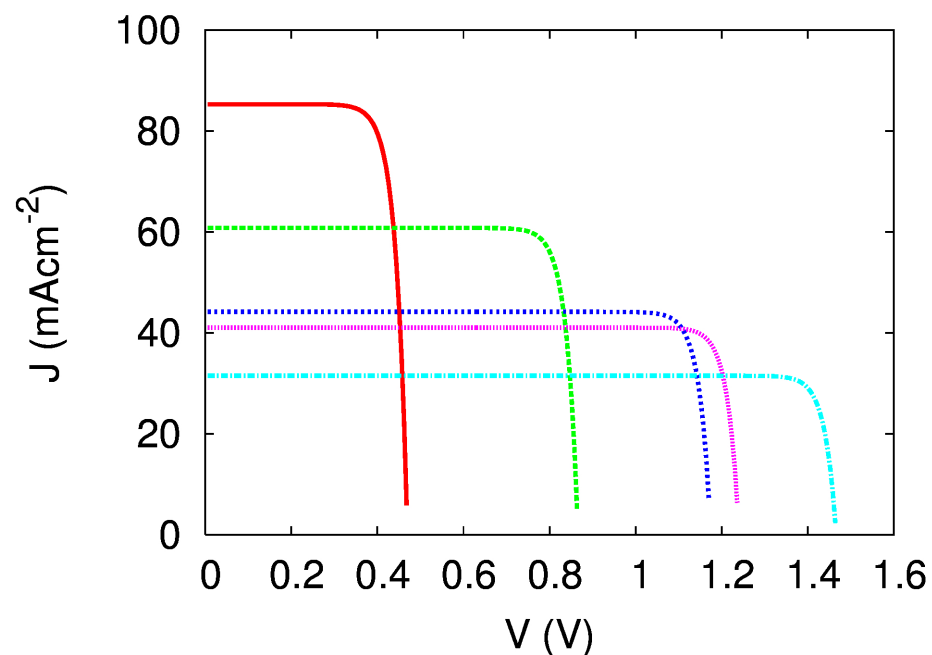$$b_s(E) = \frac{2F}{h^3 c^2} \frac{E^2}{e^{E/kT} - 1}$$

http://rredc.nrel.gov/solar/spectra/

$$dW/dS = b_s(E)E\,dE$$

ICTP The Abdus Salam International Centre for Theoretical Physics

Efficiency

$$J = J_{sc} - J_{dark}$$
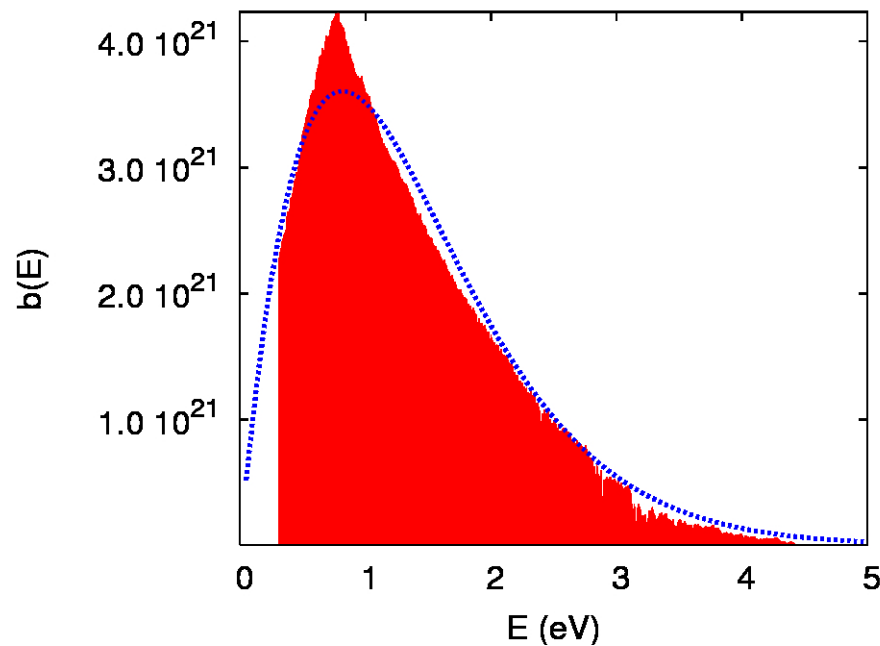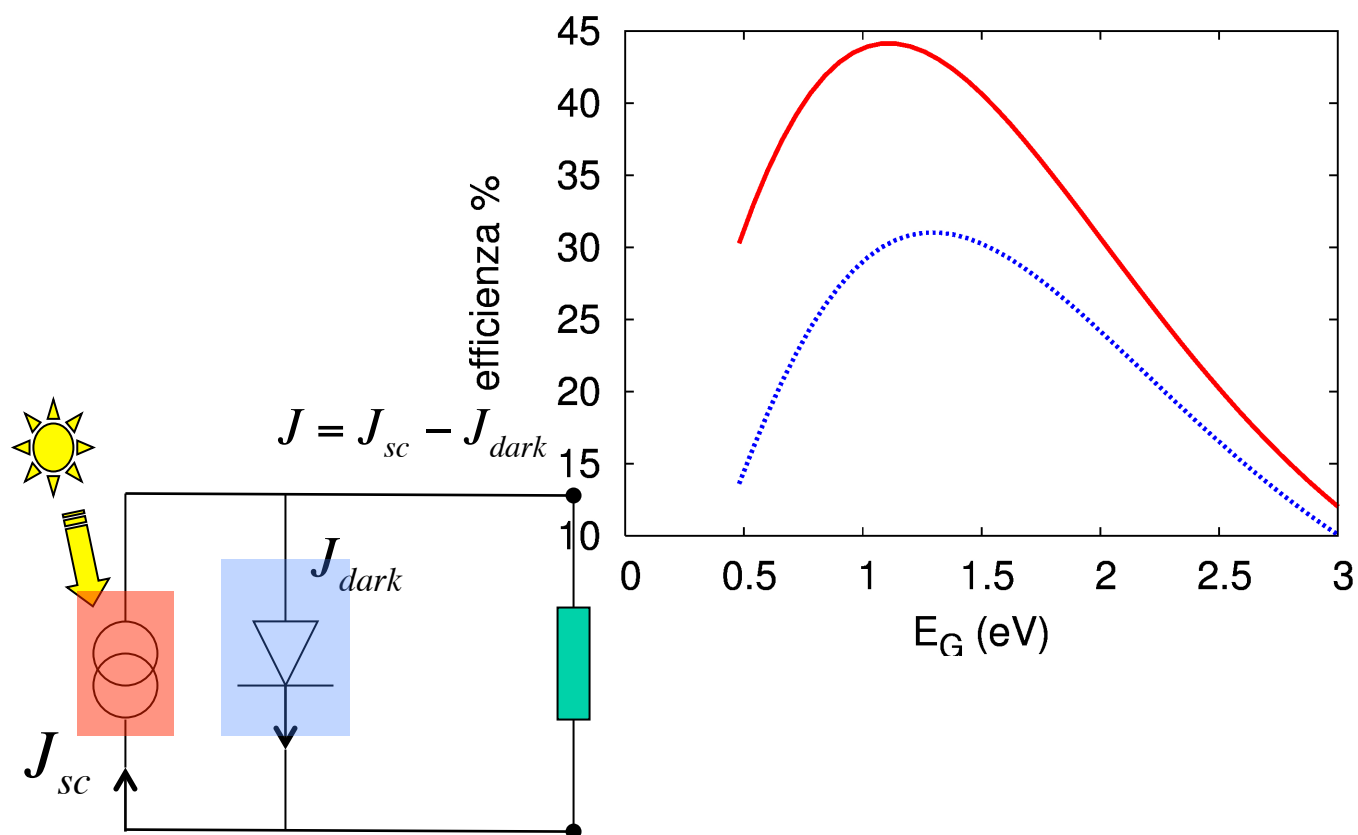
Modeling ideal materials

c-Ge ~ 0.67.eV

c-Si ~ 1.1 eV

GaAs ~ 1.43eV

a-Si ~ 1.5-1.8.eV

Se ~ 1.74eV

ICTP The Abdus Salam International Centre for Theoretical Physics

The 3rd generation of solar cells
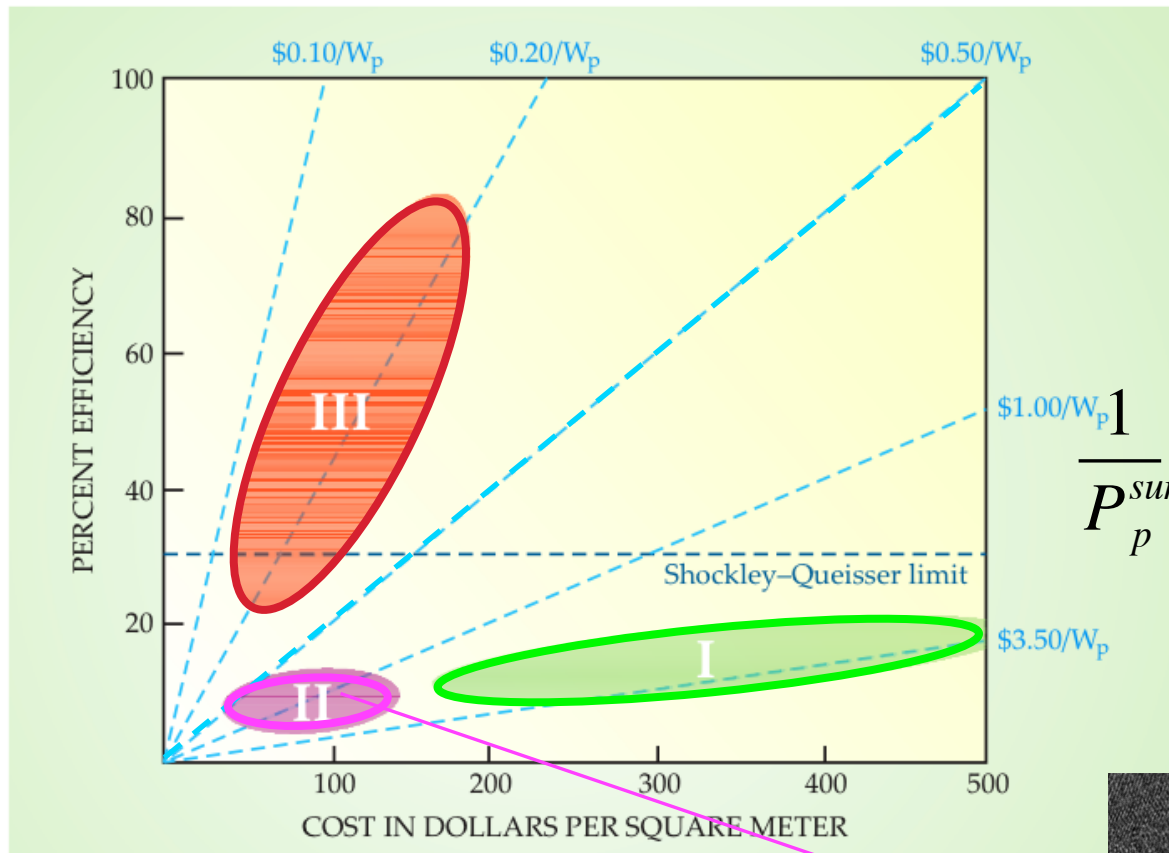
$$\frac{1}{slope} = \frac{c(\$)A^{-1}}{eff}$$

$$\frac{1}{P_p^{sun}}\frac{1}{slope} = \frac{c(\$)}{P_p^{sun}Aeff} = \frac{c(\$)}{W_p}$$

G.W. Crabtree and N. S. Lewis
Physics Today March (2007)
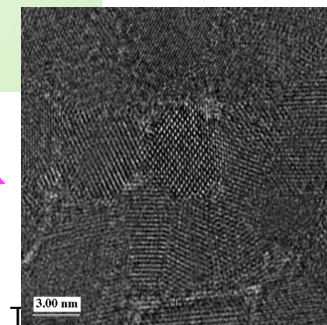
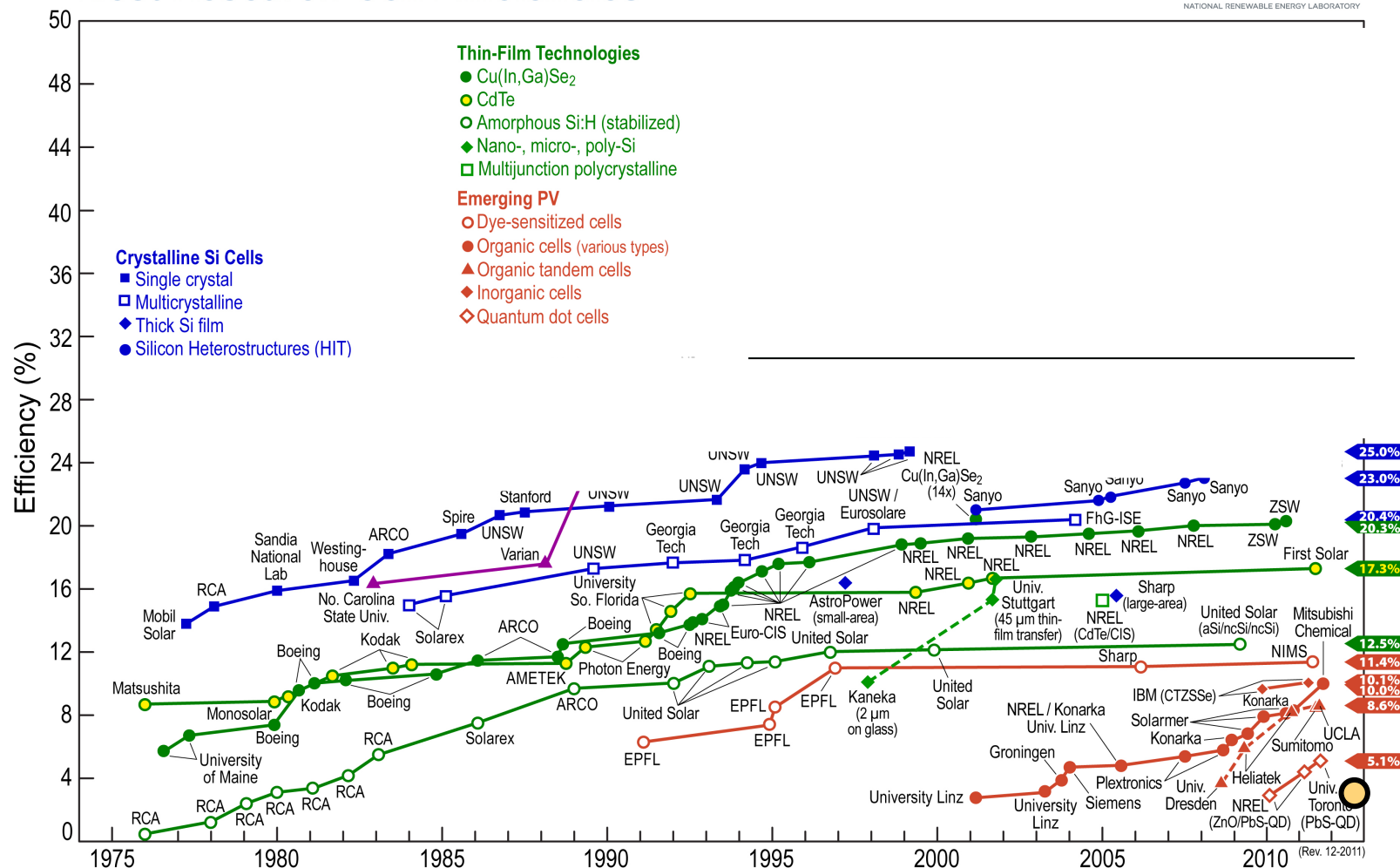# Research on photovoltaics

Best Research-Cell Efficiencies

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

MPMD simulations of nanostructured materials for photovoltaics

Trieste 26-30, November 2012

ICTP
The Abdus Salam
International Centre
for Theoretical Physics

Photovoltaic materials

Inorganic

Organic

CdTe

PbS

PbSe

C

PCBM

CIGS

GaAS

TiO$_2$

DYES

Si

P3HT

ZnO

The Abdus Salam
International Centre
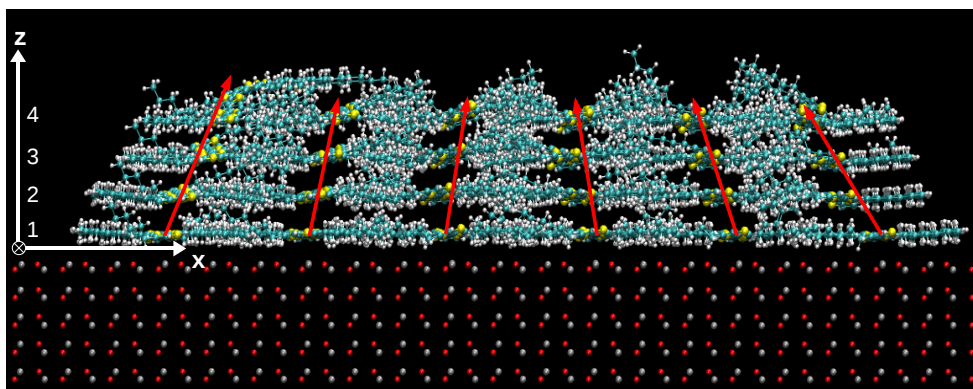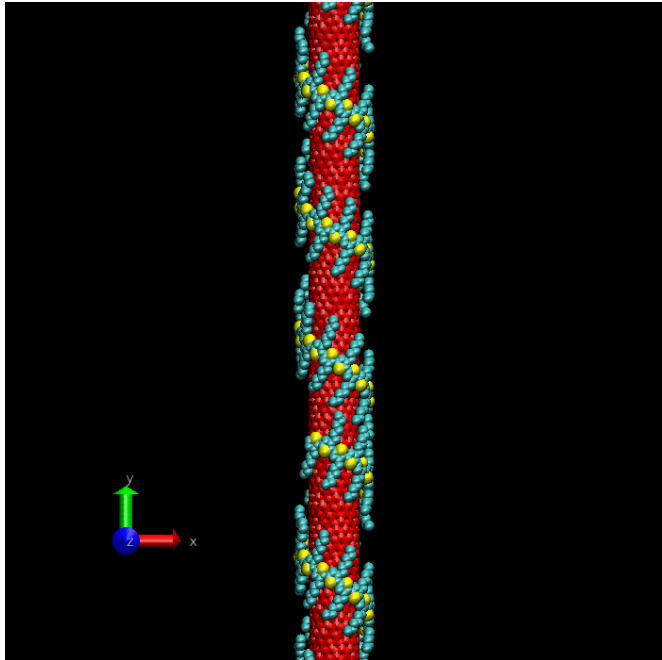for Theoretical Physics
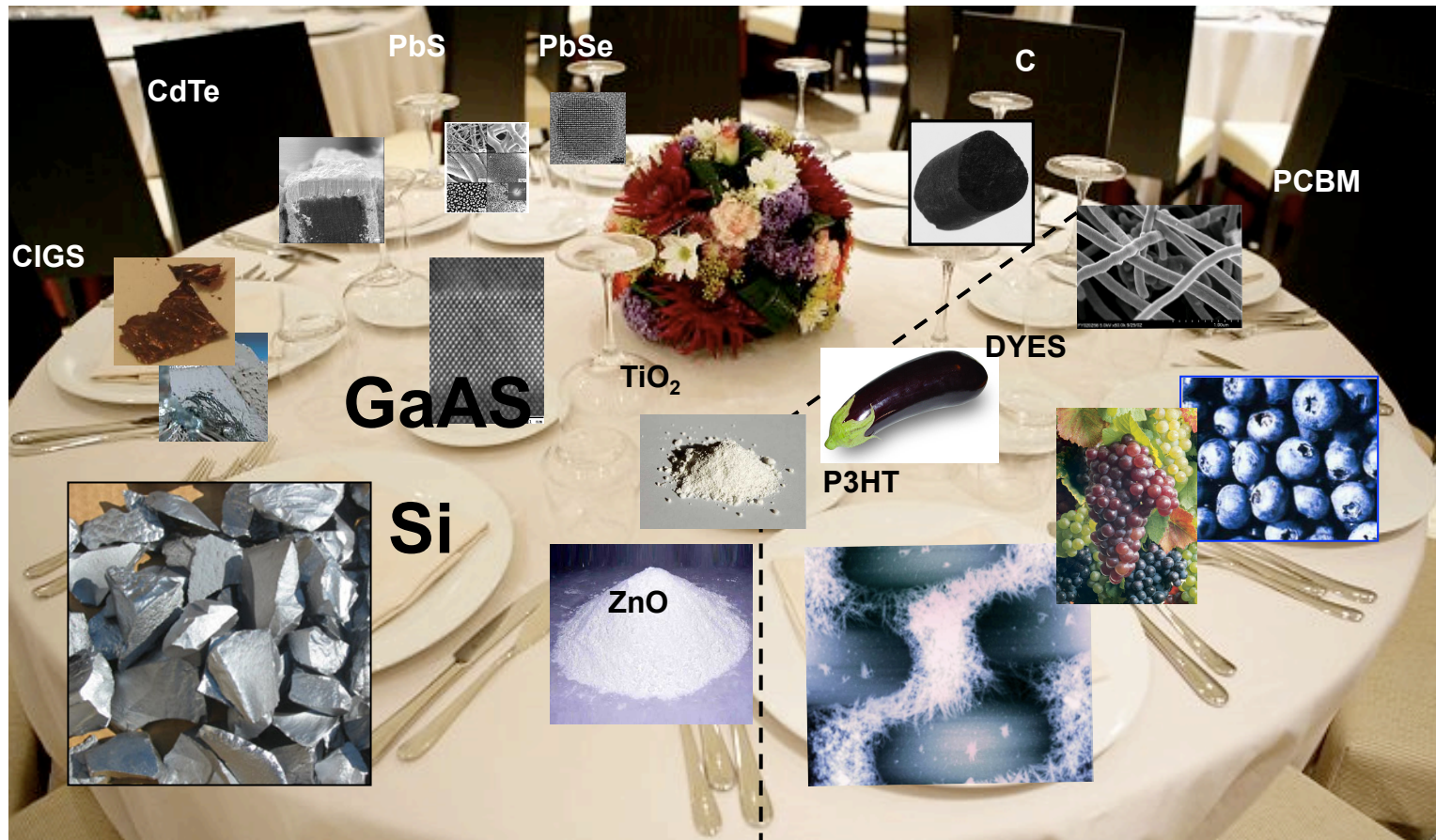
Models of interfaces (hybrids)
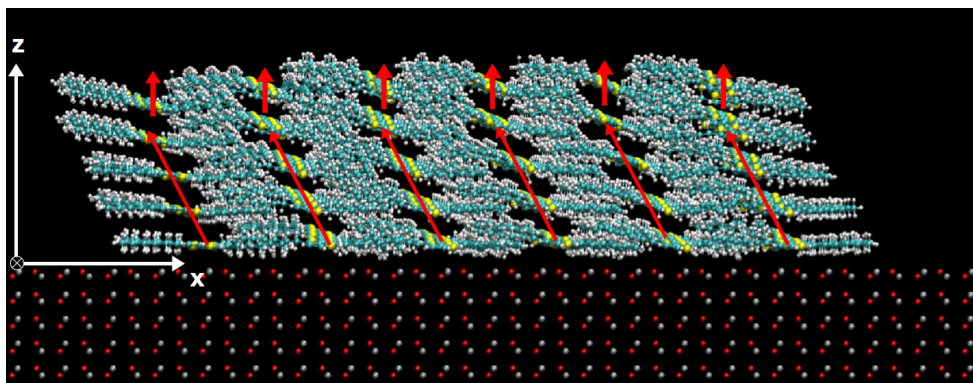
M.I. Saba, et al."Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface" *J. Phys. Chem. C* **2011, ASAP**

ICTP
The Abdus Salam
International Centre
for Theoretical Physics

# Polymer/carbon nanotubes systems

- Hybrid solar cells can be prepared by preparing blends of CNT and p3ht semiconducting polymers.
- Such hybrids are characterized by a complex morphology where the polymer wrap around the CNT surface
- Generating models realistic models of p3ht/CNT blends and their stability under thermal treatment is the object of the present investigation
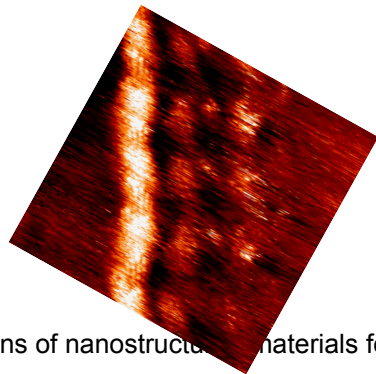
C. Caddeo et al. J. Phys. Chem. C **2010,** *114,* 21109–21113
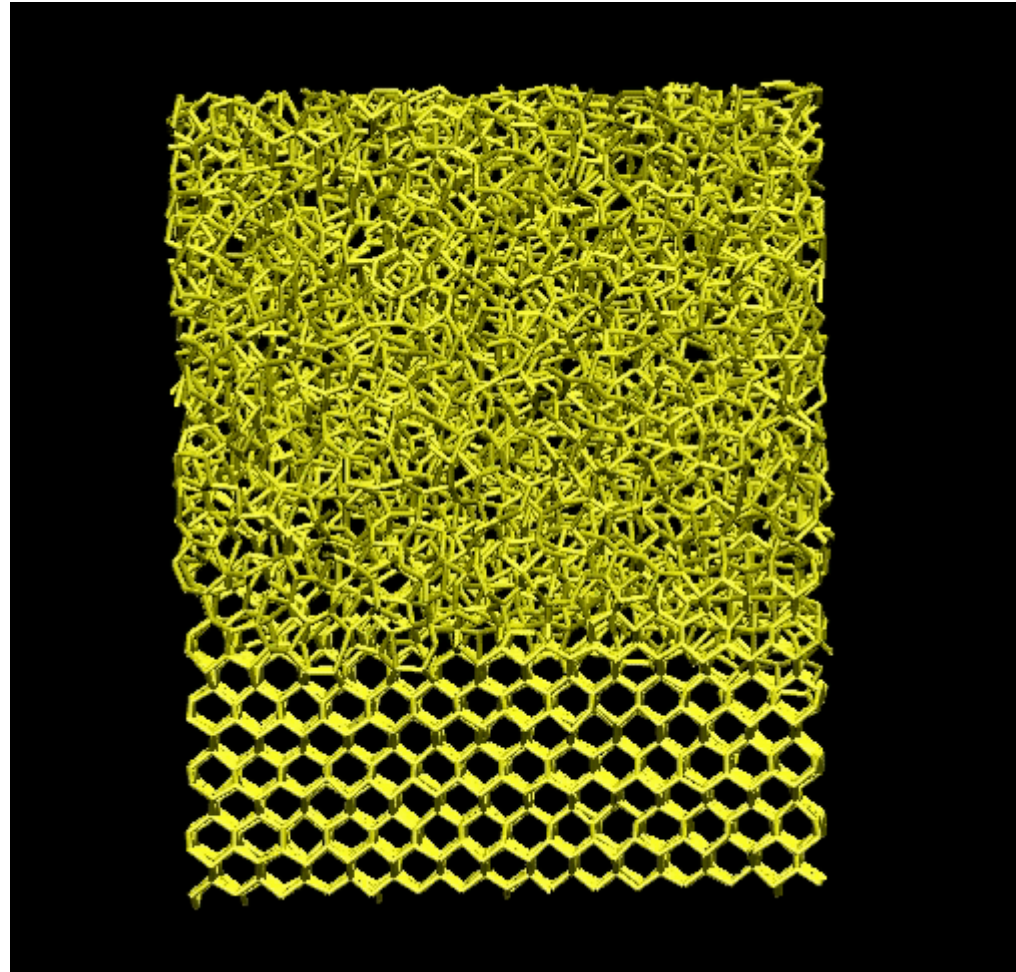
Morphology of complex interfaces

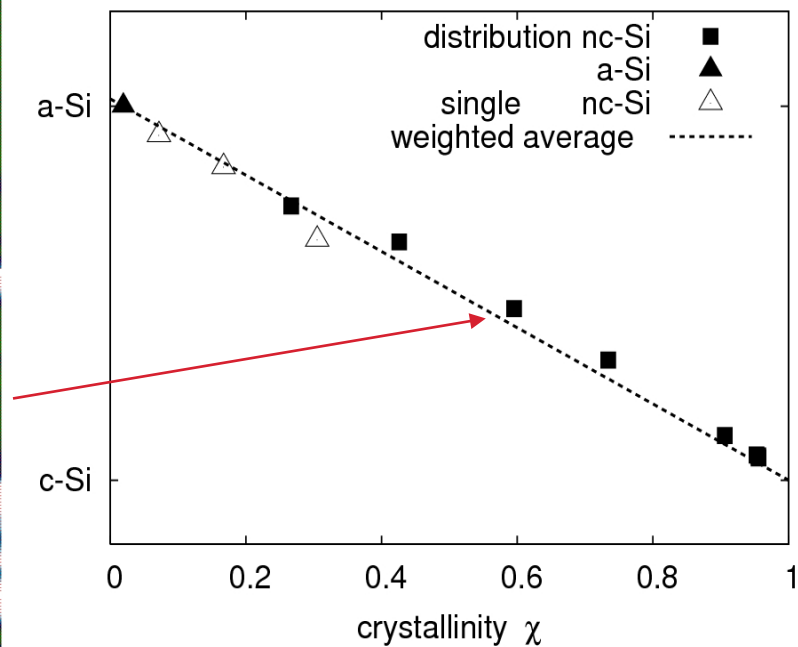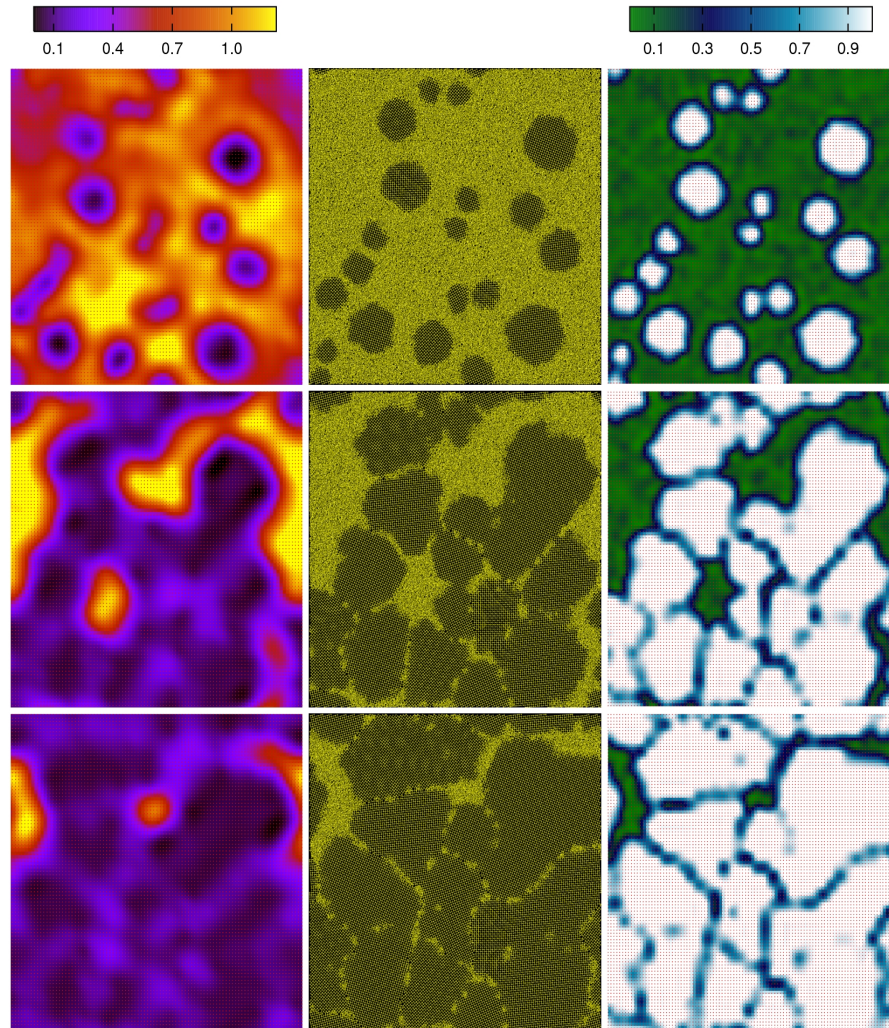*C. Melis J. Phys. Chem. C* **2010**, *114,* 3401–3406
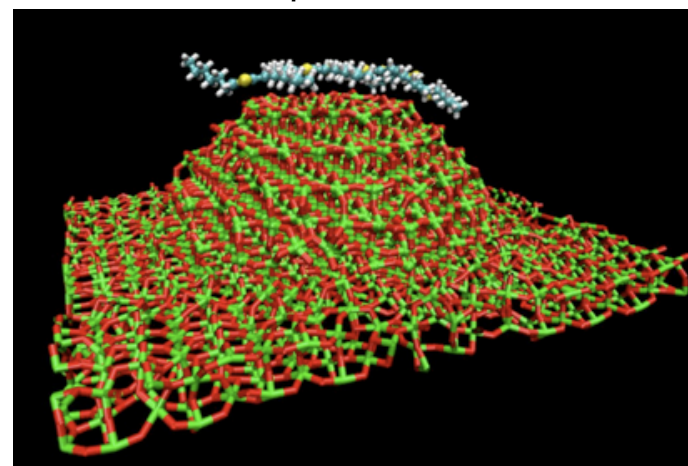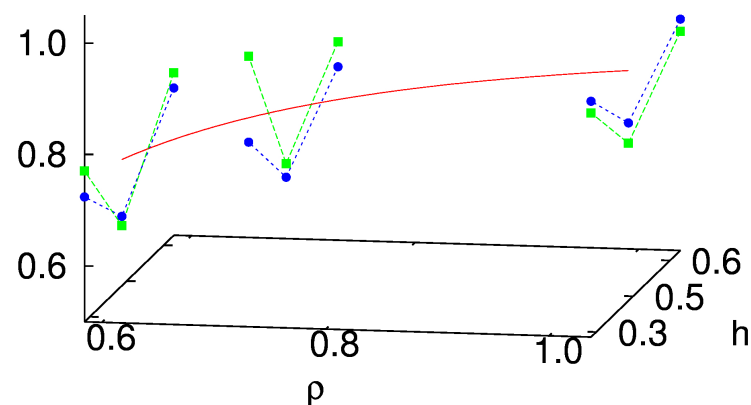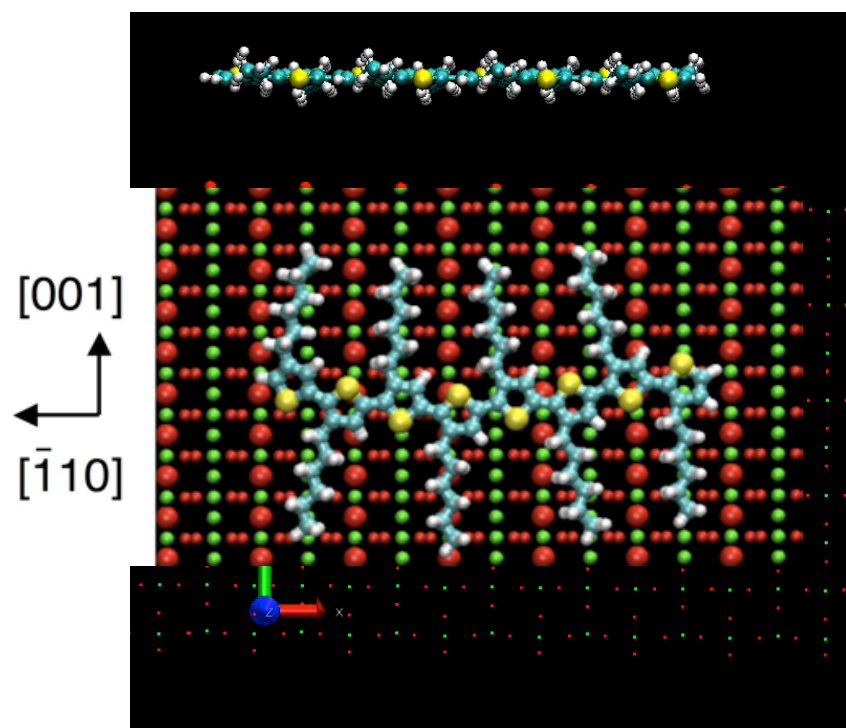
$$\gamma(\rho, h) = 1 - \alpha\rho^{-2} - \beta Q(\rho, h)$$

• **Models of interfaces (inorganic)**

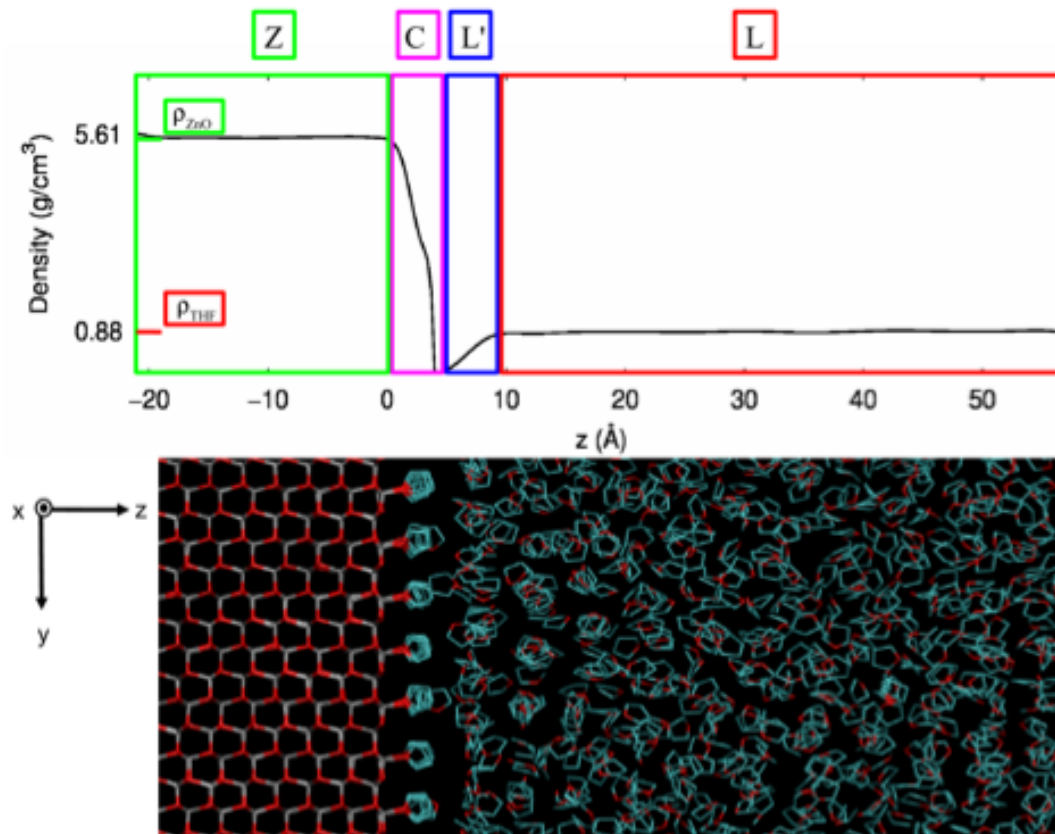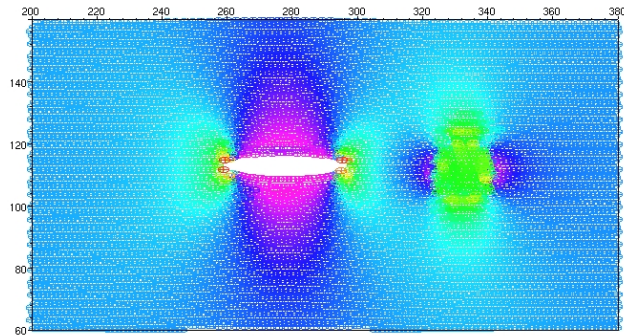**A. Mattoni et al.**
PRL 99, 205501 (2007)

Overall absorption

ICTP The Abdus Salam
International Centre
for Theoretical Physics

Solid/liquid interface

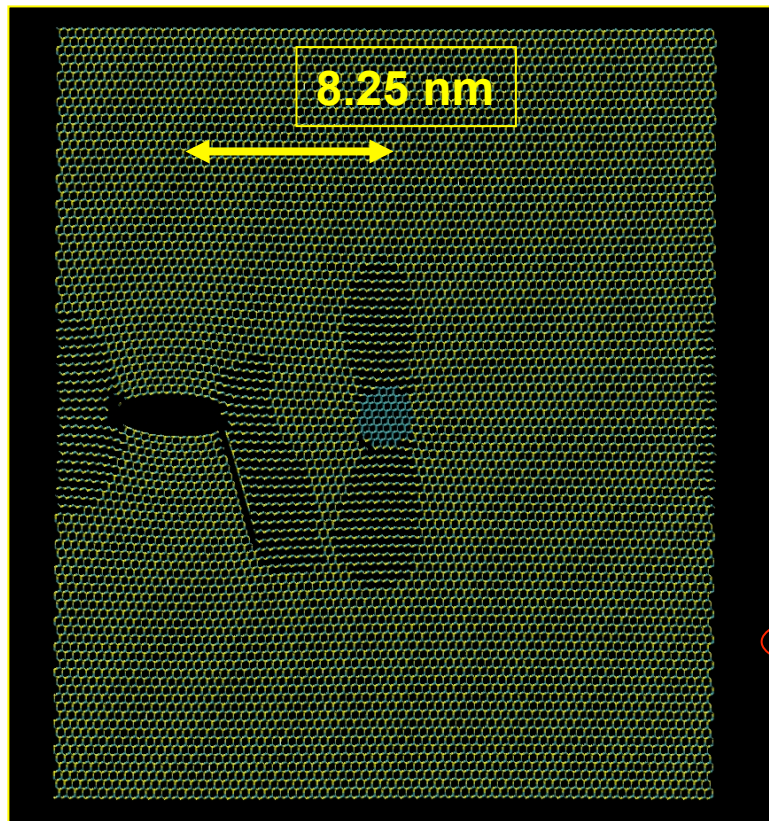**M.I. Saba et al. J. Phys. Chem. C 2012, 116, 12644−12648**

Atomic-level stress field

Mechanical properties
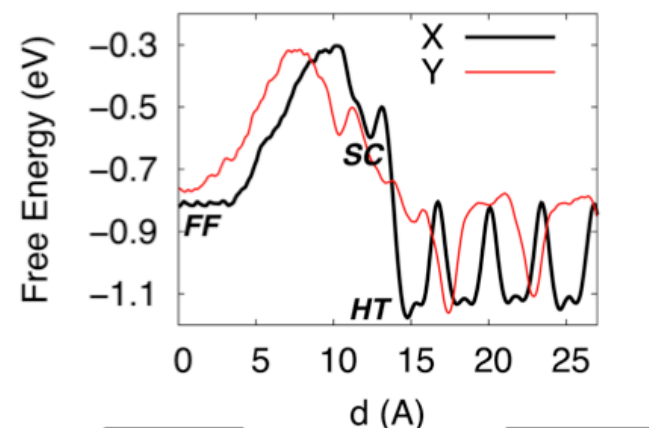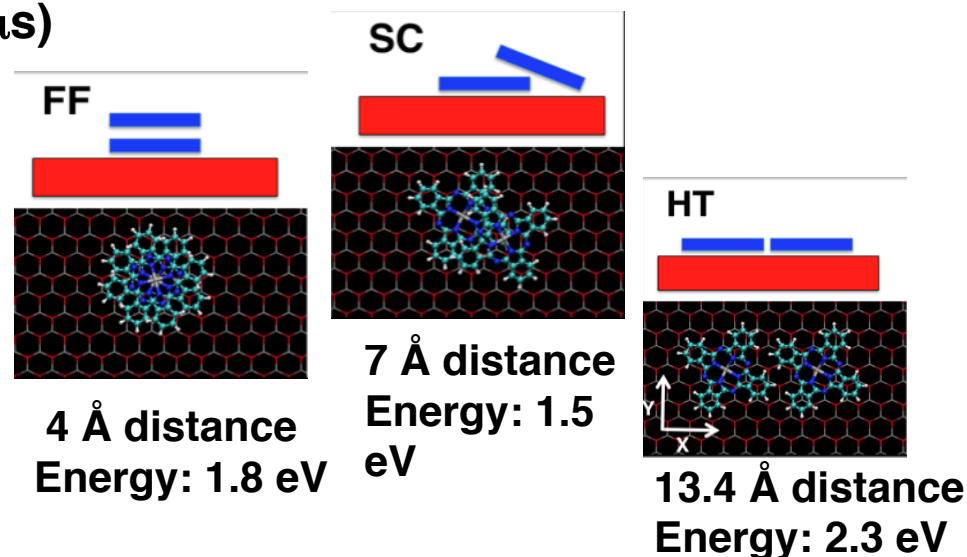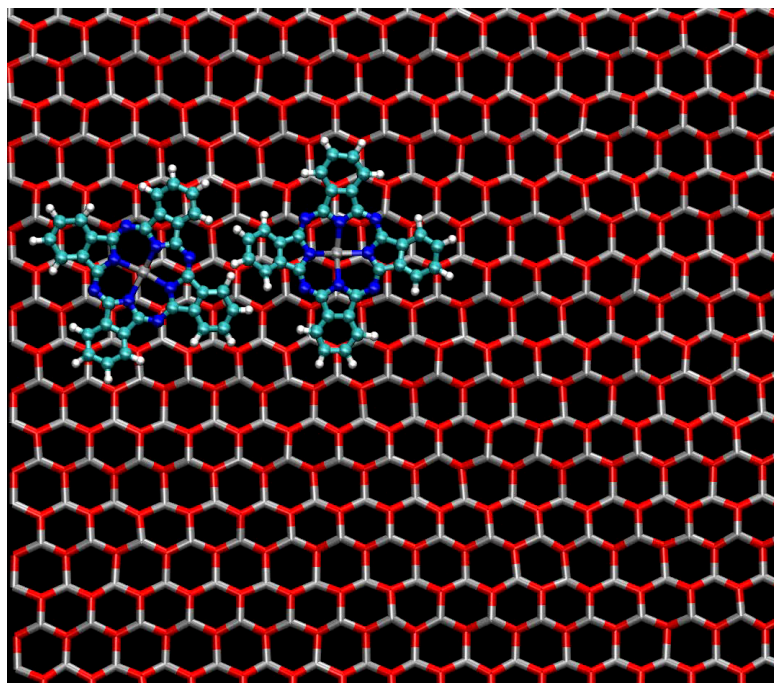
A.Mattoni et al. PRL 95, 115501 (2005)

8.25 nm

5.5 nm

Strain 16%

No crack

ICTP The Abdus Salam
International Centre
for Theoretical Physics
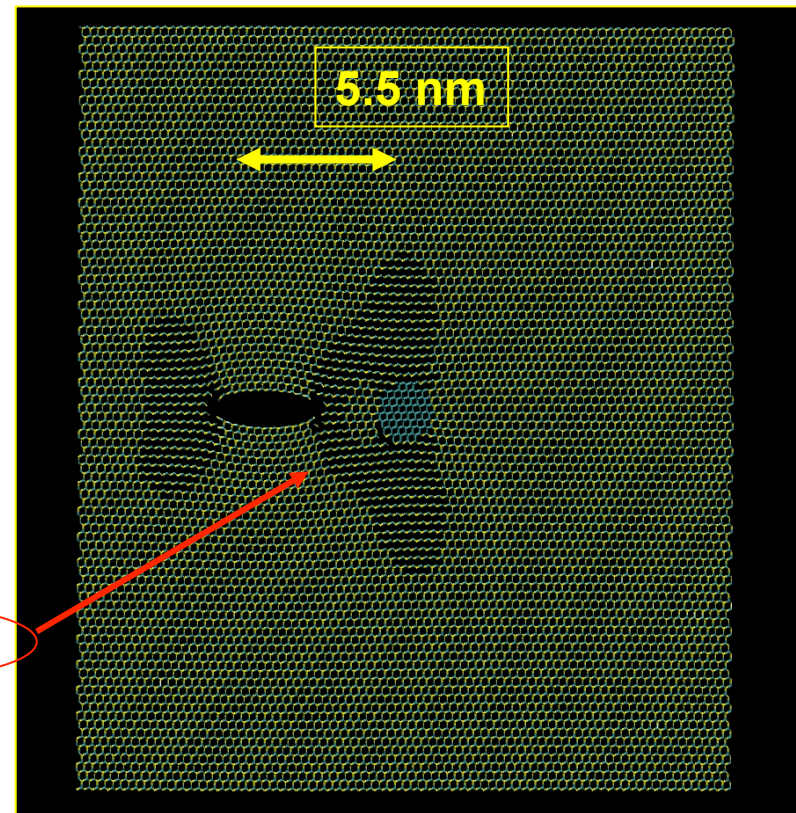
Microstructure evolution (assembling)

Metadynamics simulation 300 K(1.2 μs)

FF
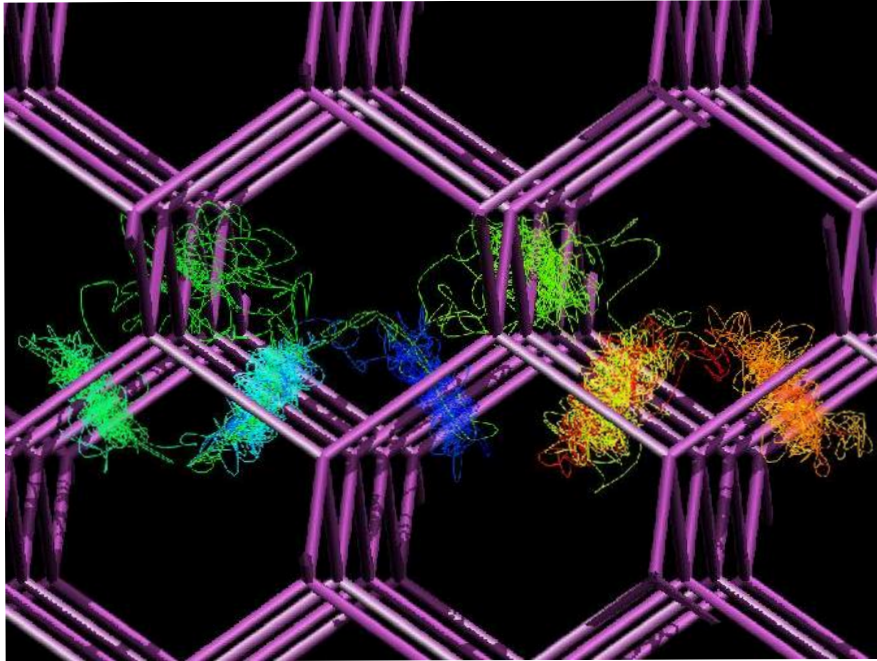**4 Å distance**
Energy: 1.8 eV

SC
7 Å distance
Energy: 1.5 eV

HT
13.4 Å distance
Energy: 2.3 eV

C. Melis et al. ACS Nano (5)12 9639–9647 (2011)

ICTP The Abdus Salam International Centre for Theoretical Physics
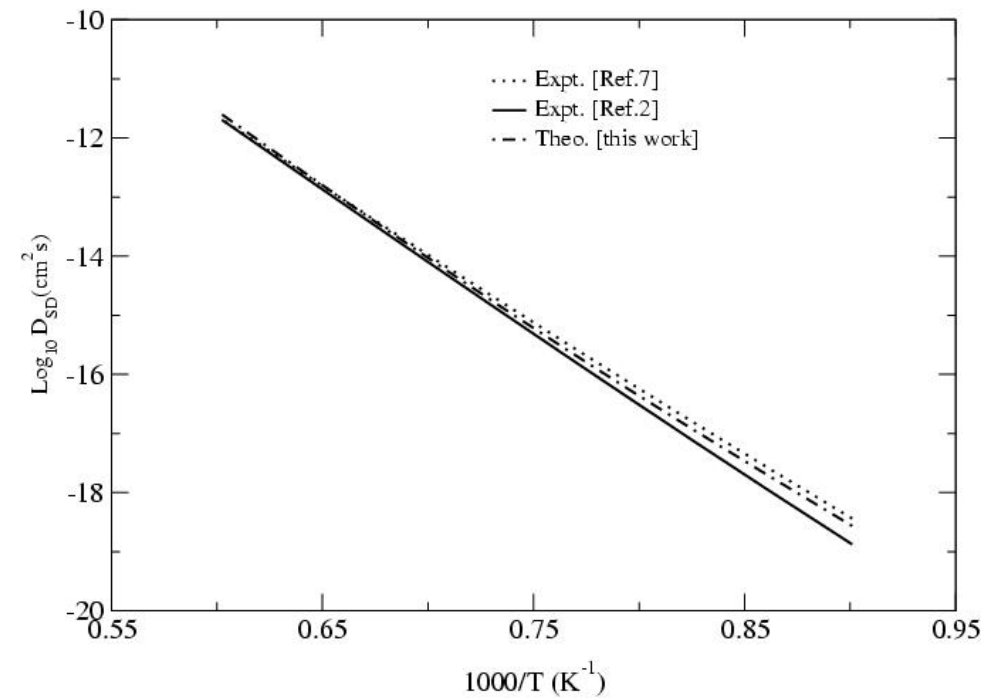
Model potential MD for…

- **Generating complex models (beyond ab initio)**

  Interfaces, defected bulk, nanocrystal

- **Microstructure evolution under controlled thermodynamical conditions**

- **Defects mobility, assembling, crystallization phenomena**

- **Link continuum models to atomistics**

  Explore continuum models at the atomic scale (grain growth, elasticity at the nanoscale)
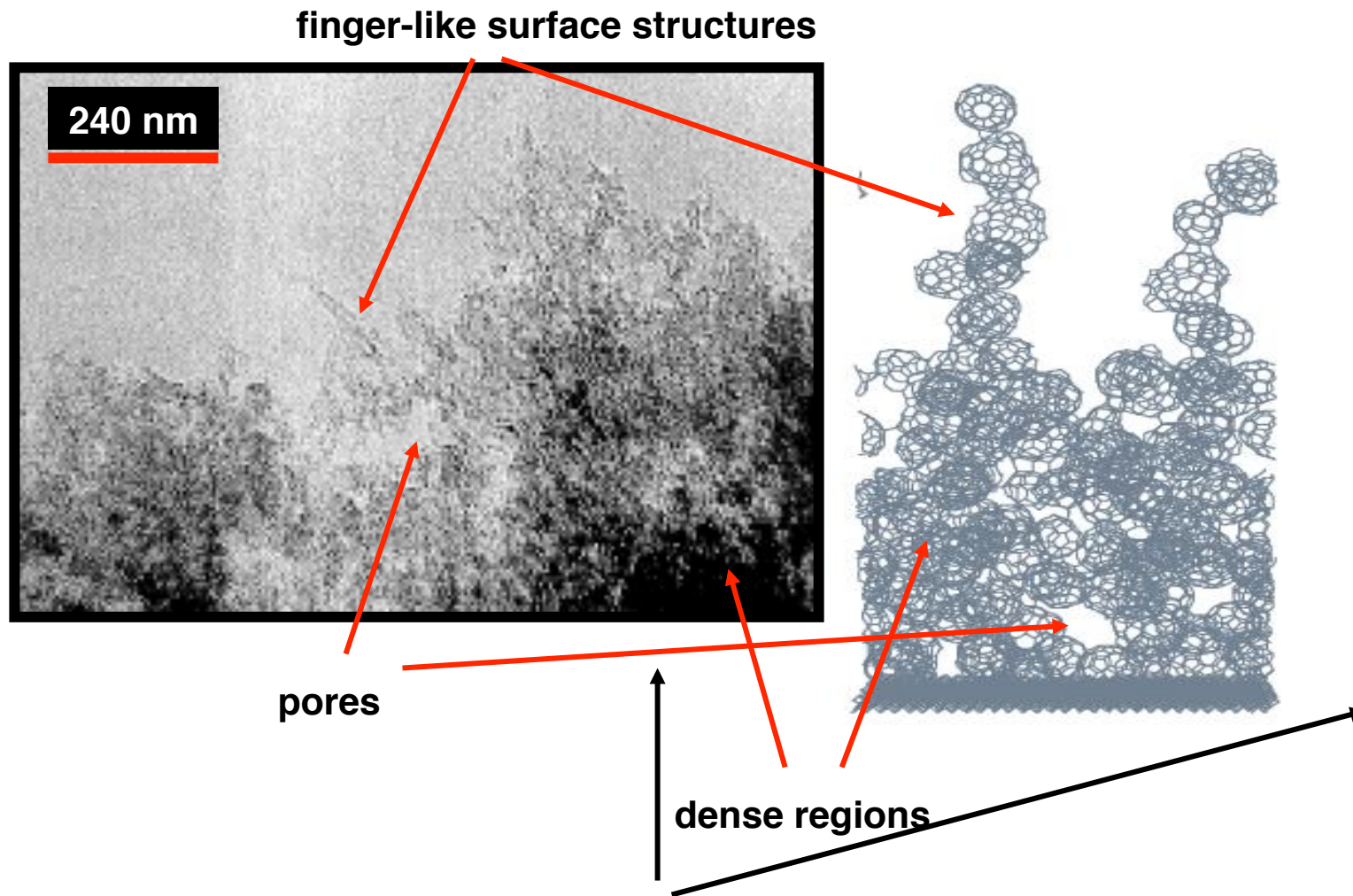
Diffusion trajectories of defects: H in c-Si

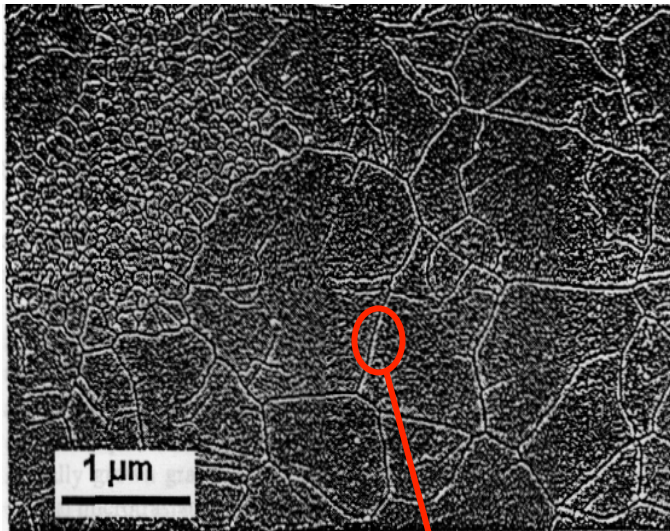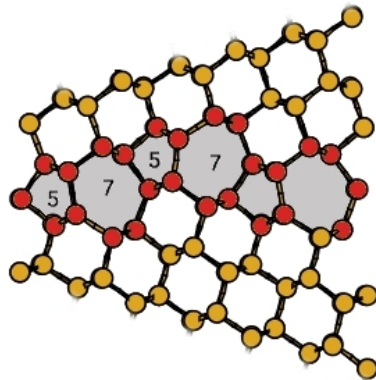**Transport coefficient: Si self-diffusion**

Simulation: ── · ──
Expt.1: ────
Expt.2 ···········

ICTP The Abdus Salam
International Centre
for Theoretical Physics

Film growth

finger-like surface structures

240 nm

pores

dense regions

ICTP The Abdus Salam
International Centre
for Theoretical Physics

Structural modelling

Physico-chemical processes

Poly-Si for solar cells

Hydrogenated ns-C

ICTP The Abdus Salam International Centre for Theoretical Physics