Condensed Matter Theory

6 faculty,13 grads, 3 postdocs.

Phillip Duxbury (5) (Statistical Physics, Complex materials)

Mark Dykman (1,1) (Nonlinear Dynamics, Many body Physics)

Bhanu Mahanti (2,1) (Electronic structure, Complex materials)

Michael Moore (2) (Atomic Physics, Quantum Optics)

Carlo Piermarocchi (2) (Quantum Optics, Control, Networks)

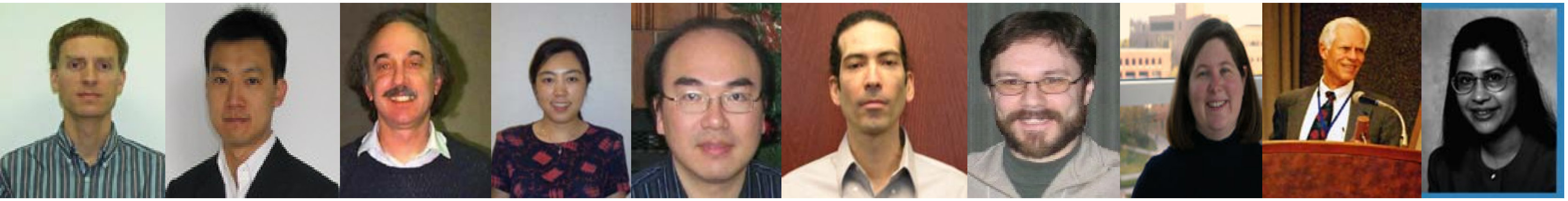
David Tomanek (1,1) (Electronic structure, Nanotubes)

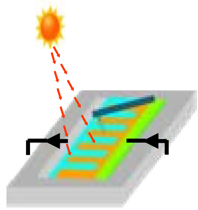
Michael Harrison, Tom Kaplan

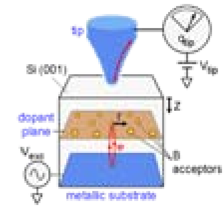
Centers: CORE-CM (Duxbury), IQS (Dykman), QBM (Quantitative Biology, Lapidus), DOE-EFRC (Morelli, Engineering), NSF-Solar (McCusker, Chemistry), NIH-GO (Worden, Engineering), GAANN (Worden, Engineering). Seminars: CMP, IQS, Physics Colloquium, Science at the Edge (SATE), CORE-CM seminar (Thursdays-Pizza!!). Active collaborations with CMPE. E.g. Ultrafast diffraction, Quantum optics, light-matter interactions, complex materials.

Condensed Matter Physics

Experiment

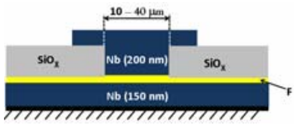


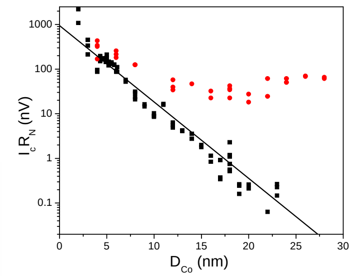




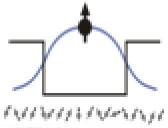
Emeritus

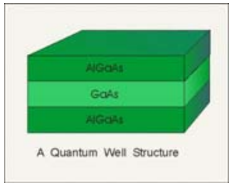
- Transport in nanostructures

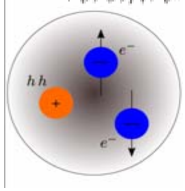


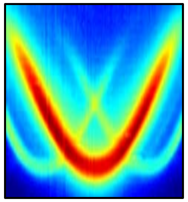


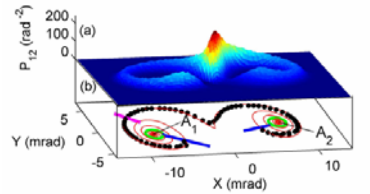
- Quantum optics



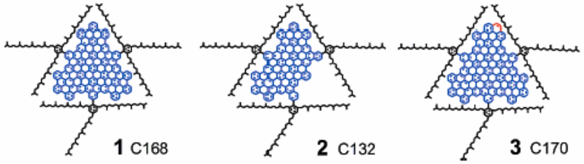


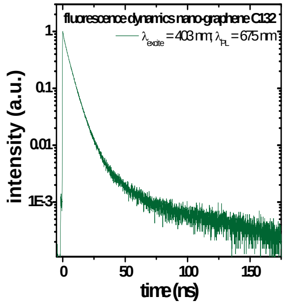


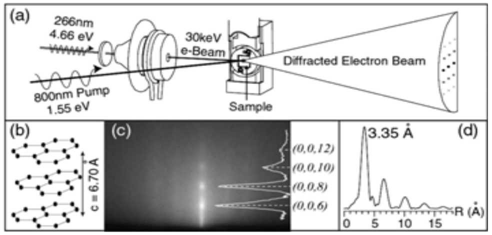


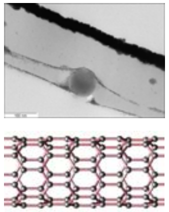


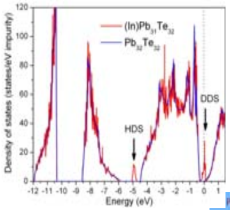
- Complex Materials



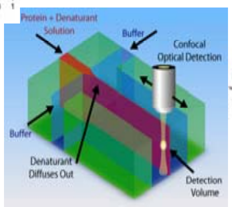








Biological Physics



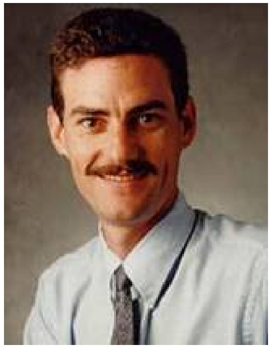
Theory

The Center of Research Excellence in Complex Materials (CORE-CM)

CORE-CM Advisory Committee

Keith Promislow

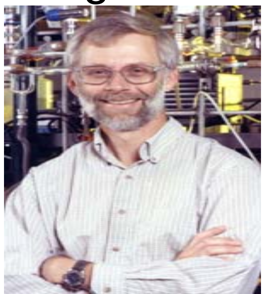
Tim Hogan



Vlad Tarabara

Phil Duxbury (Chair)

Greg Baker



Jim McCusker

Don Morelli

Center mission

The CORE-CM mission is to promote excellence in materials research on the MSU campus through high quality multidisciplinary group research, infrastructure development, training programs and technological innovation.

Externally fundable group and shared infra-structure projects are primary goals.

- Center programs
- Shared infrastructure
- Emerging groups

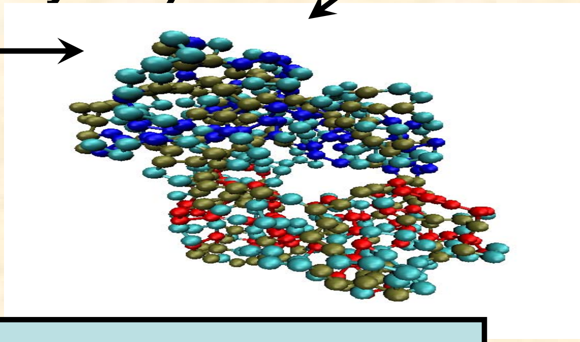
Research Directions (Duxbury Group)

Nanostructures underpin emerging technologies in the energy, medical, environmental and automotive sectors.

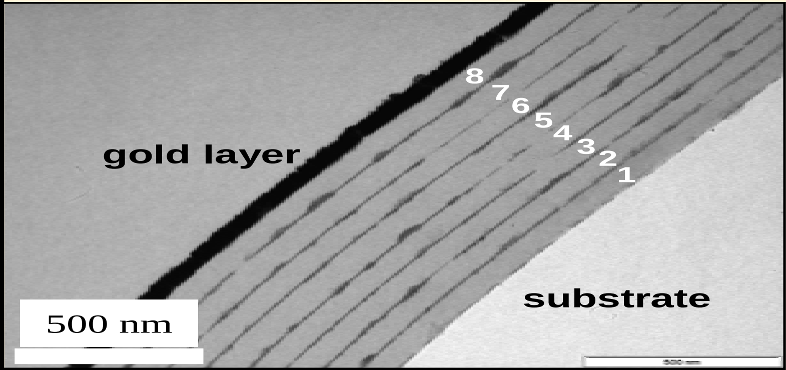
Phil Duxbury **(Physics/Ast)**
Michael Mackay **(Delaware)**
Greg Baker **(Chemistry)**
Simon Billinge **(Columbia)**
Bill Punch **(CSE)**
Bill Wedemeyer **(Biochem./Physics)**

Area 1:
Design and synthesize functional nanoparticles.
→ Drug delivery, imaging, polymer coatings, solar cells

Area 2 :
Develop methods to see atoms inside nanoparticles.
→ Nanostructure center



Area 3: Design and fabricate multilayers and other nanostructures through self-assembly.
→ Solar cells and OLEDS.



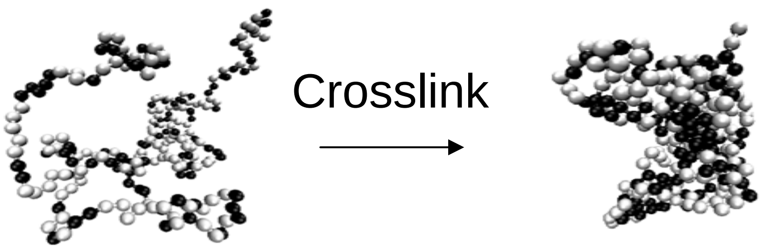
CNDA activities, current and planned:

- **-Research on nanostructured materials**
- **-Applications to energy and medical sectors**
- **-Training program in design and self assembly**
- **-Training program in nanostructure characterization**
- **-Industrial partners for SBIR etc**
- **-Outreach to MSU community, schools and public**
- **-Ongoing submission of center and training proposals to NSF, DOE, NIH and defense agencies.**

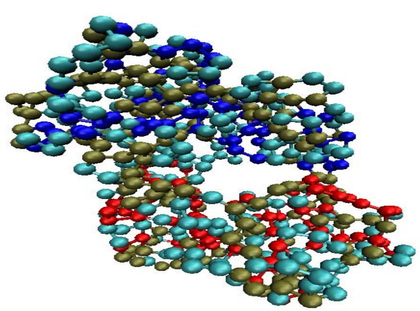
Area 1: Design and synthesize functional nanoparticles

- Functional proteins evolved through natural selection
- Can we design and fabricate functional nanoparticles?

1. Theory : Molecular Simulations of irreversible folding. Duxbury et al. ACS 2007 proceedings.

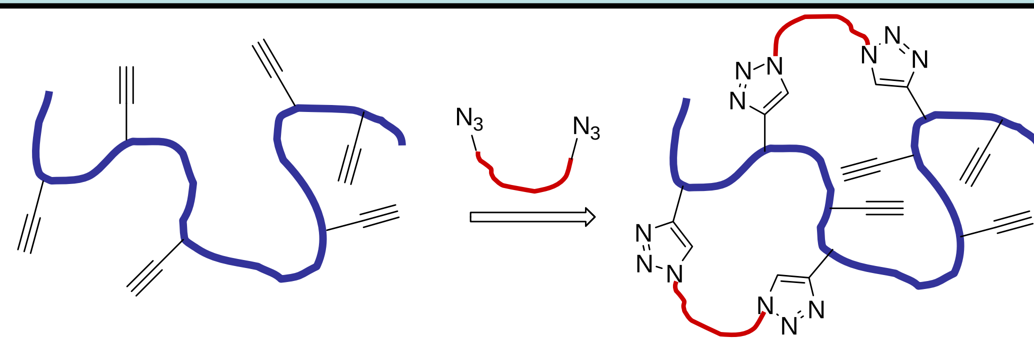


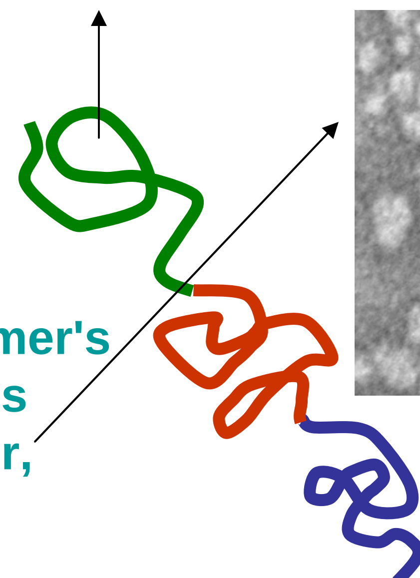
e.g. Formation of 2-faced (Janus) nano particle.

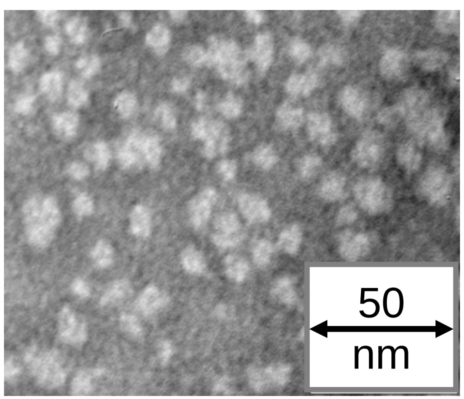


Mackay's group

2. Targeted synthesis of Nanoparticles.
Baker, Smith



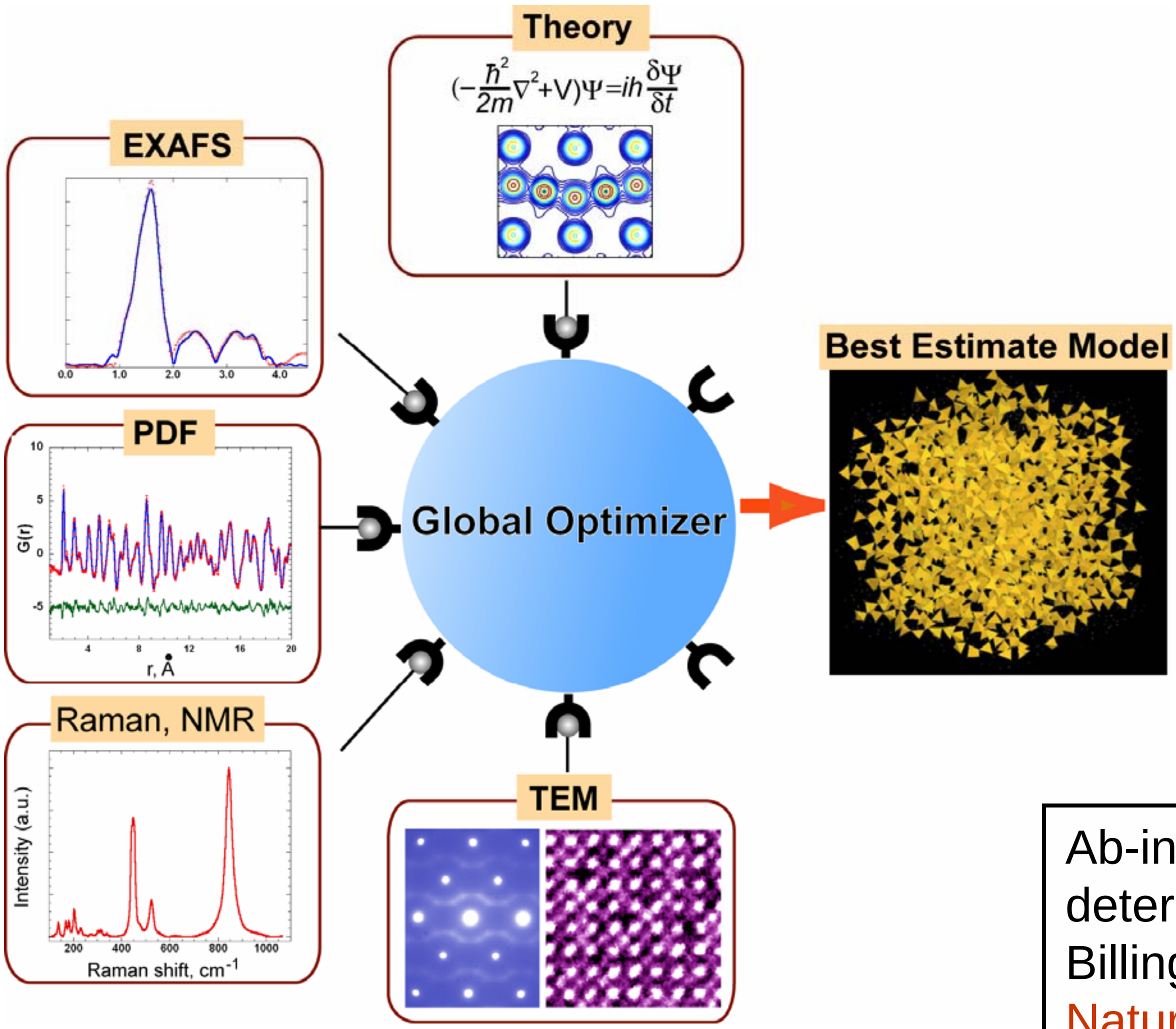




Drug delivery for Alzheimer's disease via nanoparticles (NIH proposal: Baker, Smith, C. Chan, Pat Walton in CHEMS)

Area 2 – Seeing inside nanoparticles

Grand challenge to see atoms in non-crystalline materials:
Billinge, Science `07.



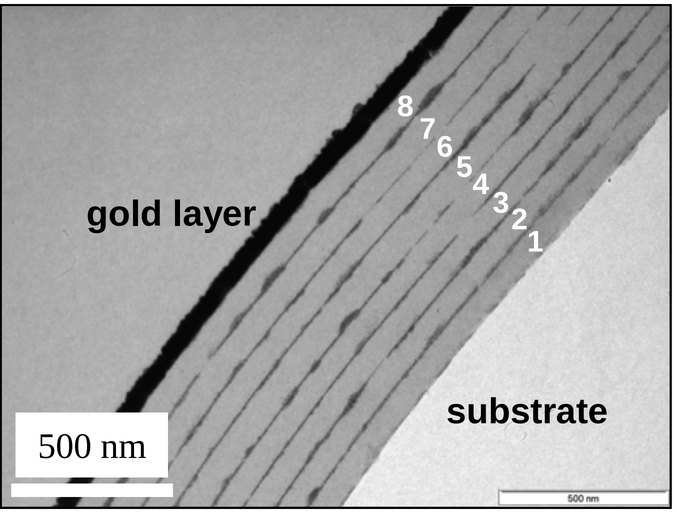
Unified
Modeling
Framework

Co-refinement

Ab-initio nanostructure determination – hard materials.
Billinge, Punch, Duxbury
Nature, 2006

Area 3 : Manufacturing efficient plastic electronics

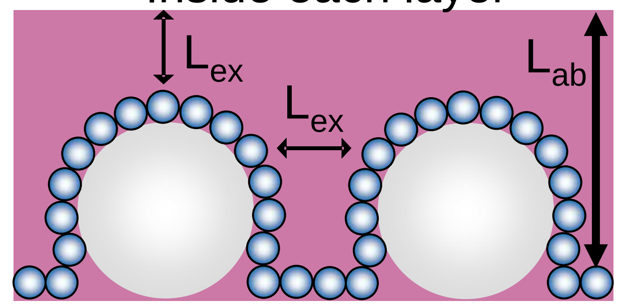
- Can we can direct nanoparticle self-assembly?
- Can we use this to make better plastic solar cells and OLEDS?

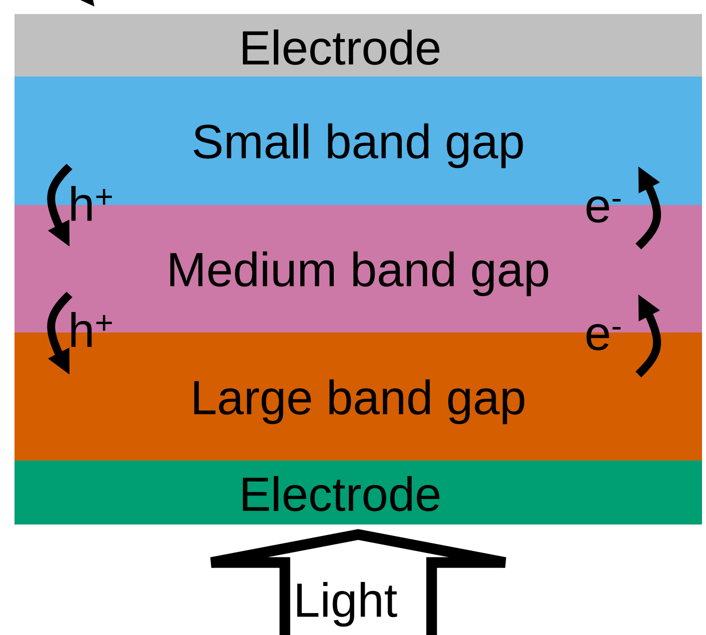


Self-assembled multilayers
Mackay, Duxbury et al.,
Science 2006, Nano Letters 2007
Mackay - Patent pending

Proposed optimal solar cell. Mackay's group will make this

Inside each layer





Computational effort:
- Simulate self-assembly
- Design optimal nanostructures
- Carry out device simulations

New DOE-EFRC on Novel Thermoelectrics

EFRC – Energy Frontier Research Center

Morelli (Engineering, MSU): Transport measurements, synthesis

Sakamoto (Engineering, MSU): Synthesis, device physics

Chemistry (NW) Kanatzidis: Material Synthesis&Characterization

Physics (MSU) **Mahanti**: Theory of Structure and Transport

Physics (UM) Uher: Transport measurements

Engineering (MSU)Hogan: Transport measurements

Schock: Devices (small and large scale)

Engineering (Iowa S) Shi: Modeling heat flow in anisotropic media

Theoretical Studies of Electronic Structure and Transport Properties of (AgSb)$Pb_{2n-2}Te_{2n}$ Compounds

PI: S. D. Mahanti, Michigan State University

Science Objectives

To understand

• Why these systems show large *ZT* at high T

• The underlying electronic structure – role of microstructure, structural stability

• How the resulting electronic structure controls charge and energy transport

Recent Accomplishments

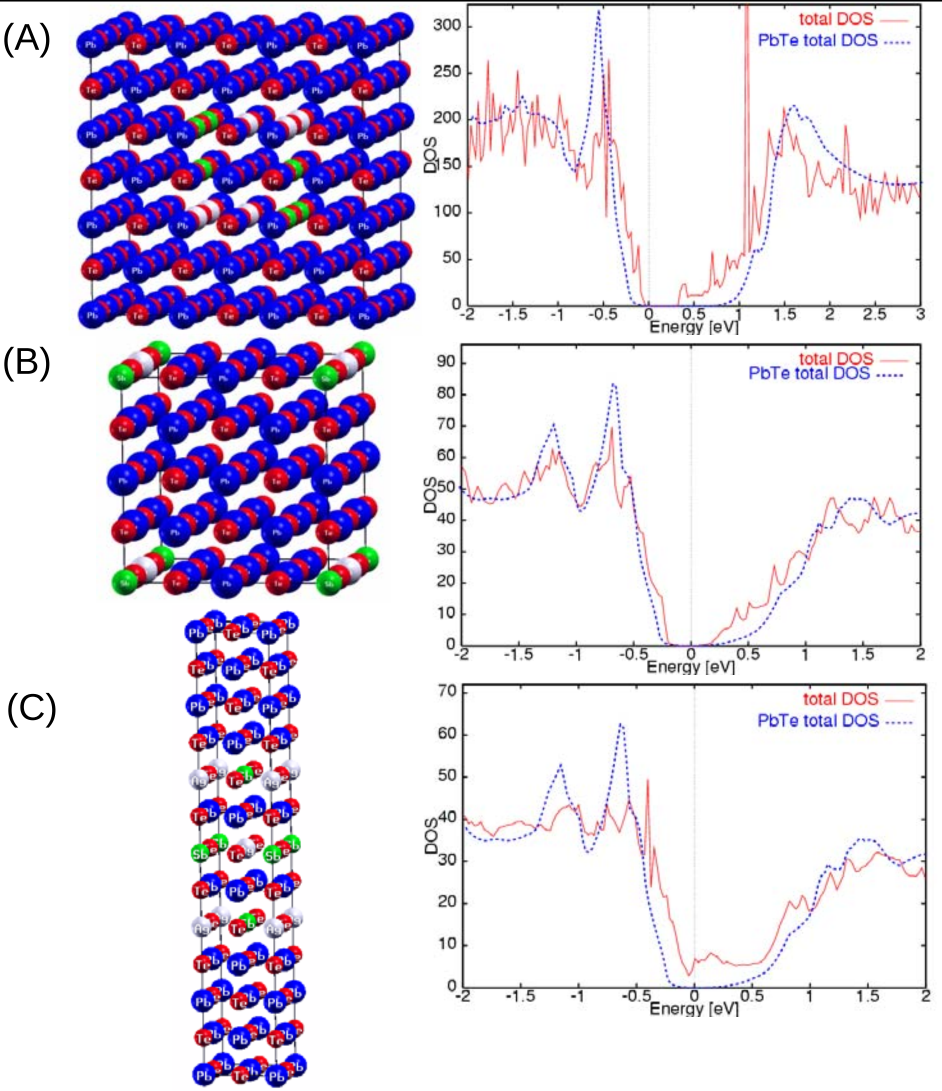
- Found that Sb and Ag introduce new resonant states near the band gap region – dramatically modifying the gap and the density of states near the gap
- Electronic structure near the gap depends sensitively on the micro-structure of Ag and Sb atoms
- MC simulation of Coulomb Lattice Gas model gives layered (2D) structures

Approach

• Monte Carlo (MC) Simulation of Coulomb Lattice Gas (CLG) model to probe ordering of Ag and Sb ions

• *Ab initio* all electron calculations using density functional theory for electronic and ionic structure

• Transport theory in semiconductors



Ag-Sb cluster model (A), chain model (B) and layer model (C). The corresponding density of states (DOS) compared with that of pure PbTe. The Ag, Sb, Pb and Te are shown in grey, green, blue and red colors. (A) without spin-orbit, (B,C) with spin-orbit interaction.

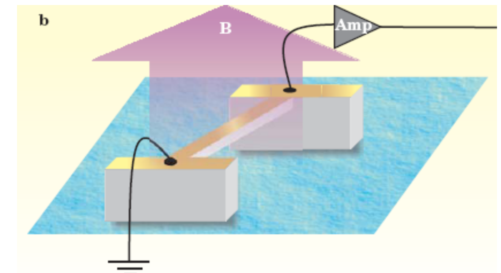
Nonlinear Dynamics: Noise-induced switching in nano-oscillators

Noise-induced switching between co-existing vibrational states is

- **A ubiquitous fundamental phenomenon in nano-systems**
- **Underlies one of the most sensitive means of quantum measurements**

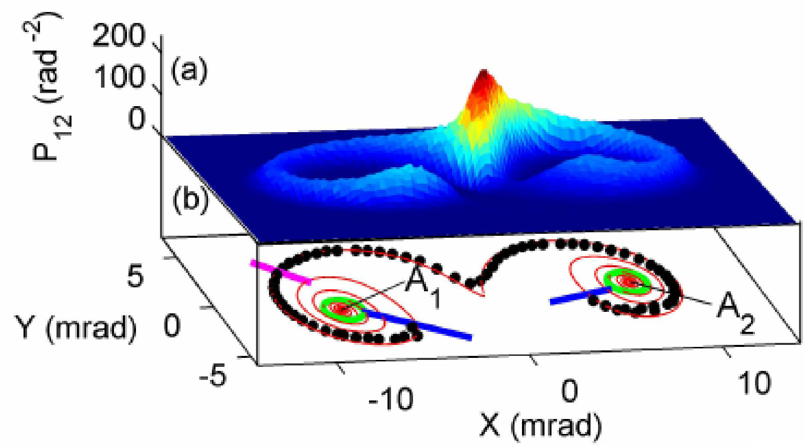
(based on the theory by Dykman and Krivoglaz)

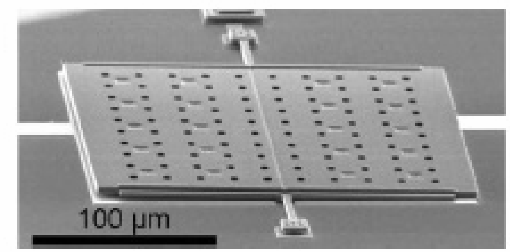
Switching is a random event, but the system follows a well-defined path!



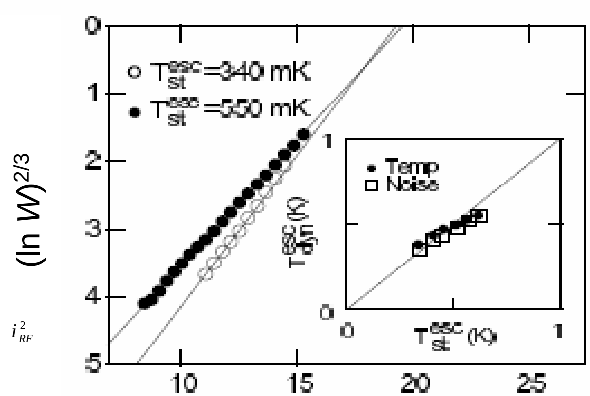
Typical size: $1\times 0.1 \times 0.1\ \mu$m

First theoretical prediction and experimental observation of the distribution of paths followed in switching (Chan, Dykman, & Stambaugh, PRL 2008)

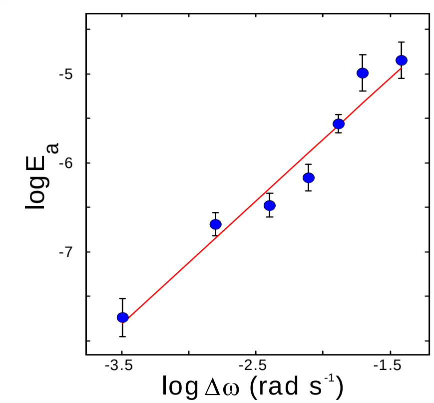




The universal scaling predicted at MSU has been now observed in many nano- and micro-oscillators



Josephson junctions (Siddiqi et al., 2005)



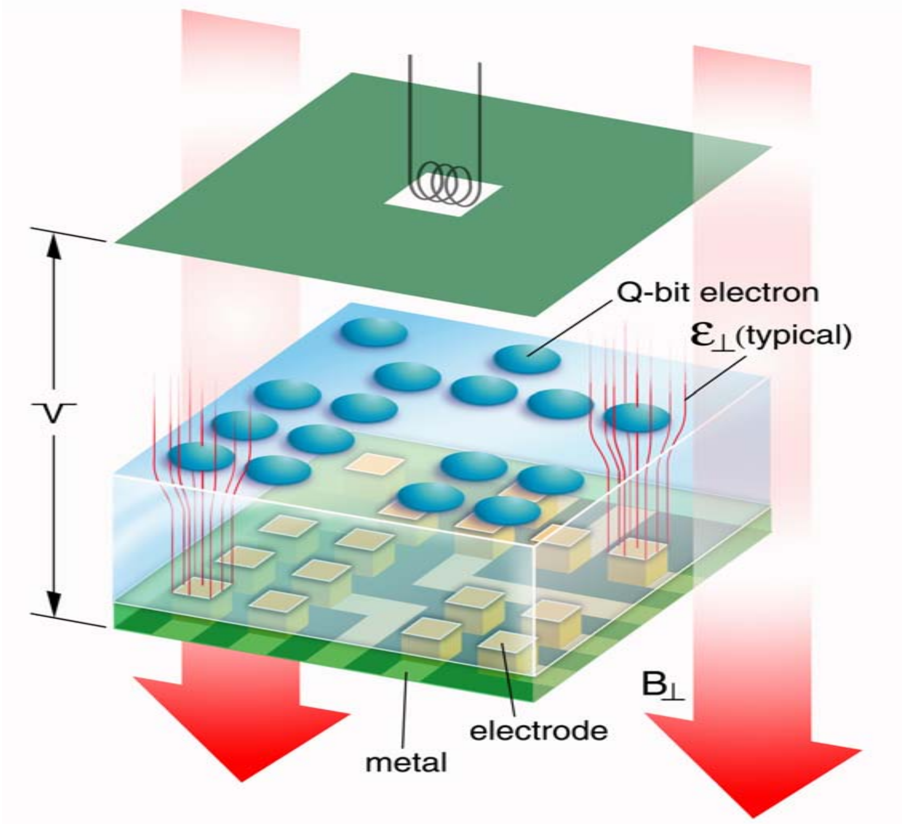
MEMS (Chan & Stambaugh, 2005)

Dykman

Mark Dykman
Carlo Piermarocchi

-Theory of quantum computing with electrons on helium
-Theory of tunneling decay in correlated many-electron systems
-Scaling theory of activated switching in modulated systems
-Theory of many-particle localization

16 bit quantum computer based on electrons on liquid helium

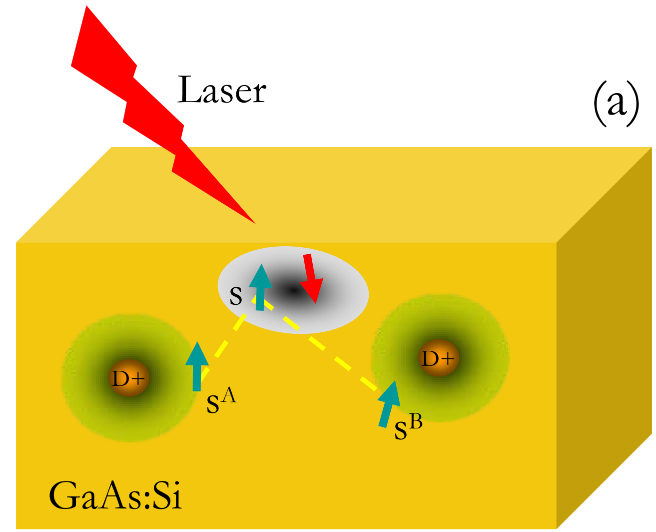


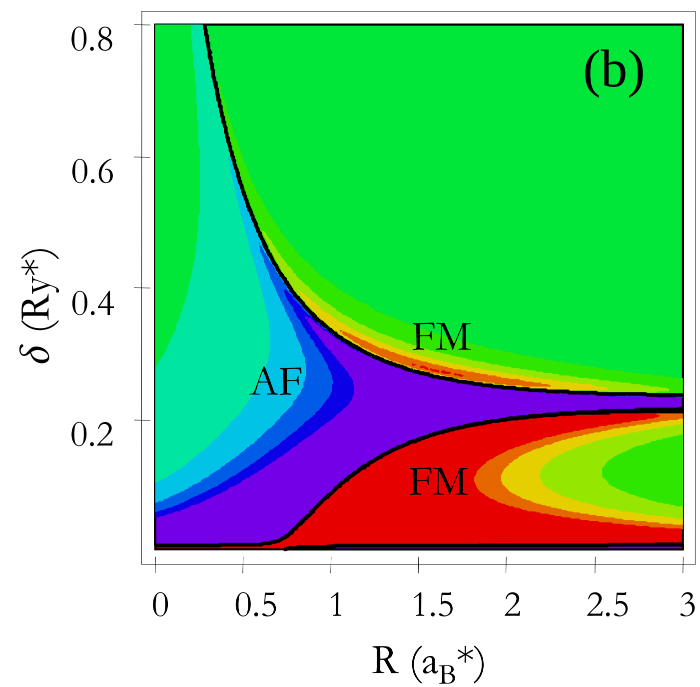
-Brage Golding

CMPT: Carlo Piermarocchi

We study the light-induced interaction between spins localized by impurities in a semiconductor host. Fig. a: the laser creates electron-hole pairs in the semiconductor and mediates a spin-spin coupling between electrons in donors. Fig. b: the coupling depends on the frequency of the laser δ and the distance R . Ferromagnetic (FM) and Anti-Ferromagnetic (AF) coupling are possible. This mechanism can be used to control qubits stored in the impurities and process optically quantum information; it also opens to new controllable materials whose magnetic properties can be controlled by changing the spin-spin coupling with lasers.

Basic applications of optics in quantum information technology have been included in the list of topics of the undergraduate class I taught in the Fall Semester (Optics I).



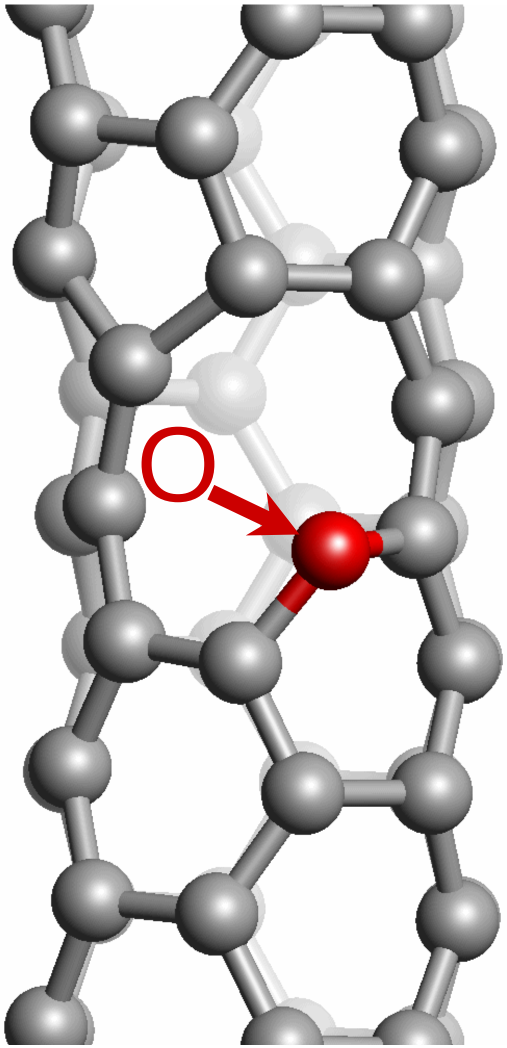


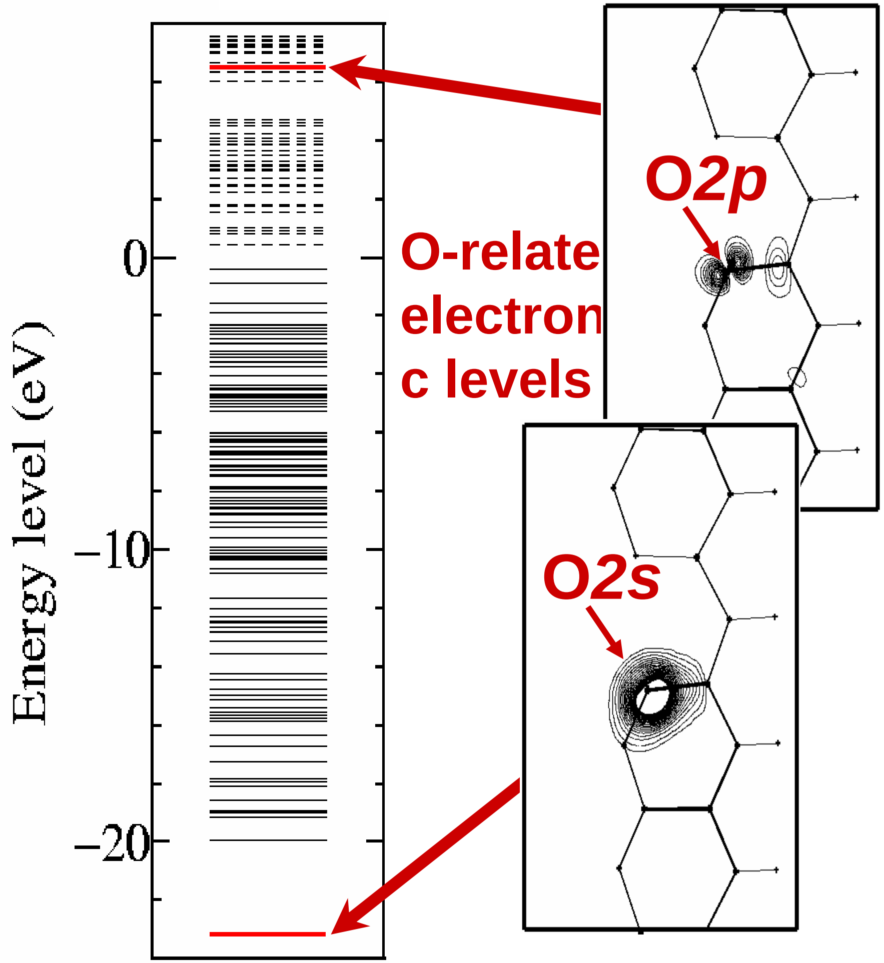
Removal of Oxygen Defects from Nanotubes

Alternative to thermal and chemical treatment:

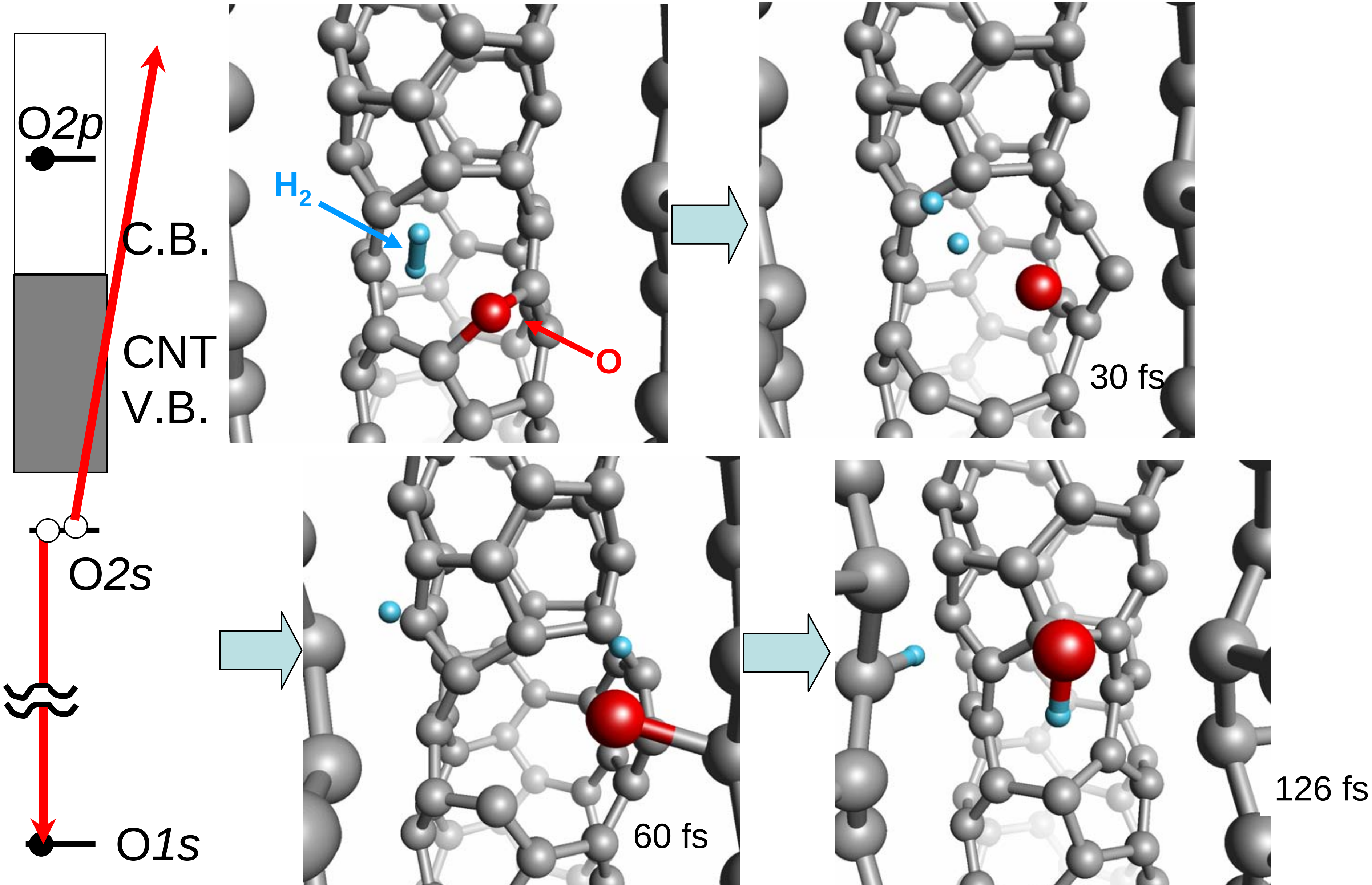
Electronic excitations!

David Tomanek





Auger decay following the O1s → 2p excitation (~520 eV)



- Removal of oxygen by photo-surgery

(Tomanek, MSU, 2004)

Quantum Atom Optics Theory Group

Prof Michael Moore

– Yuping Huang (Grad)

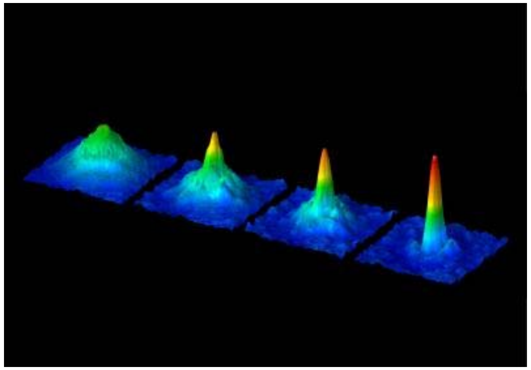
– Steven Wolf (Grad)

- **Research Topics**
  - **Bose-Einstein Condensation**
  - **Optimal quantum measurement**
  - **Quantum information processing with single-atom qubits**
  - **Nonlinear mixing of coherent matter and light**
  - **Nonlinear mixing of atomic and molecular matter-waves**

- **Bose-Einstein Condensation**
  - **A phase transition occurs when a trapped gas of atoms is super-cooled to the nano-Kelvin regime**
  - **All atoms jump into a single macroscopic (~1 mm) orbital**

Decreasing T →

Thermal cloud

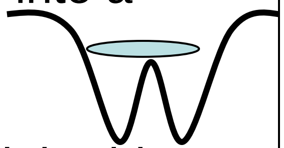


BEC

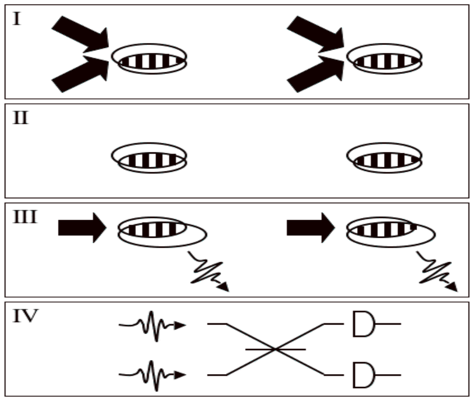
Rempe group, MPQ

Some of our Projects

- BEC double-well interferometry:
  - A BEC can be loaded into a double-well potential



  - Raising the barrier height drives a Superfluid-Insulator transition
  - We have developed a protocol to create optimal input states for sub-shot-noise phase measurements in double-well BEC systems

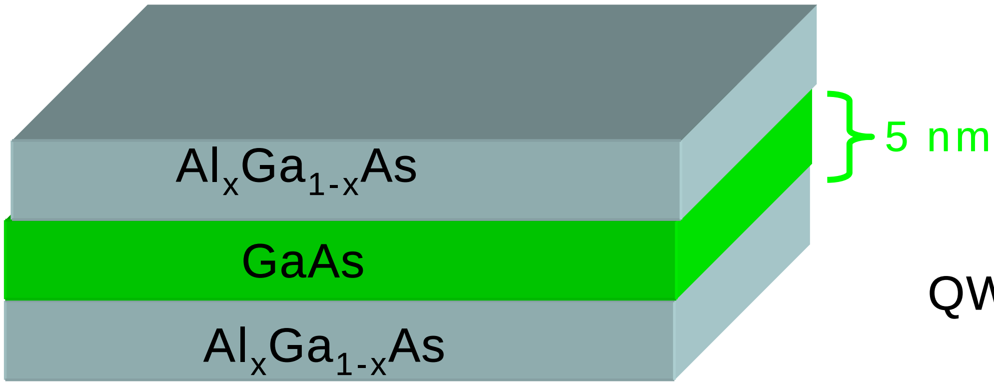


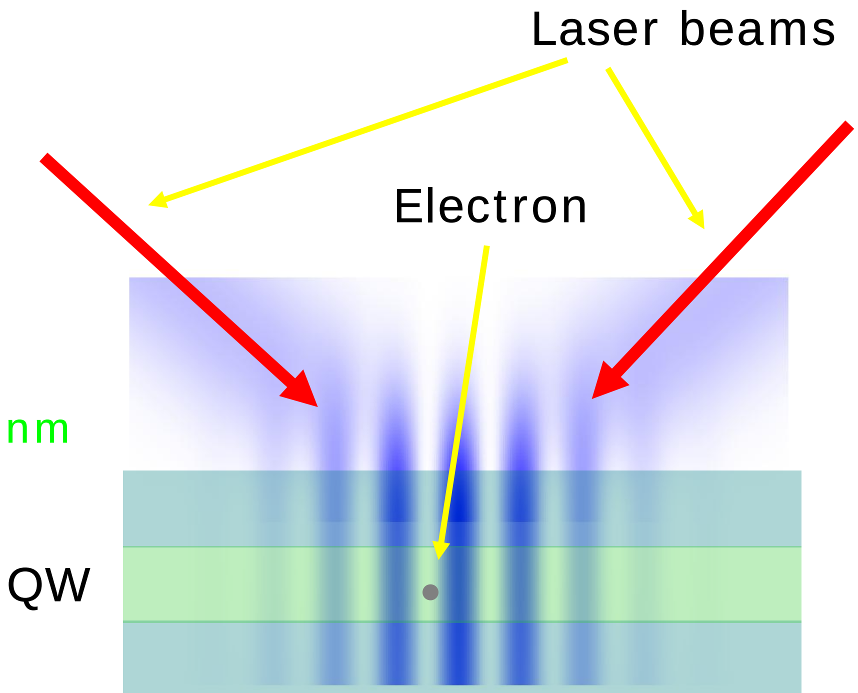
- Non-linear mixing of matter and light waves
  - The development of BEC places atomic matter waves and light waves on equal footing
  - From this perspective, the processes of Rayleigh and Raman scattering can be viewed as nonlinear four-wave mixing involving 2 matter and 2 light waves
    - Starting with 2 light and 1 matter generates 2nd matter wave
    - Imprints quantum phase information from laser onto BEC
    - Starting with 2 matter and 1 light generates 2nd light wave
    - Transfers quantum phase from BEC onto laser
  - Using this coherent phase transfer between matter and light, we are designing and modeling hybrid atom-photon interferometers

Optical tweezers for electrons in quantum wells

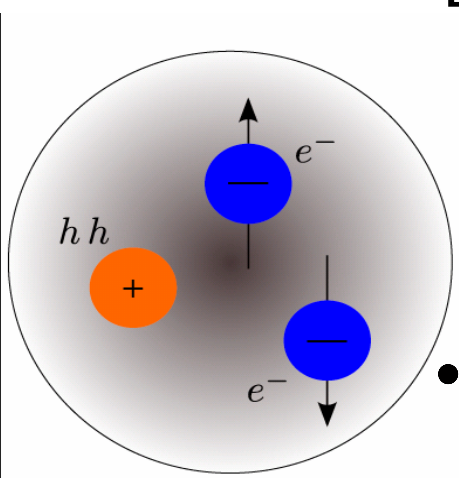
M. Moore and C. Piermarocchi

- Semiconductor Quantum Well:
  - 2-dimensional system
  - Electron moves in x-y plane

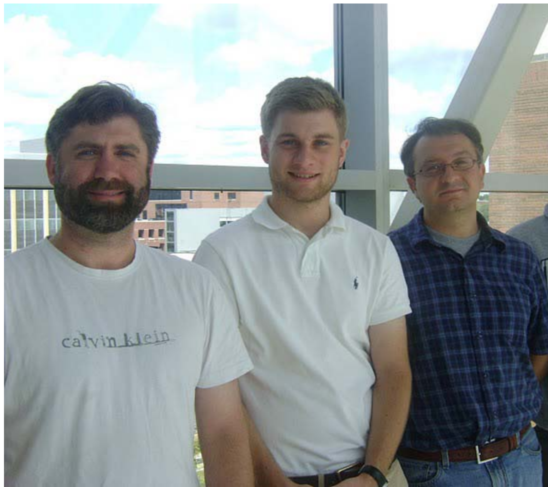




- Electron Optical Lattice:
  - Electron is trapped due to laser intensity modulation
  - Strong potential due to “trions”



- Trion: two electrons and one hole bound together



Condensed Matter Theory: This talk is online:
www.pa.msu.edu/~duxbury/MSUCMPToverview.pdf

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