Materials Simulations for LIGO

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LSC meeting, MIT-Boston
July, 2007

LIGO-G070564-00-Z

Research Group & Funding

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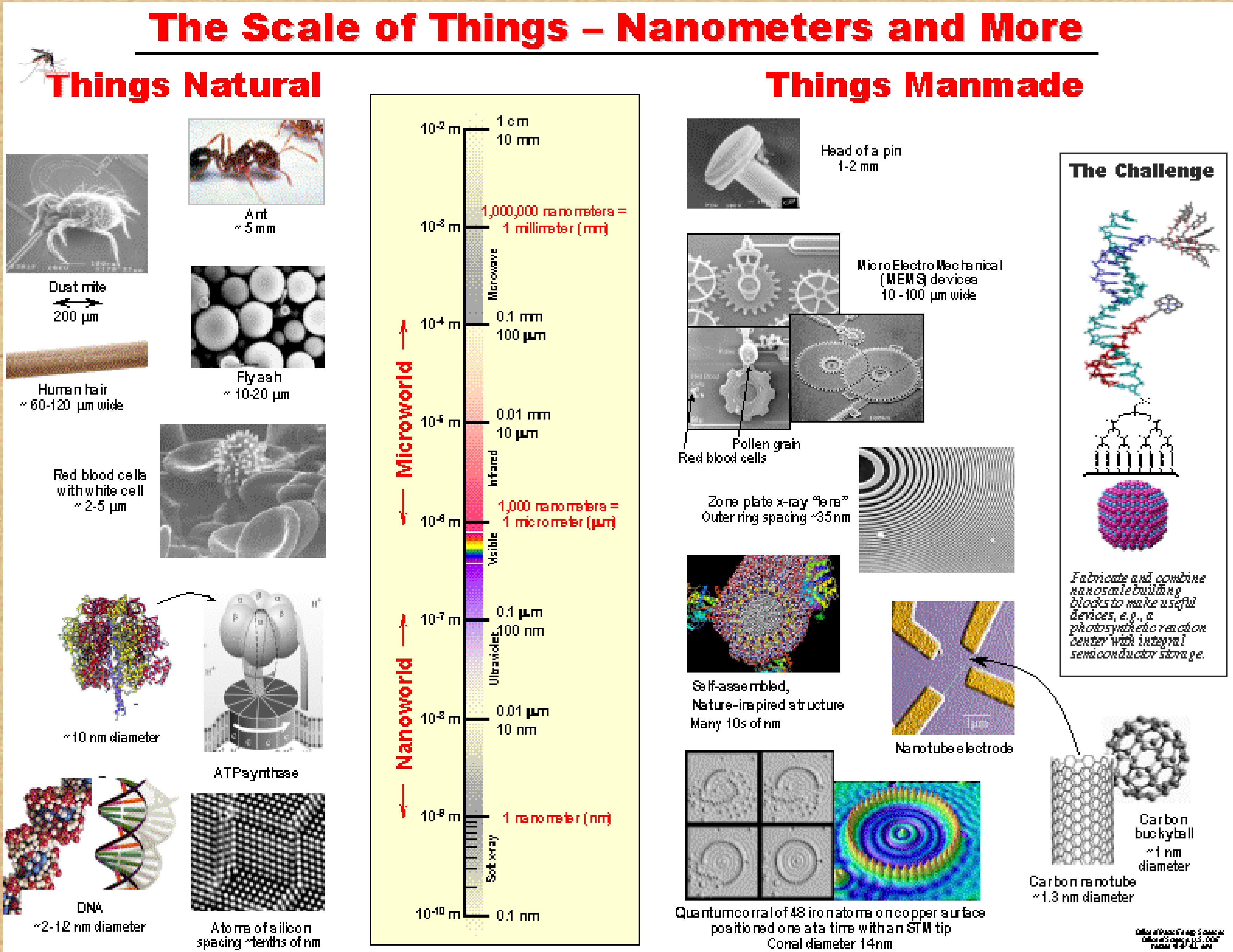
Funding

Department of Energy /Basic Science
National Science Foundation/ITR
(Information Technology Research)
University of Florida
UF/LIGO seed support 7/07-

Computer Centers
DOE/NERSC, ORNL/CCS, UF/HPC
http://www.nersc.gov

Allocation: 1 million CPU hours on nersc in 2007; have been using ~20-30% of UF/HPC center (~2000 CPU)


The Scale of Things – Nanometers and More
Things Natural
Things Manmade
Dust mite
200 µm
Ant
~ 5 mm
Fly ash
~ 10-20 µm
Human hair
~ 60-120 µm wide
Red blood cells
with white cell
~ 2-5 µm
~10 nm diameter
ATP synthase
DNA
~2-1/2 nm diameter
Atoms of silicon
spacing ~tenths of nm
10^{-2} m
1 cm
10 mm
1,000,000 nanometers =
1 millimeter (mm)
10^{-3} m
Microwave
10^{-4} m
0.1 mm
100 µm
10^{-5} m
0.01 mm
10 µm
Infrared
1,000 nanometers =
1 micrometer (µm)
10^{-6} m
Visible
10^{-7} m
0.1 µm
100 nm
Ultraviolet
10^{-8} m
0.01 µm
10 nm
10^{-9} m
1 nanometer (nm)
Soft x-ray
10^{-10} m
0.1 nm
Microworld
Nanoworld
Head of a pin
1-2 mm
MicroElectroMechanical
(MEMS) devices
10 -100 µm wide
Pollen grain
Red blood cells
Zone plate x-ray "lens"
Outer ring spacing ~35 nm
Self-assembled,
Nature-inspired structure
Many 10s of nm
Nanotube electrode
Quantum corral of 48 iron atoms on copper surface
positioned one at a time with an STM tip
Corral diameter 14 nm
Carbon nanotube
~1.3 nm diameter
Carbon
buckyball
~1 nm
diameter
The Challenge
Fabricate and combine nanoscale building blocks to make useful devices, e.g., a photosynthetic reaction center with integral semiconductor storage.

Current projects in the group

- New directions: Thermal noise in SiO2 and optical coating Ta_2O_5.

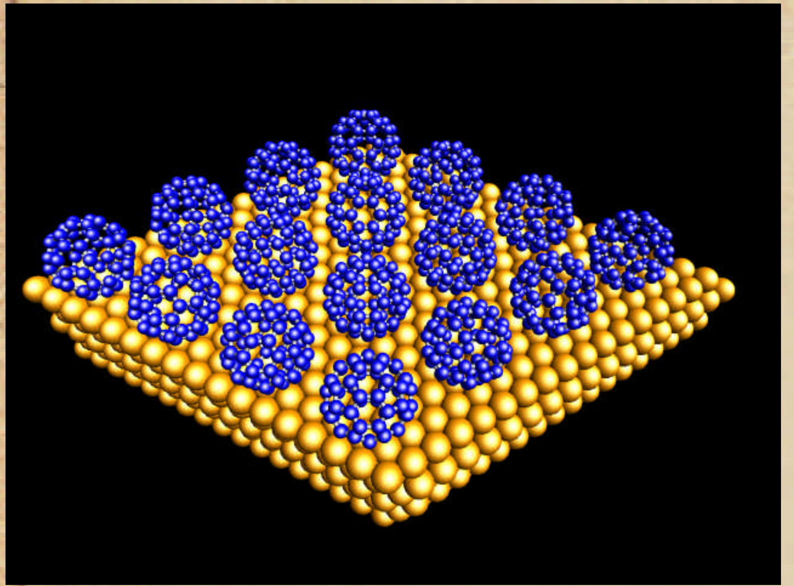
- Electron Transport properties at molecular- and nano-junctions

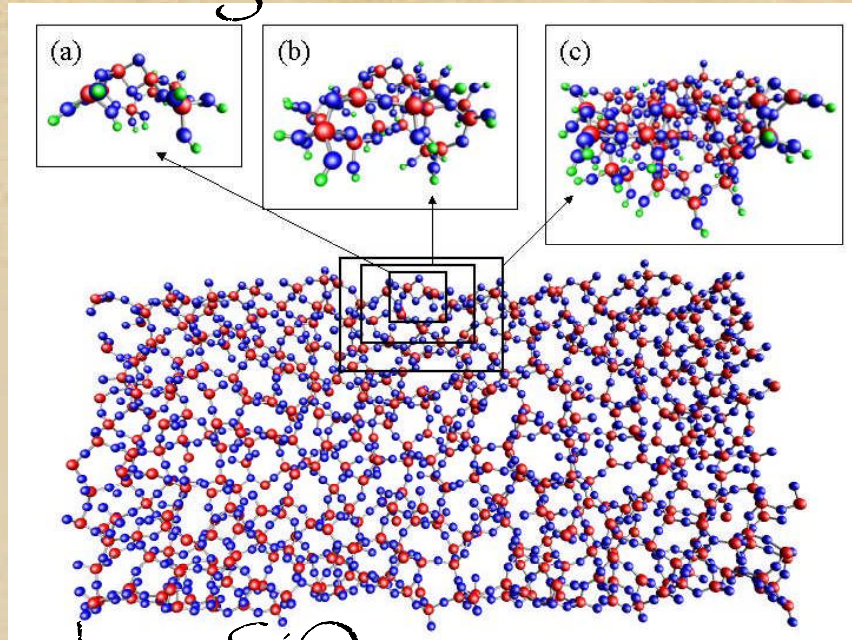
- Structure and Electron structure at surfaces and interfaces

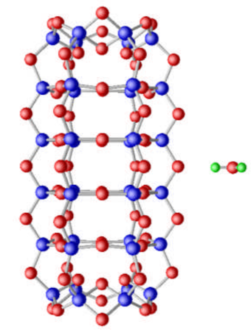
- Multi-scale simulation of hydrolytical weakening in silica and other materials under stress

- Relation of structure and eLectronic properties of cuperates to STM experiments

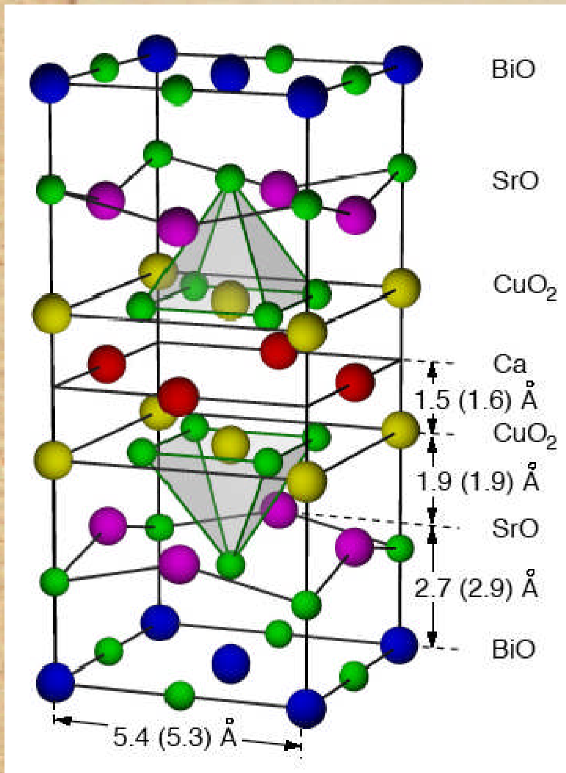
Atomistic modeling and simulation

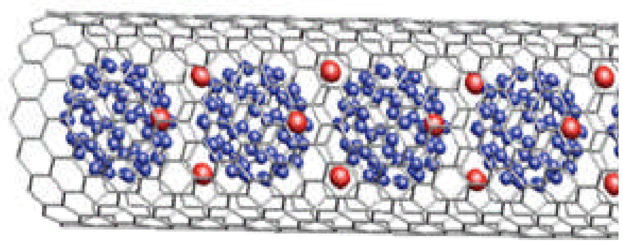


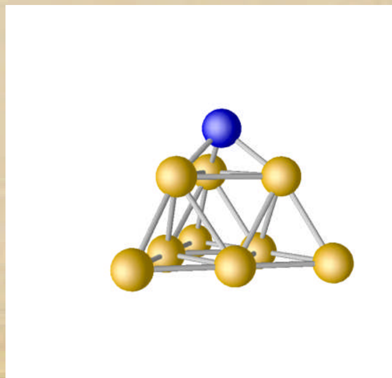


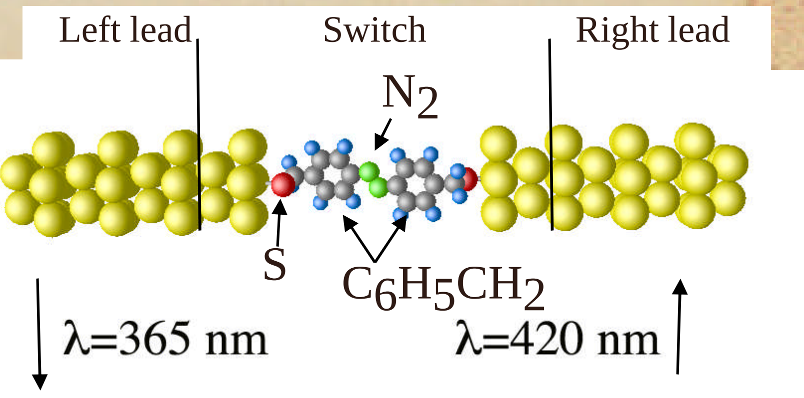


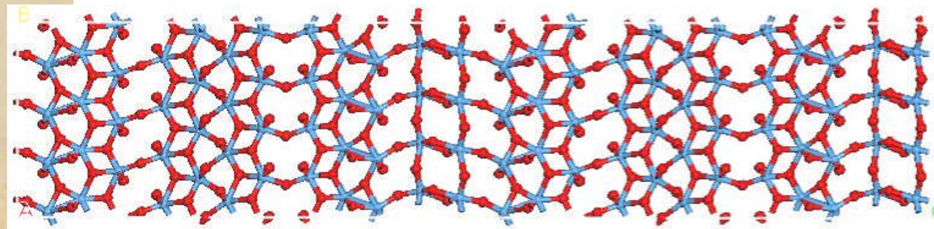
Amorphous SiO_2









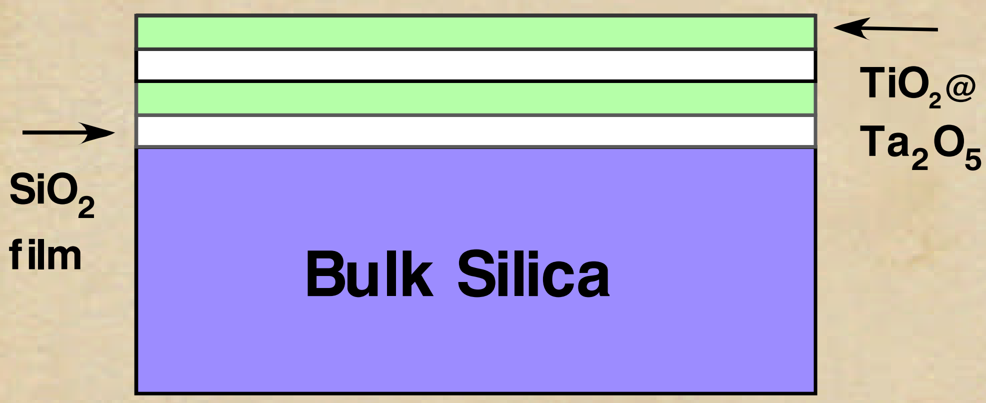


Ta_2O_5

Why we are interested in LIGO coating thermal noise?

Thermal Noise is a limiting noise source for graviational wave detection!

Experimental fact: Bulk silica has small thermal noise, but SiO_2 film has larger noise than the bulk, TiO_2 doping can reduce noise in Ta_2O_5 film.



Why? How do we find coating materials that has reduced/minimal thermal noise?

What can we do for LIGO?

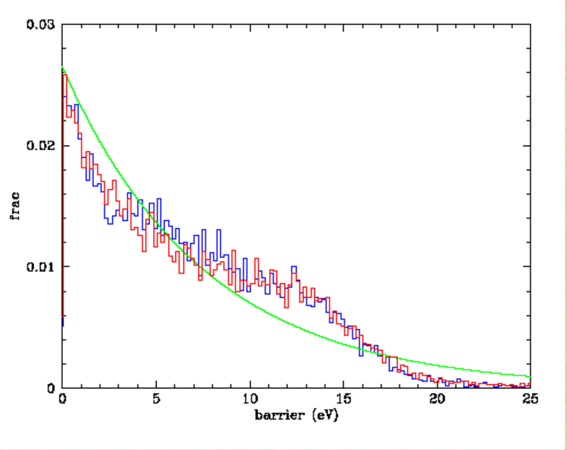
Relaxations of glasses affect:

Neutron and light scattering   Sound wave   attenuation   Dielectric loss

A direct relation between a microscopic quantity V and a macro-scopic measurement " is

(Wiedersich et al. PRL (2000) 2718

$$\chi''(\nu) \propto Q^{-1} \propto \int_0^\infty \frac{2\pi\nu\tau}{1+(2\pi\nu\tau)^2} g(V)\,dV$$



Also related to thermal noise are Young's moduli and Poisson ratio, can also be calculated.

Macroscopic models of thermal noise that accurately predict thermal noise, rely on our understanding of physical parameters. Microscopic, predictive model is lacking. Goal: to develop a working microscopic simulation model which i) can probe dissipative mechanisms (ie, bond angle relaxation) ii) can be correlated against experiment and iii) add predictive power to new recipes for low noise coatings."

Simulation road map

Classical MD
known $U(\{R_I\})$

Constructing U
for classical MD

Difficult!

Quantum
model system

Amorphous materials
barrier distribution

Crystal or local structure
Young's moduli, Poisson ratio
electronic properties

State-of-the-art:
10^6-10^8 particles;
10^3-10^4 needed for
amorphous silica

State-of-the-art:
10^3 electrons

Working Plan

If funded by NSF

One student: working classical simulation and barrier determination
One postdoc: working on quantum calculation of dielectrics and effect of doping
Hai-Ping Cheng: Start with 25-30% of time on the LIGO project, re-evaluate as project evolves (will keep the LIGO team informed).

Before getting NSF funding, the student and postdoc will work at somewhat reduced pace.

Will submit a proposal to NSF September 2007!