Institute for the Theory of Advanced Materials in Information Technology

(NSF DMR-0325218*)

Walter Library, Digital Technology Center at the University of Minnesota

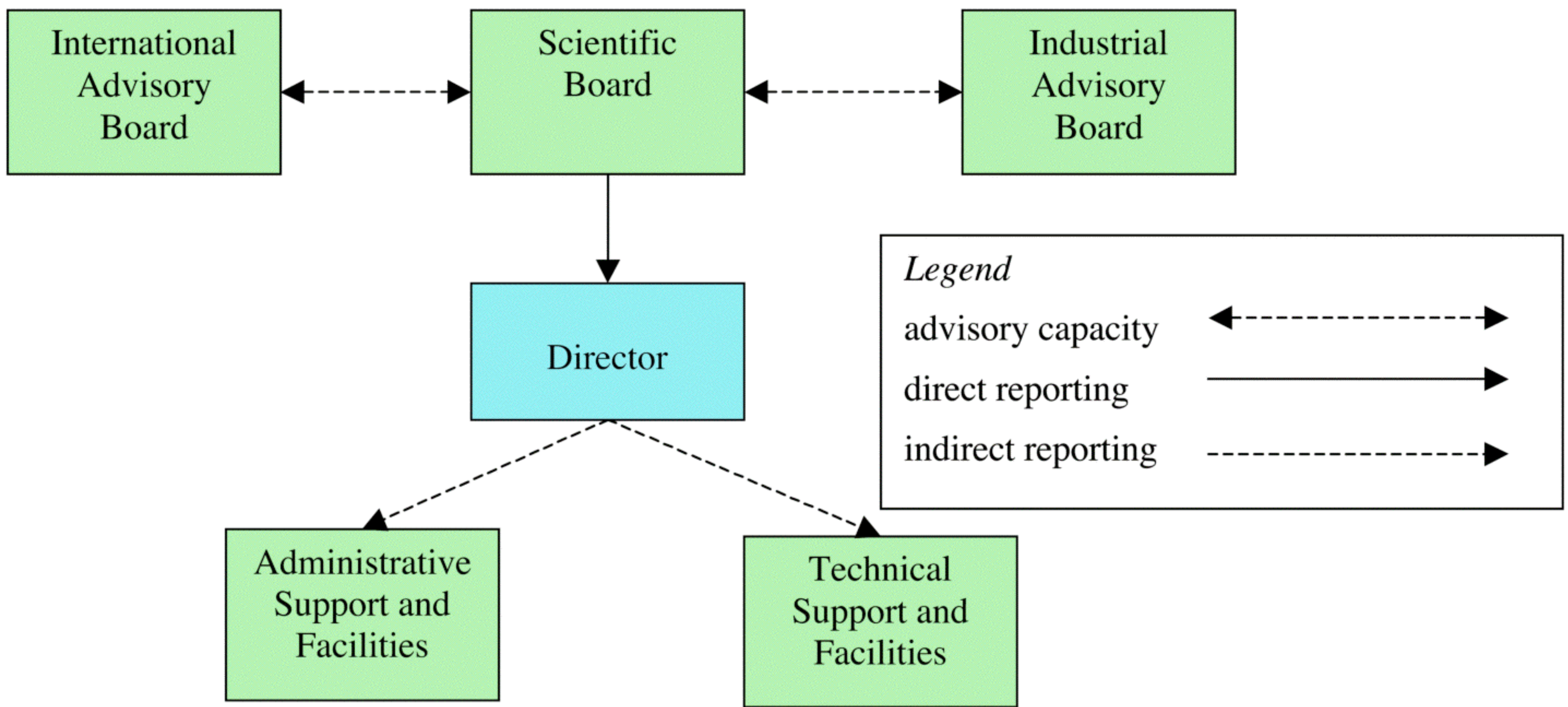
Mission:

The Institute is dedicated to promoting research on understanding and predicting the properties of materials used in information technology.

http://www.itamit.dtc.umn.edu/

***Funded by the National Science Foundation for 5 years (3+2) for a total of $3M**

Organization



Computational Resources from the Minnesota Supercomputing Institute. Staff/Office support from the Digital Technology Center

Science Board

Yousef Saad
University of Minnesota

Jim Chelikowsky
University of Minnesota

Steve Louie
UC Berkeley

Renata Wentzcovitch
University of Minnesota

Efthimios Kaxiras
Harvard University

Andreas Stathopoulos
William and Mary

Industrial Board

Dr. James Chadi, Chief Scientist, Science Division, NEC
Dr. Ken Hass, Manager, Chemistry & Environmental Science Department, Ford Motor Company
Dr. Alex Demkov, Principal Staff Scientist, Motorola Physical Sciences Research Laboratories
Dr. Doug Allan, Research Associate, Corning
Dr. Cristina Thomas, Senior Research Specialist, 3M
Dr. John R. Smith, Group Manager, Manufacturing Processes Research, Delphi Automotive Systems
Dr. Gaddi Haase, Staff Scientist, Texas Instruments
Drs. Y.-K. Kwon and S.-H. Jhi, Nanomix
Dr. S. Shankar, Intel

International Board

Professor Achi Brandt (Weizmann Institute of Science, Rehovoth Israel)
Dr. Nadia Binggeli (International Center for Theoretical Physics, Trieste, Italy)
Dr. Leeor Kronik (Weizmann Institute of Science, Rehovoth, Israel)
Professor Jose Luis Martins (Instituto Superior Tecnico, Lisbon, Portugal)
Professor Angel Rubio (University Pais Vasco, San Sebastian/Donostia, Spain)
Professor Matthias Scheffler (Max Planck Institute, Berlin Germany)

Outreach and Education Activities

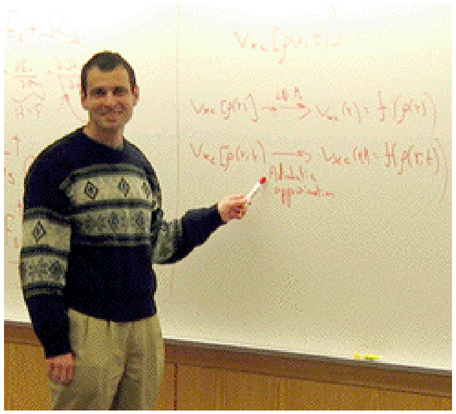
European Commision/National Science Foundation Workshop on "Computational Methods in Materials Science." San Francisco, April 15 and 16.

Coordination Meeting: August 6 and 7 (Science, Industrial and International Boards)

Software link:

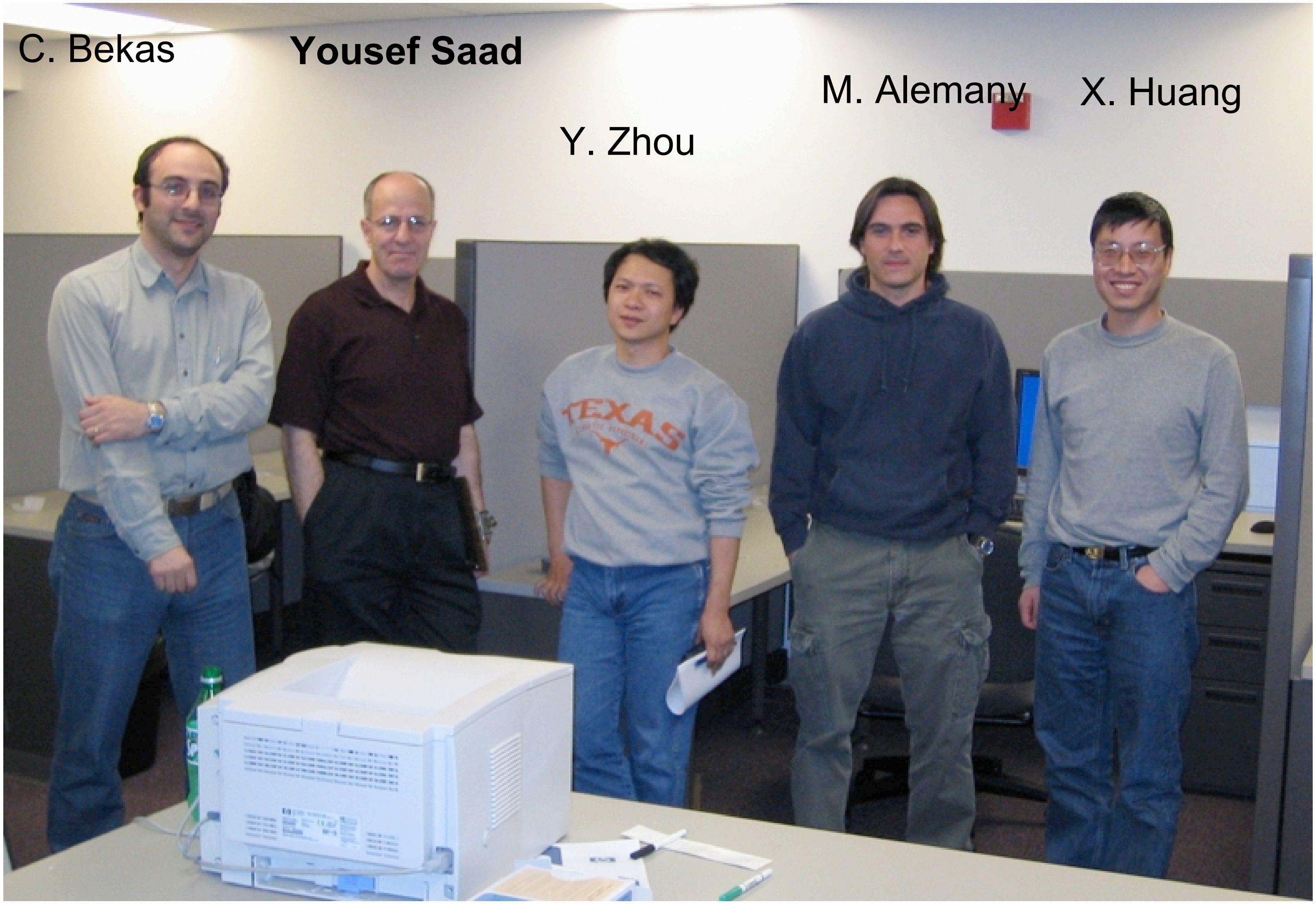
http://www.itamit.dtc.umn.edu/software.html

Summer Intern Program:
Eric Lindgren
Carleton College



Visitors: Leeor Kronik and Adi Makmal from the Weizmann Institute; Serdar Ogut from University of Illinois, Chicago

Postdocs/Students



Lingzhu Kong

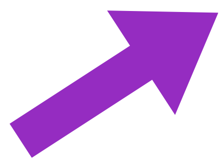
Marié López del Puerto

Shiv Gowda

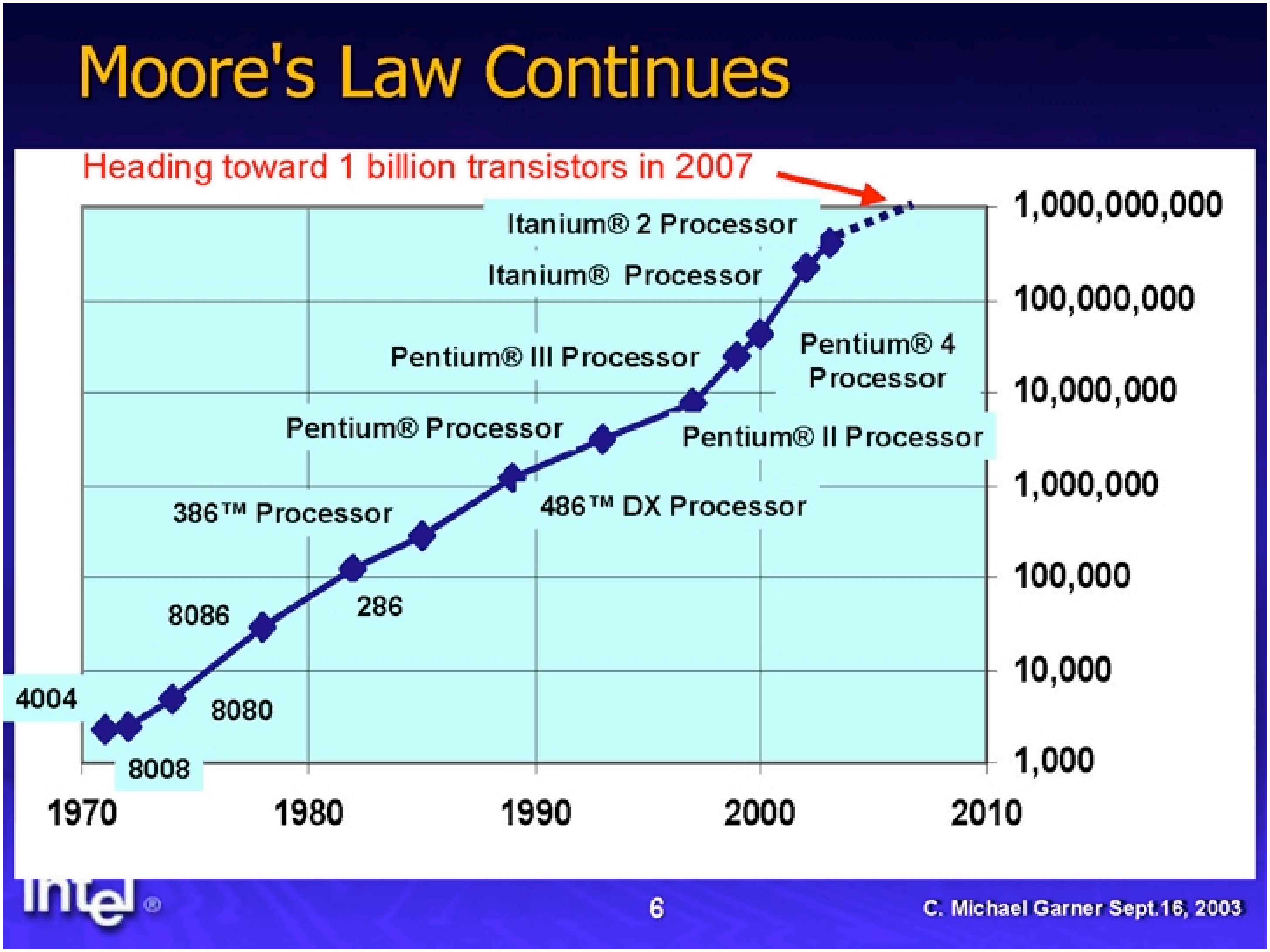
Shen Li

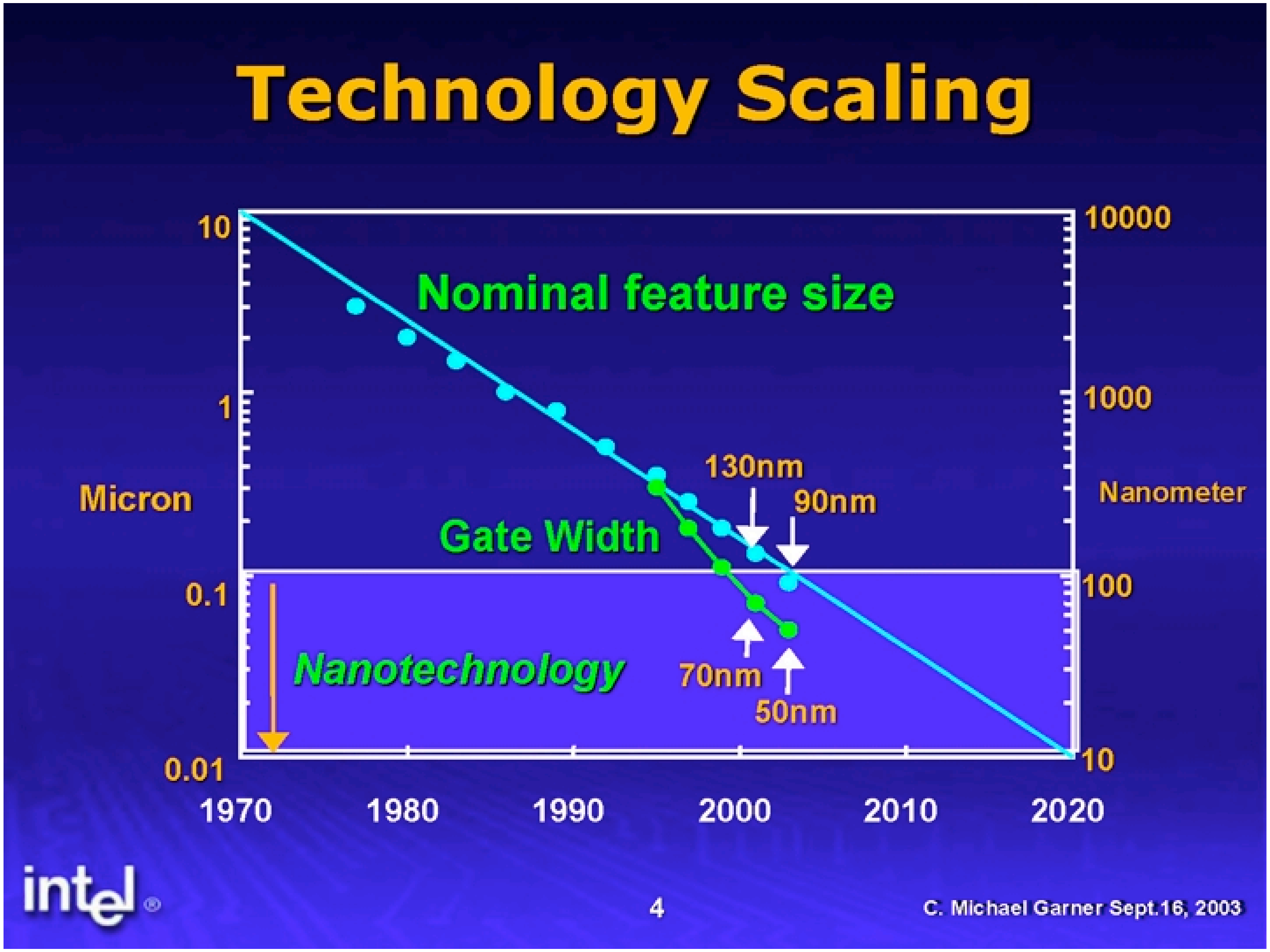
Chemical Engineering, Chemical Physics, Materials Science, Physics, Scientific Computation and Computer Science

One of the greatest accomplishments of humankind: Changing silicon from beach sand to the stuff of supercomputers



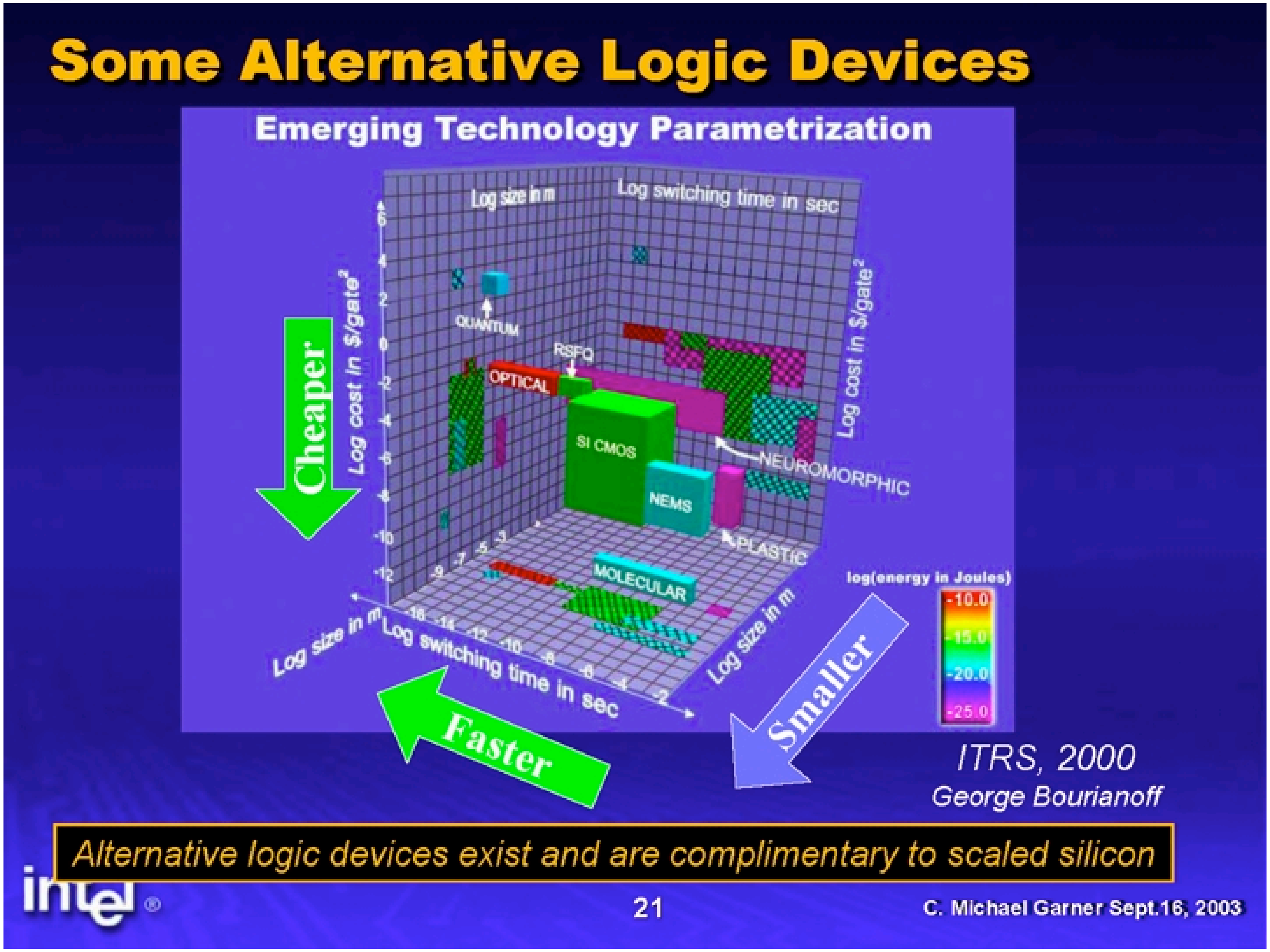
Heading toward the nanoscale.....





Intel is now a "nanotechnology company."

Examples of Materials of Interest to Intel....



Turning wafers into microprocessors costs $1 billion per acre of silicon. - Gordon Moore, *BusinessWeek*, 1996.

Research Programs

Surfaces: Adsorption, defects and growth
Liquids: Microstructure, growth
Molecular electronics
Dielectrics: Defects in silica
Clusters and quantum dots:
Optical, structural and magnetic properties

Spintronic materials:

- $Co_{1-x}Fe_xS_2$ **half metals (Renata Wentzcovitch)**
- **Growth of Mn:Ge Surfaces (Efthimios Kaxiras)**
- **Mn:ZnSe Quantum dots (Xiangyang Huang)**

High performance algorithms!

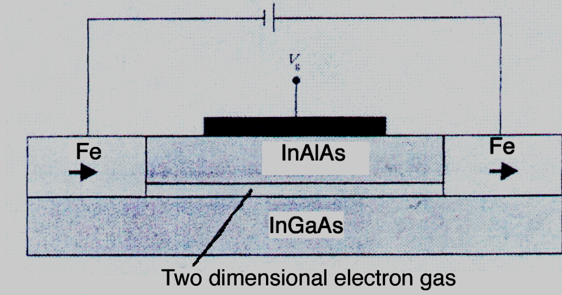
Spintronics

Can we "inject spin" into electronic devices?

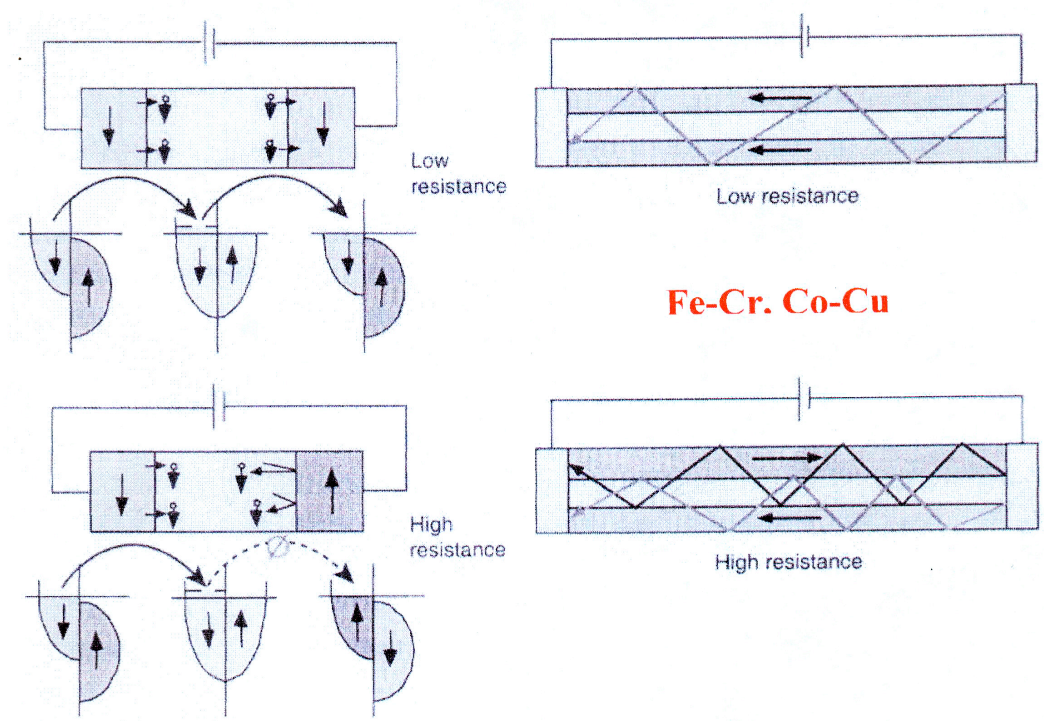
Spintronics !!

e.g., The spinFET

Datta & Das, APL, 1990



The spin valve – a memory element

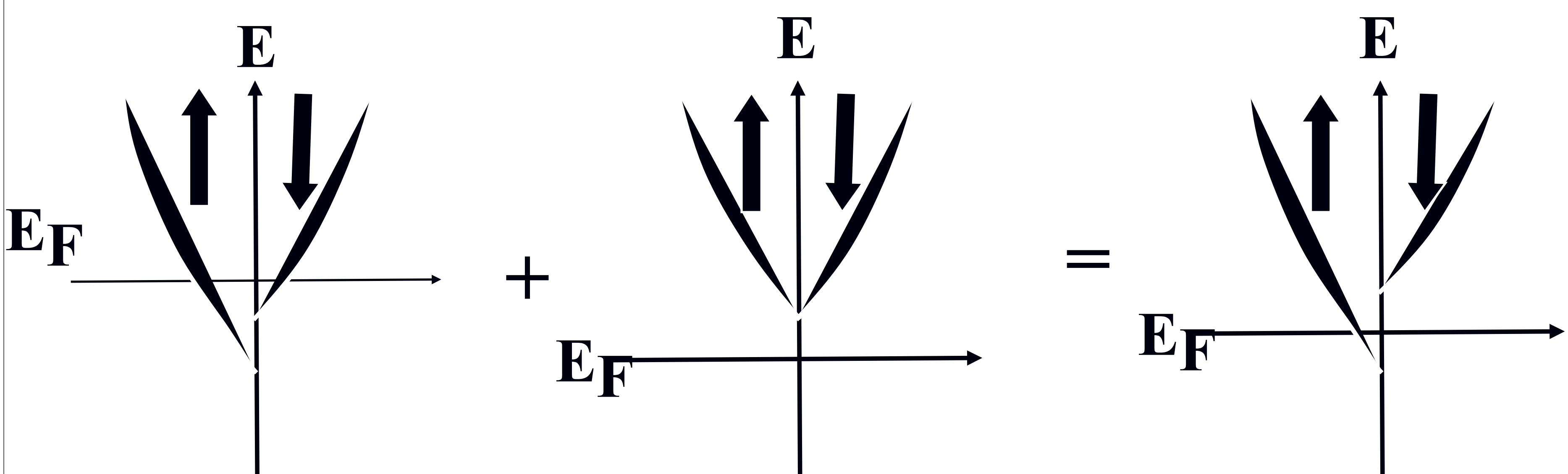


Search for materials with 100% polarization:

$$P = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}} = 1$$

Engineering a half metal ferromagntic material – $Co_{1-x}Fe_xS_2$

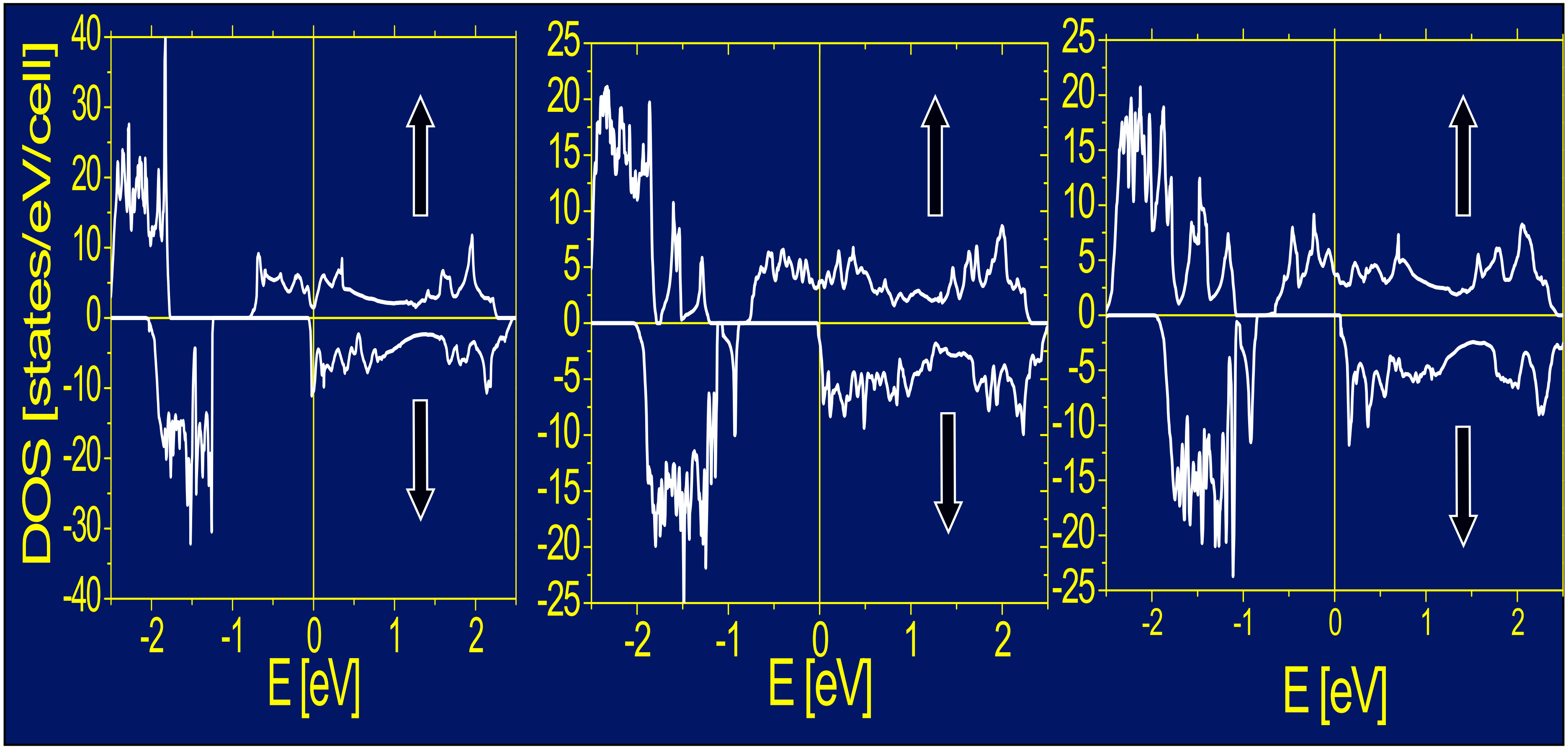
- CoS_2 Metallic ferromagnet
- FeS_2 Diamagnetic semiconductor
- $Co_{1-x}Fe_xS_2$ Half-Metallic Ferromagnet?



Electronic structure calculations

- **Pseudopotentials, plane-wave expansion, and the LSDA**

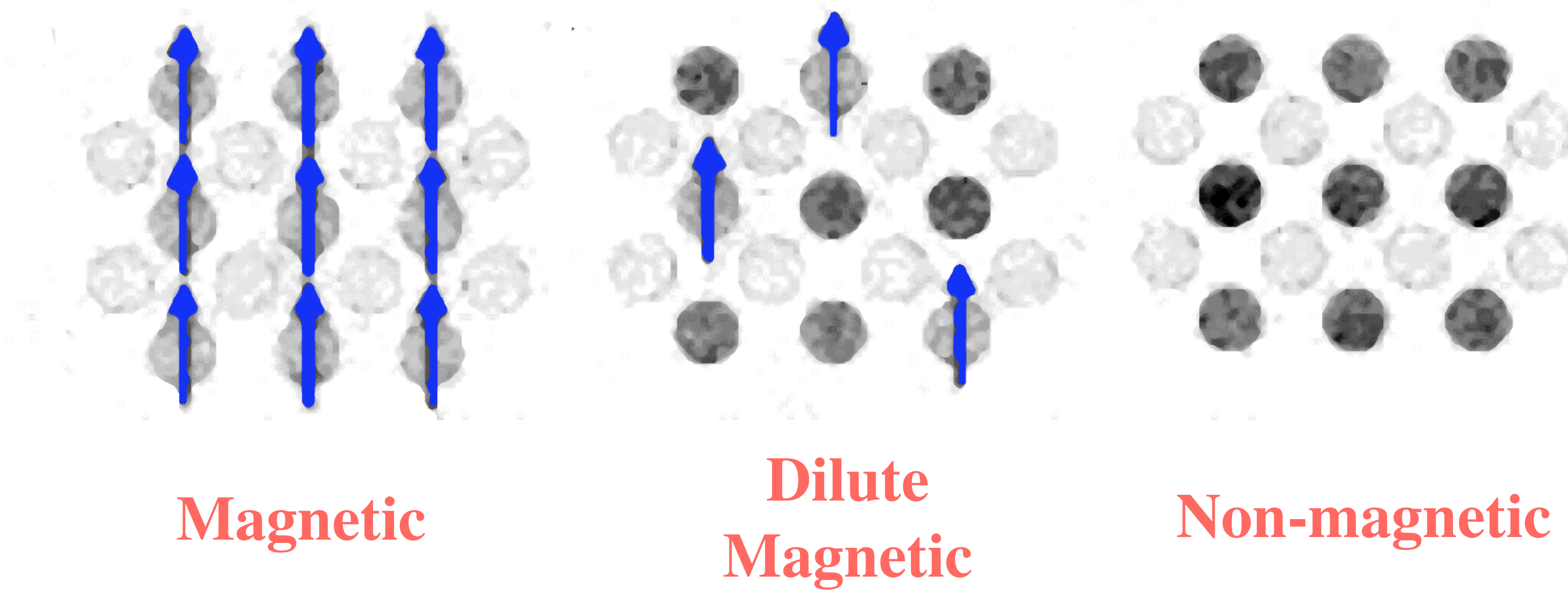
x = 0.0 **0.125** **0.25**



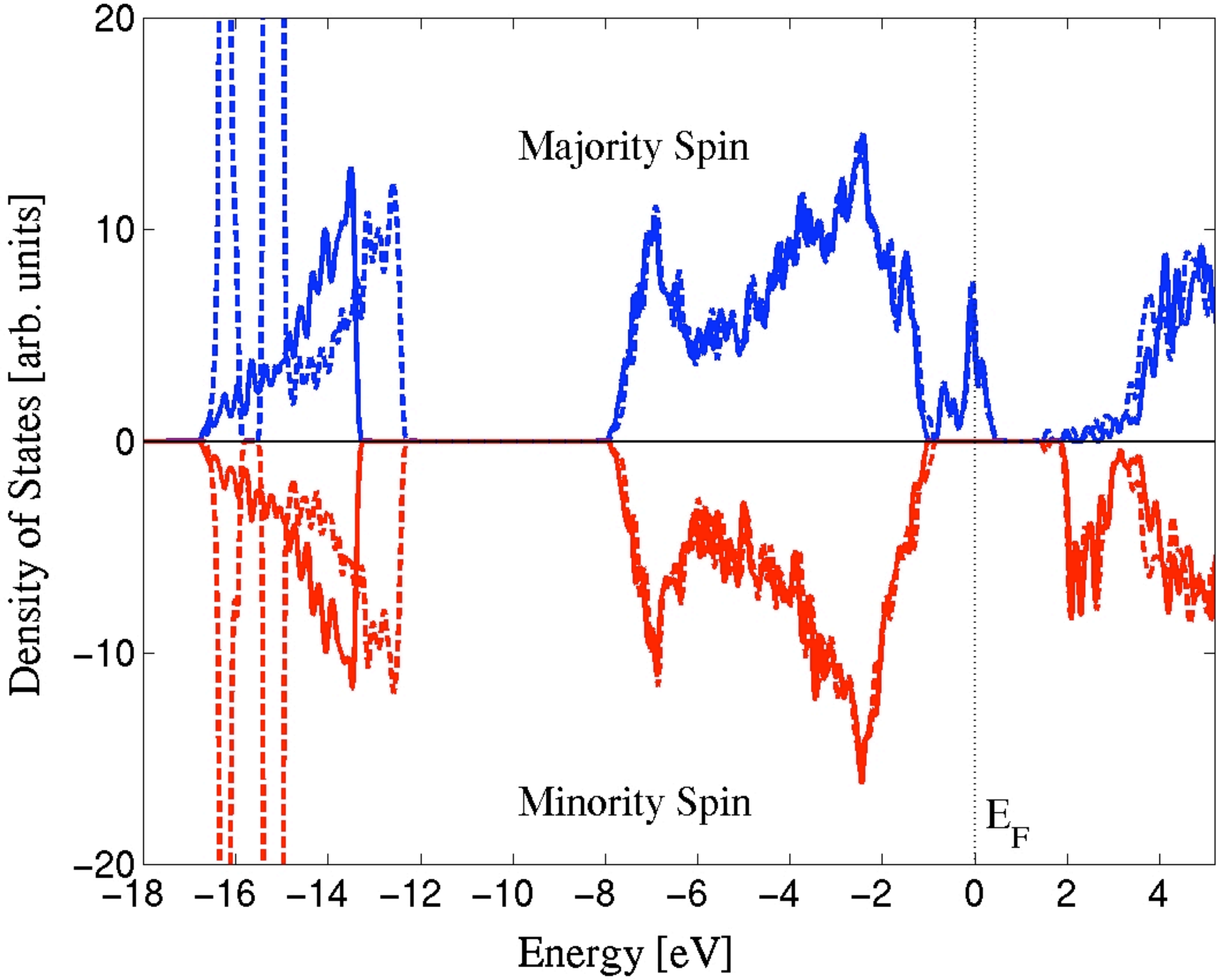
P = -70% **+ 40 %** **+100 %**

Wentzcovitch et al.

Spintronic materials are often made of dilute magnetic semiconductors alloyed with a magnetic element. These alloys are both ferromagnetic and semiconducting, opening the door to exciting "spintronics" applications - devices based on both electron charge and spin.



MnGaN: Role of Ga 3d States



Dashed line with 3d state treated explicitly.

Key results:
-Valence band not polarized.
-State in the gap "half-metallic".
-Minority polarization in conduction band states.

Ga 3d and N 2s states do interact, but effect on band gap energy is minimal

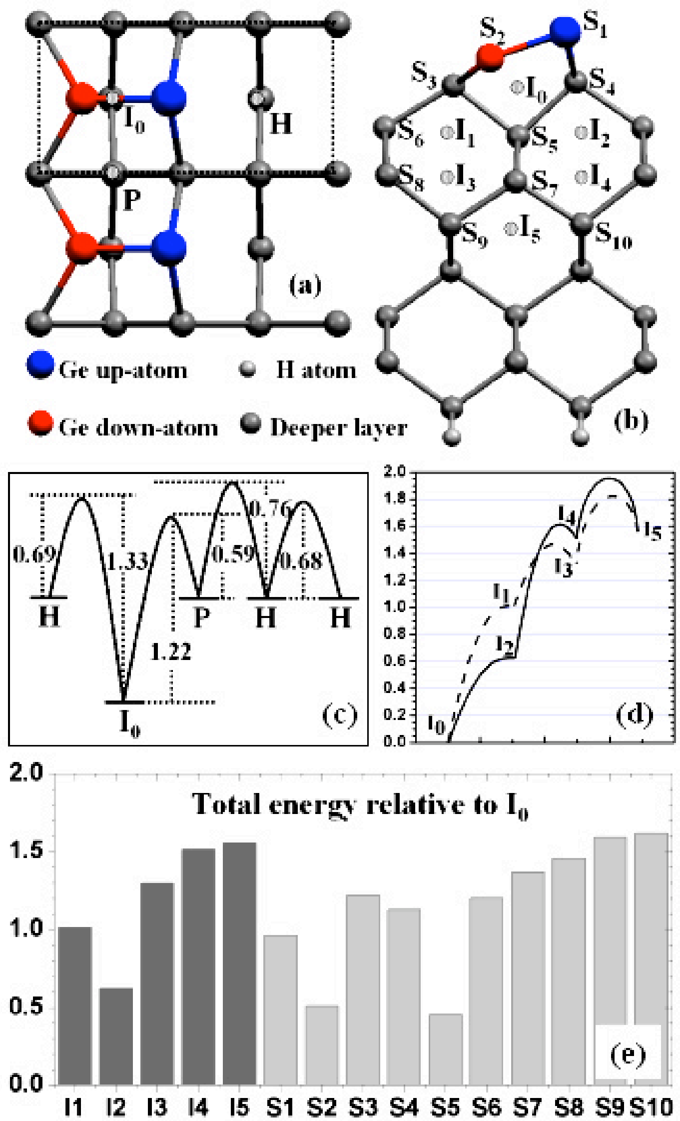
Kronik, Jain and Chelikowsky

Growth Modes of Mn on Ge (100) and Ge (111) Surfaces

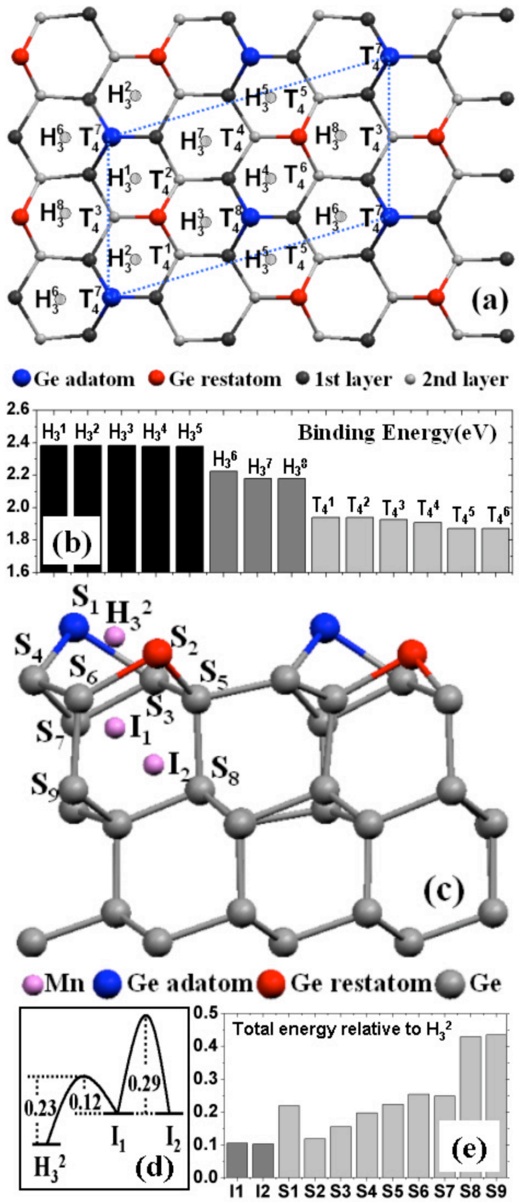
- Growth mechanisms, important but largely unexplored.
- Use pseudopotential-density functional theory to examine the growth of Mn on Ge surfaces
- Low Mn doses on Ge (100) initiates novel subsurface growth whereas Mn on the (111) surface can diffuse into the bulk via interstitial sites.

Kaxiras et al.

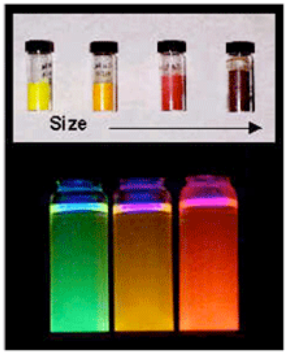
(100) Ge Surface



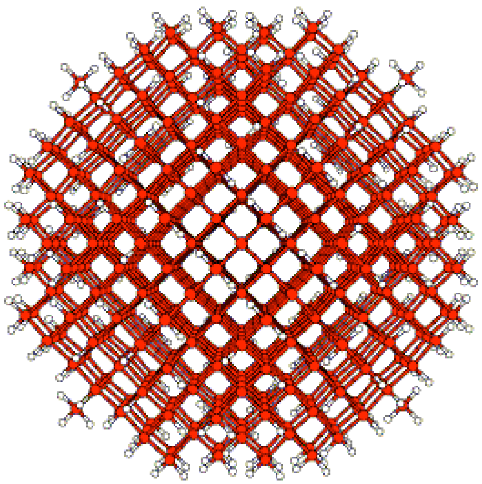
(111) Ge Surface

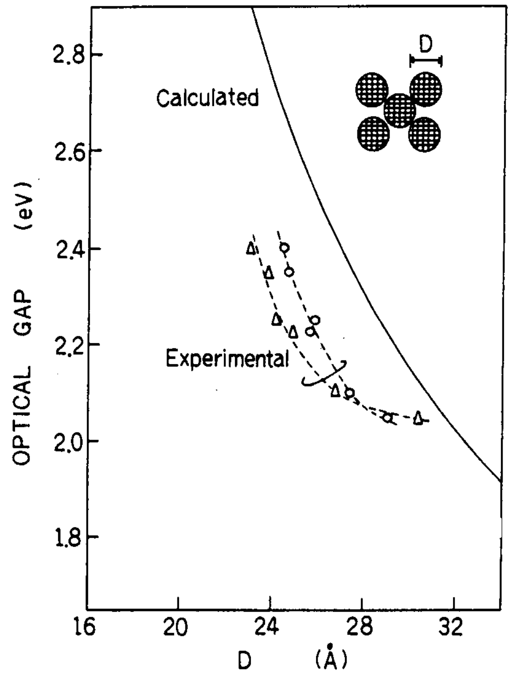


Quantum Dots: Optical and Magnetic Properties

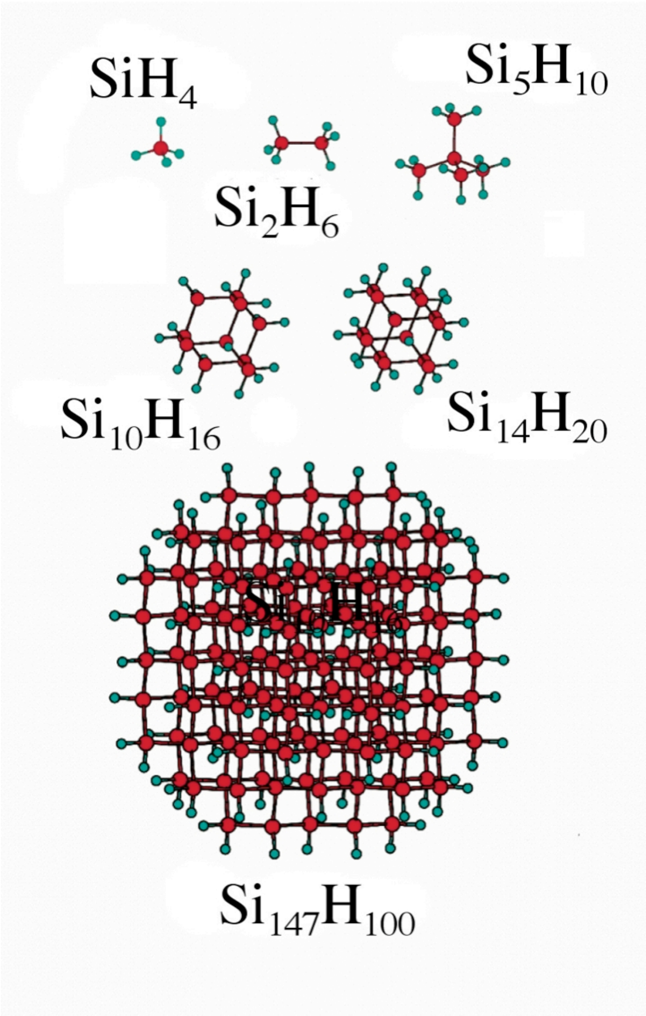


Examine the role of quantum confinement
- Profound effect on the optical properties of nanocrystal





Hydrogenated Semiconductor Clusters and Quantum Dots

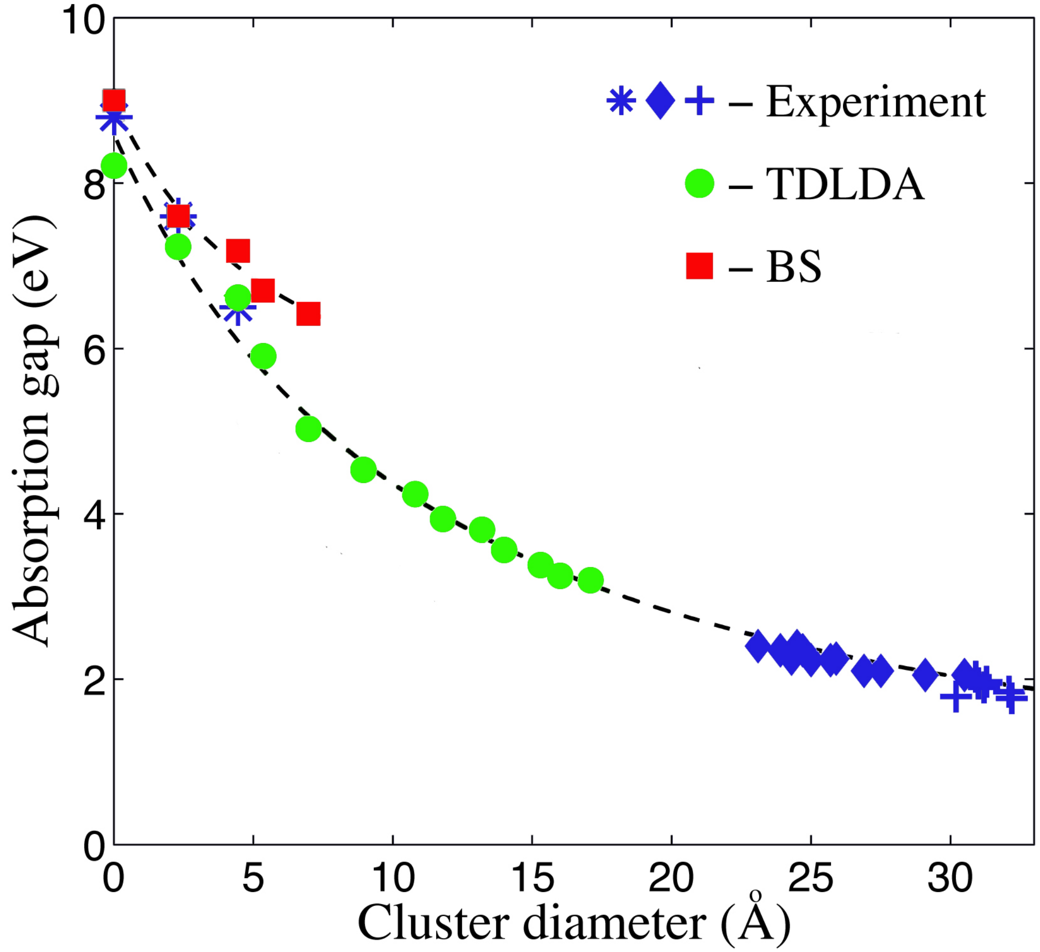


Consider bulk fragments of silicon passivated with H atoms.

What are the characteristic spectra of these objects?

How do they evolve to the bulk spectra?

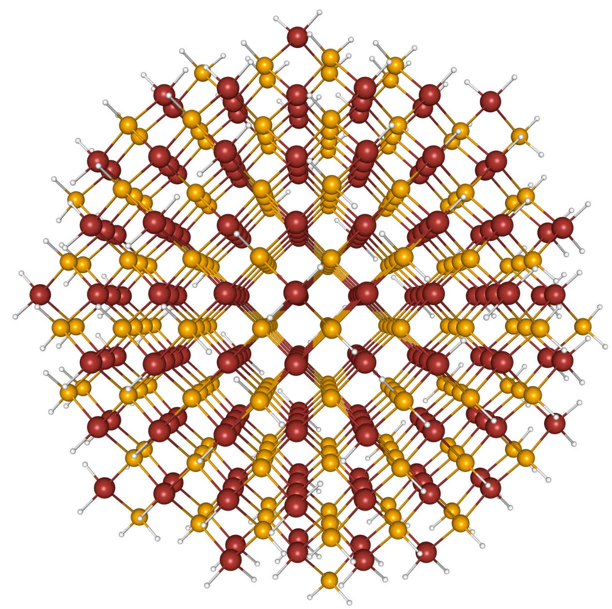
Absorption Gap Compared to Experiment



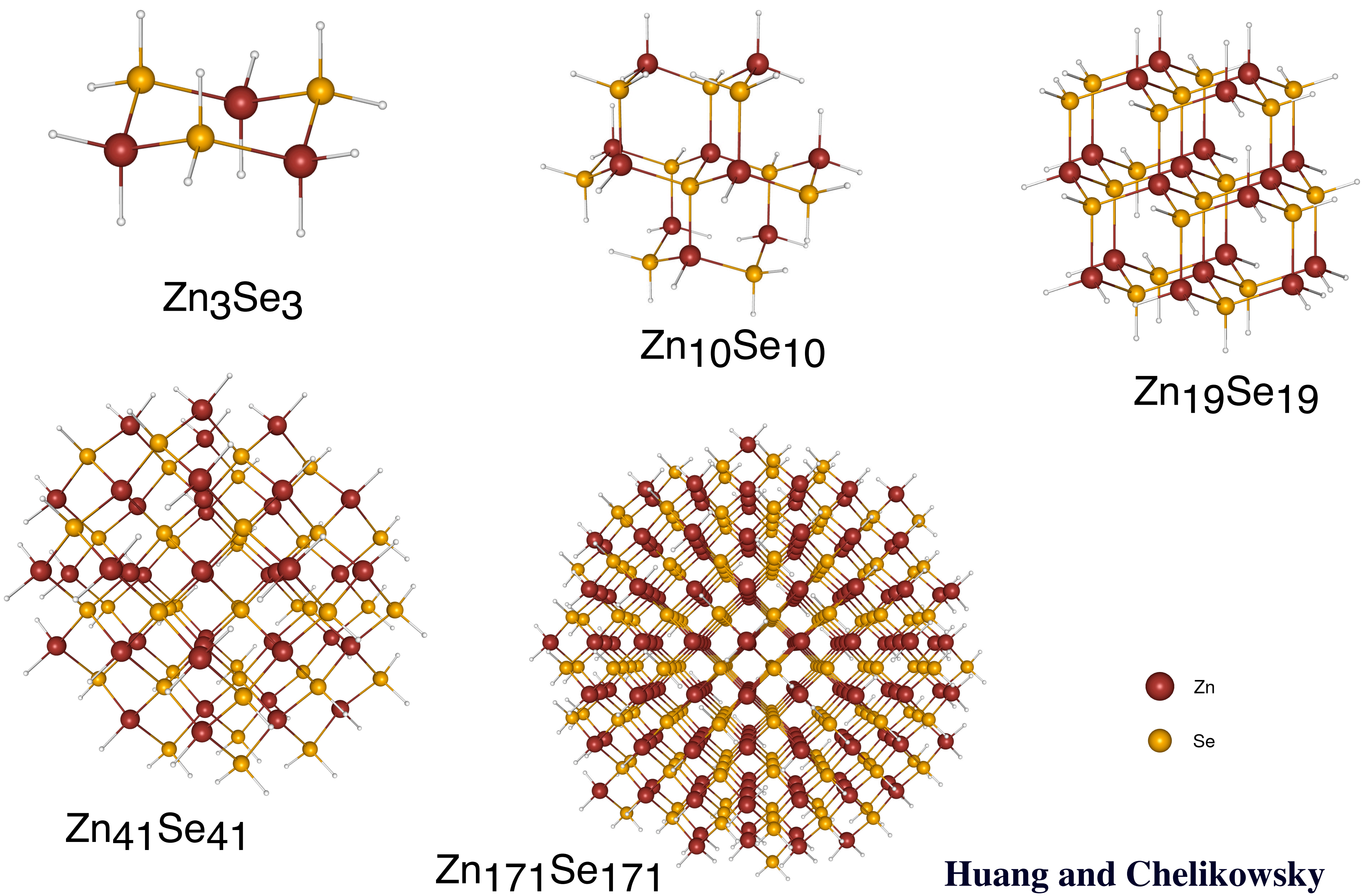
Quantum Dots: Optical and Magnetic Properties

Confinement should also have
strong effect on spin-spin exchange.

- Study and manipulate a single spin in a semiconductor box.
- Serve as a model for spintronic materials.

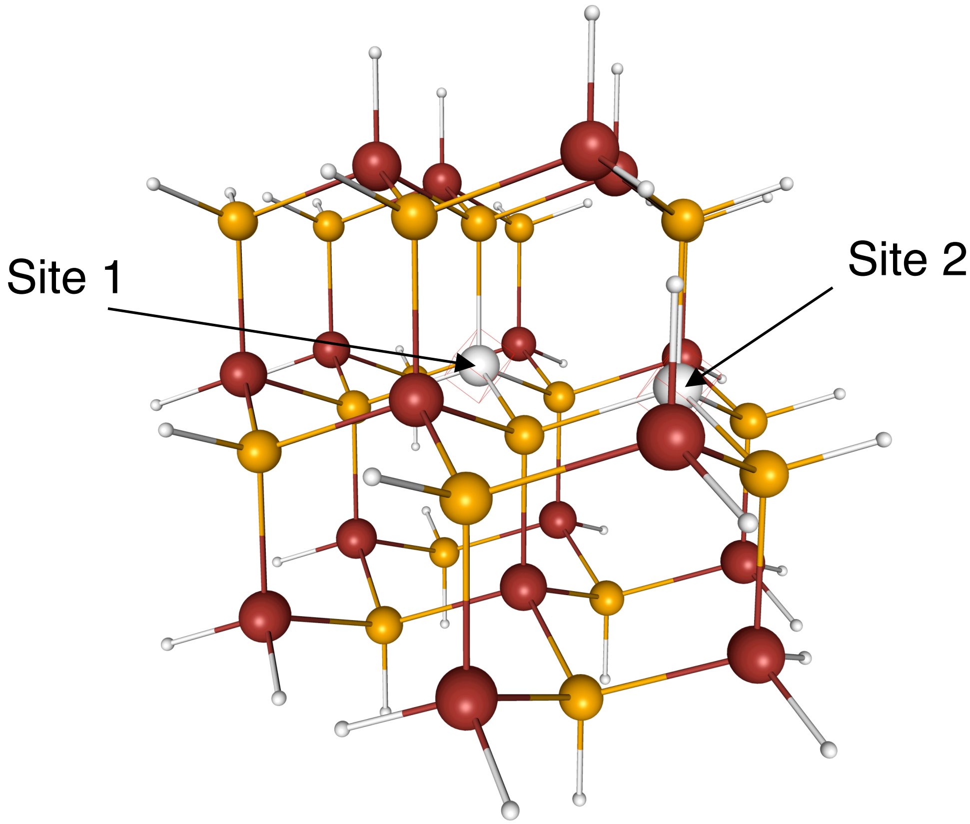


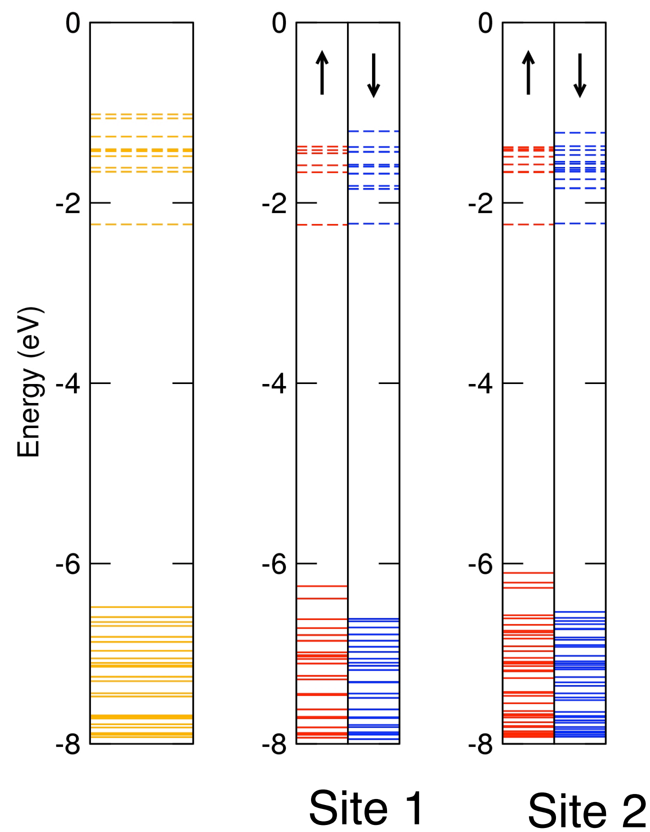
Structure of Zn_mSe_m clusters



Huang and Chelikowsky

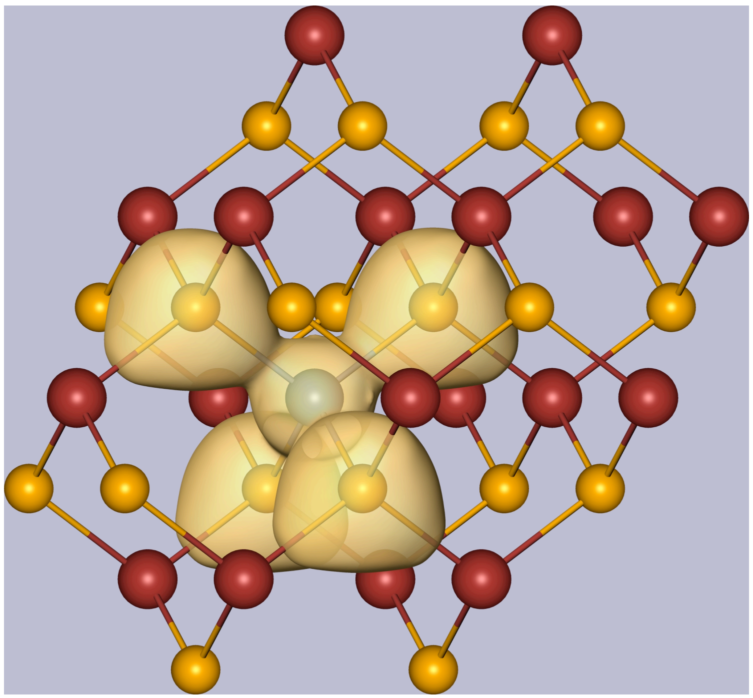
$MnZn_{18}Se_{19}$ quantum dots



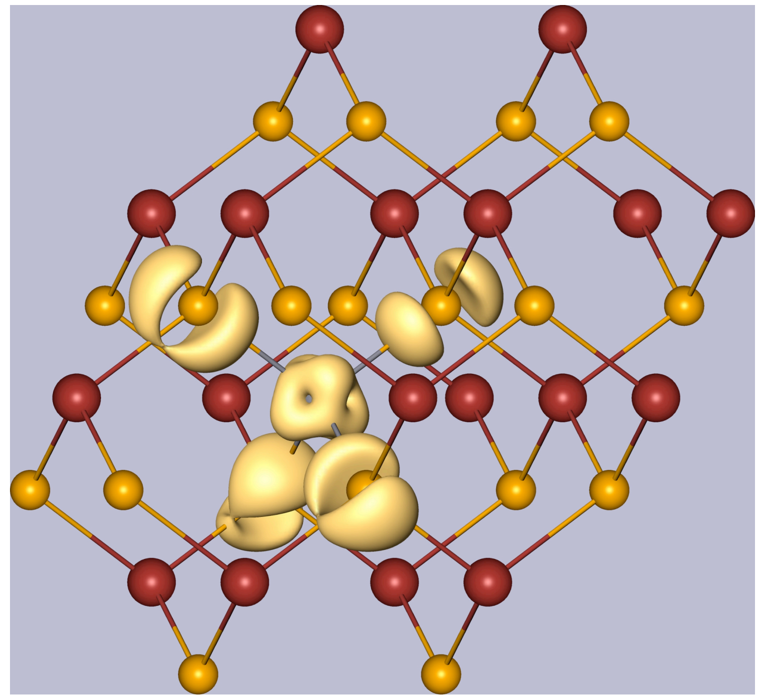


- Mn impurity in the ZnSe quantum dot has a high spin state
- The impurity levels are not sensitive to the impurity position in the cluster

Impurity state in the $MnZn_{18}Se_{19}$ quantum dot



Isosurface of charge density in the vicinity of the Mn atom



Isosurface of summation of wave function square of impurity levels

- Bonding between Mn and Se atoms
- Impurity levels are highly localized around Mn

Goals of this Meeting

- Review and coordinate activities
- Receive input and suggestions from international and industry boards
- Boards meet in executive session tomorrow. 9 a.m., same place.