Toward ORNL/TAMU Collaborative Research (maybe on scientific simulation?)

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Texas A&M is interested in pursuing collaborative research with ORNL.

- I am here to explore potential areas for collaboration.
- One possibility: Large-scale scientific simulations.
  - ⇒ ***A strength of both organizations***
  - ⇒ ***Preliminary explorations in progress***
  - ⇒ ***Can effectively employ Leadership Computing Facility?***
- Another possibility: Materials for extreme environments
  - ⇒ ***I hope to become educated on ORNL interests while I'm here***
- Intriguing possibility: Large-scale materials simulations
  - ⇒ ***combines both of the above***
  - ⇒ ***TAMU has some strengths here***
- I am interested in hearing other possibilities.
- In this presentation I will focus mostly on TAMU capabilities in scientific simulation.

Before we begin: A few words about successful university/lab collaborations.

- I have opinions about what makes such collaborations succeed. These are born from my thoughts and my experiences:
  - ⇒ ***Employee at LLNL 1986-1992***
  - ⇒ ***Collaborator with LLNL and LANL since 1992, and to some extent with SNL since 2000***
  - ⇒ ***Member of many review panels at LLNL, LANL, and SNL***
- What does not work well:
  1. ***University sends proposal***
  2. ***Lab sends money***
  3. ***University writes papers***

- What can work well:
  1. ***Faculty member spends time at lab learning problems.***
  2. ***Lab recognizes need to support graduate research.***
  3. ***Faculty and staff collaborate to guide grad students (usually including grad student time at lab).***
  4. ***Everyone takes long-term view!***

How do we get started?

- Here is a relatively simple plan:
  - ⇒ ***Identify an area of mutual interest for collaboration***
  - ⇒ ***Identify a handful of representative individuals in the area at the lab and at the university***
  - ⇒ ***Lab folks host a workshop attended by university folks:***
    - 1 – 1.5 days of presenting key problems and interests
    - 1 – 1.5 days of informal discussion
    - Includes brainstorming about funding opportunities
    - Concludes with a few proposal topics and investigators tentatively identified
  - ⇒ ***For a few months, proposals are iterated via distance***
  - ⇒ ***Then each collaborative team assembles somewhere to finalize a proposal***
  - ⇒ ***It would also help if the lab could host a faculty member or two for 6-10 weeks during the summer***

- Admittedly, this is a lot of work. I think that's what it takes.

A few more comments about universities and labs. These are all just my opinions!

- Some say universities are more cost-effective than labs. I don't say that! I find that:
  - ⇒ ***Students are inexpensive but slow (in general)***
  - ⇒ ***Lab FTEs are expensive but fast and competent (in general)***
- The main product of universities: students (not research).
  - ⇒ ***Labs need pool of educated, talented, interested people***
  - ⇒ ***To get a student interested in your problems: fund him/her to work on it!!***
  - ⇒ ***To keep a faculty member working in an area of interest: fund his/her students to work in that area!!***
  - ⇒ ***Students and faculty must focus on funded areas!***
- Universities ***are*** good at research. But so are most labs. I think a lab/university team is better than either alone.
- Universities need multi-year projects, consistent with theses and dissertations.
- It takes considerable effort to establish collaborative teams.

Texas A&M University is a well-kept secret. We hope to change that!

- USN&WR: TAMU Engineering in top 10 among public schools.
- Research expenditures: more than $500,000,000/yr (top 10 among public schools and sometimes top 10 among all schools)
- Everything's big in Texas:
  - ⇒ ***TAMU has ≈45,000 students (and may approach ≈50,000 before long)***
  - ⇒ ***We are increasing our T/TT faculty from 1800 to 2250***
  - ⇒ ***Engineering T/TT faculty is growing from 280 to 400***
  - ⇒ ***TAMU System has nine universities, a Health Science Center, and eight state agencies***
  - ⇒ ***TAMU is a land-grant, sea-grant, and space-grant institution***
- Acknowledgements:
  - ⇒ ***UT-Knoxville's football stadium is bigger than A&M's.***
  - ⇒ ***The football champs are from that other Texas school – another orange UT.***

Texas A&M has an institutional commitment to scientific simulation.

- Institute for Scientific Computation (ISC)
  - ⇒ ***In operation since 1992.***
  - ⇒ ***Headed by Dick Ewing (now V.P. for Research).***

- Center for Large-scale Scientific Computing (CLASS)
  - ⇒ ***Expect final approval this week***
  - ⇒ ***Will focus multi-disciplinary teams on largest-scale simulations (Today this means peta-scale.)***
  - ⇒ ***Addresses education needed to be productive on today's large simulation code teams, including coupled-physics considerations***
  - ⇒ ***Grew from successful NE/CS/Math collaborations***

- Deans and VP-Research are committed to multi-disciplinary research. They recognize that large-scale scientific simulation (especially multi-physics) is a multi-disciplinary problem.

In the remainder of the talk I will discuss some specific simulation efforts at TAMU.

- Hope to spark interest in potential collaborators or at least prompt ideas about potential collaborators.

- I lack both time and knowledge to be comprehensive.
  - ⇒ ***Don't want to keep you here for hours.***
  - ⇒ ***Don't know everything that's going on at A&M.***
  - ⇒ ***Woefully ignorant about breadth of ORNL activities. (Help me!)***

- Will discuss a few TAMU efforts:
  - ⇒ ***Computational Chemical/Materials Engineering (Cagin et al.)***
  - ⇒ ***Computational Design and Analysis of Catalysts (Balbuena et al.)***
  - ⇒ ***Standard Template Adaptive Parallel Library: STAPL (Amato, Rauchwerger, Stroustrup, others)***
  - ⇒ ***Parallel Deterministic Particle Transport (Adams, Morel, STAPL team)***

Much activity in computational chemical/materials engineering.

- Tahir Cagin, Chem E, works with many others at TAMU. A goal:

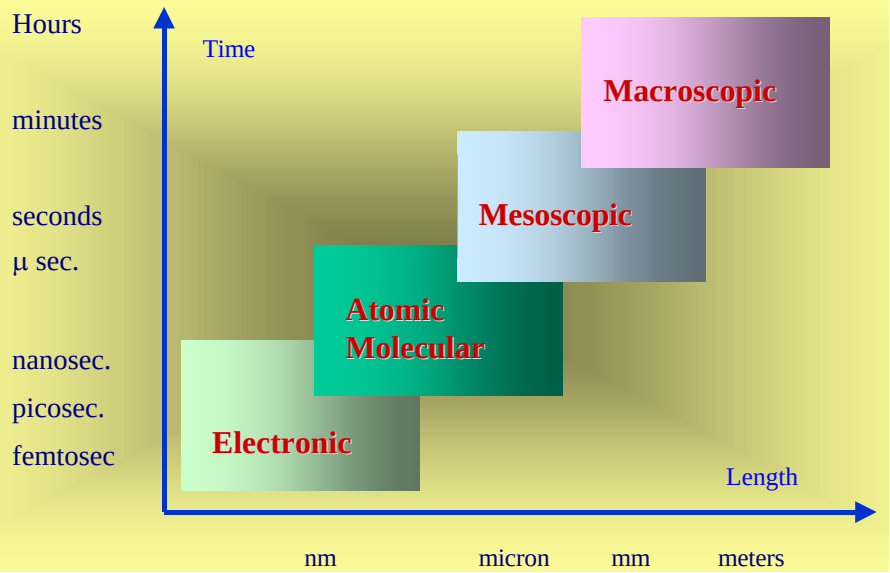
  Develop and apply simulation and modeling techniques to illuminate mechanisms and optimum parameters for processing materials with better performance.

- Multi-scale modeling is a buzzword of the day. In this case:

  ⇒ Electronic Structure Level Modeling
  - *Ab initio* Quantum Chemistry
  - Density Functional Theory
  - Tight Binding Theory

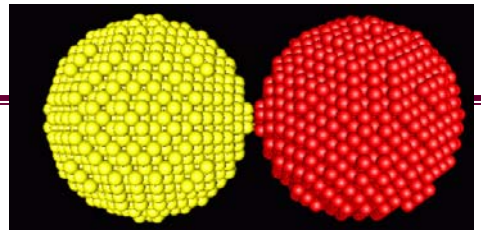
  ⇒ Atomistic Detail Modeling
  - 1st-Principles Force Fields and Molecular Mechanics
  - Monte Carlo
  - Molecular Dynamics

  ⇒ Mesoscopic Level Modeling
  - Kinetic Monte Carlo
  - Langevin Dynamics
  - Dissipative Particle Dynamics
  - Phase Field Theory

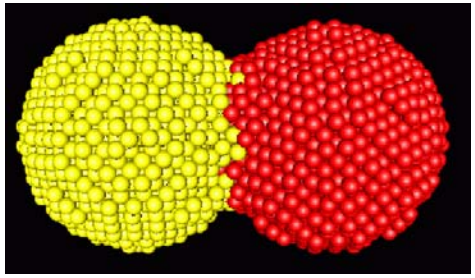


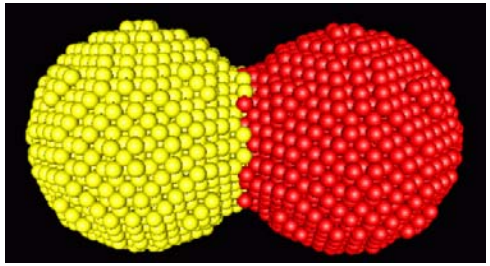
- I borrowed the following slides from a Cagin presentation ...

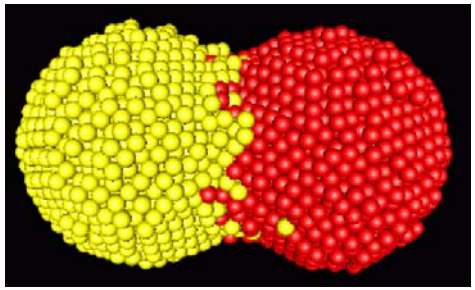
Development and Characterization of Bulk nano-crystalline metals and alloys



With Hartwig, Karaman, Zhang, and Srinivasa - TAMU





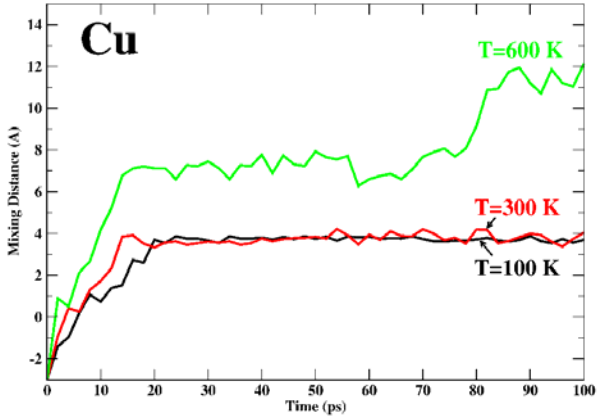


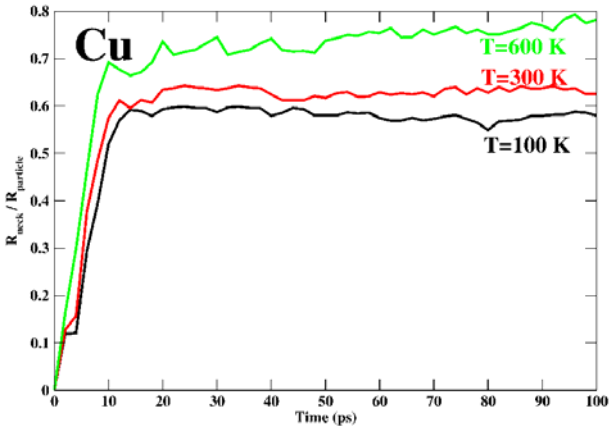
Process Parameters:

1. **Particle size**
2. **Particle shape**
3. **Temperature**
4. **Load**
5. **Size Distribution**
6. **Agglomeration**

Characterization

1. **Mechanical**
2. **Thermal**





Development & Characterization of Epoxy/α-ZrP nanocomposites

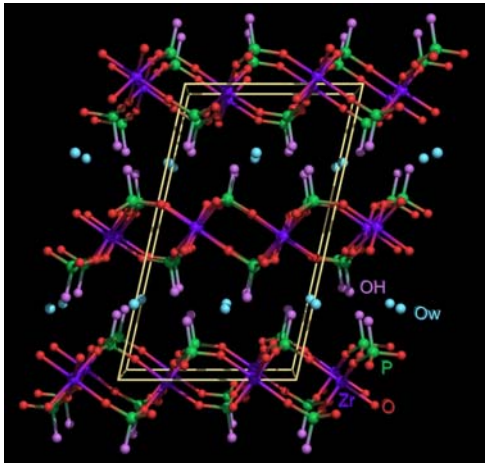
With Sue, Clearfield, and Miller -TAMU

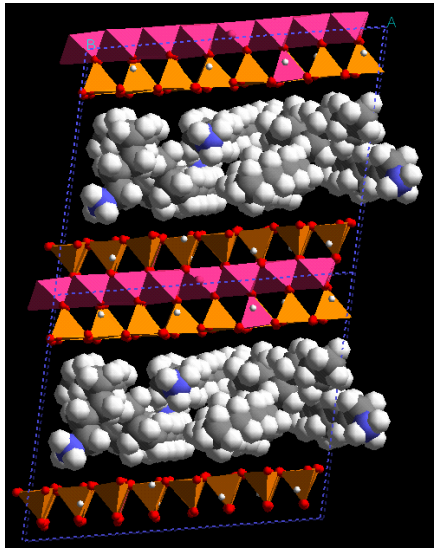
Characterization:

1. **α-ZrP structure and properties**
2. **Characterization of Clays**
3. **Comparison of Exfoliation enthalpies and free energies**
4. **Surface modification**
5. **Functional group search for polymers**

Methods:

1. ***Ab initio* Quantum Chemistry**
2. **Density Functional Theory**
3. **Molecular Dynamics**
4. **Thermodynamic analysis**





Electro- and/or Magneto-Active nano-composites

With Boyd, Ouaneis, Lagoudas, Karaman, (TAMU) and Ramamurthy (UH)

Characterization:

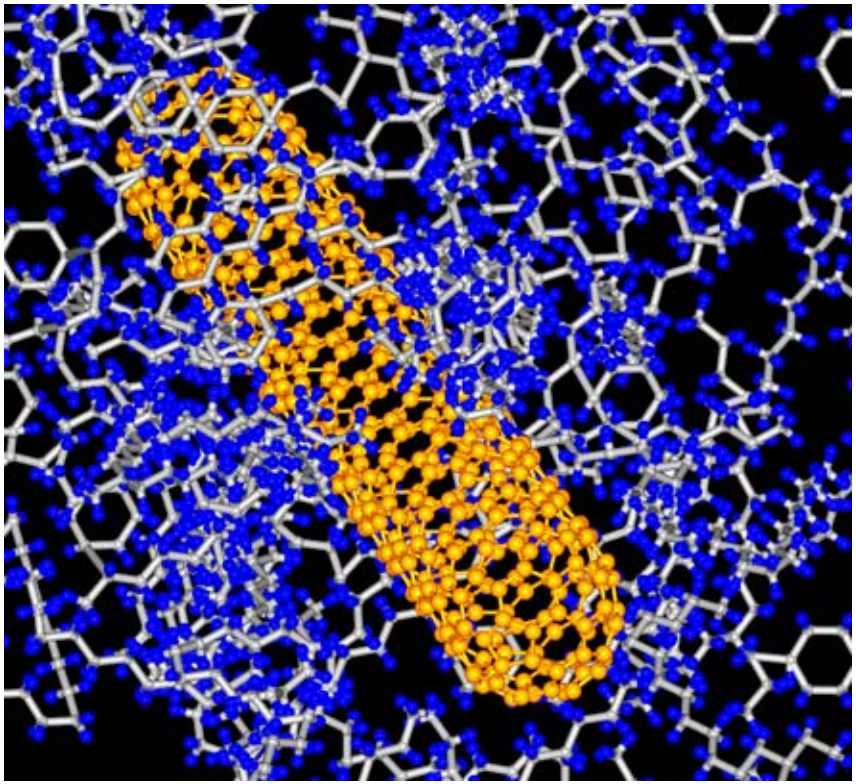
1. **of piezo-, ferro-electrics …**
2. **of High Temperature Shape Memory Alloys (SMA), magnetic SMA s**
3. **of interfacial thermodynamics of inclusions and polymers**
4. **of melt processing of polymers and inclusions**
5. **of ordering and size/shape dependence of ordering**
6. **of behavior under applied mechanical loads, electrical and magnetic fields**

Methods:

1. **Density Functional Theory**
2. **Molecular Dynamics**
3. **Micromechanics, Atomistically informed continuum electrodynamics**
4. **Thermodynamic and micromechanical analysis**

Polyimide-nanotube composites for electro-active materials

- (ß – CN)APB/ODPA Polyimide
- Piezoelectric polyimide
- Exceptional thermal, mechanical, and dielectric properties
- Amorphous in nature
- Potential use in high temperature applications



Predicting Real Optimized Materials - DARPA

With Caltech, USC, JPL, Rutgers, Purdue

Development of materials with targeted merits

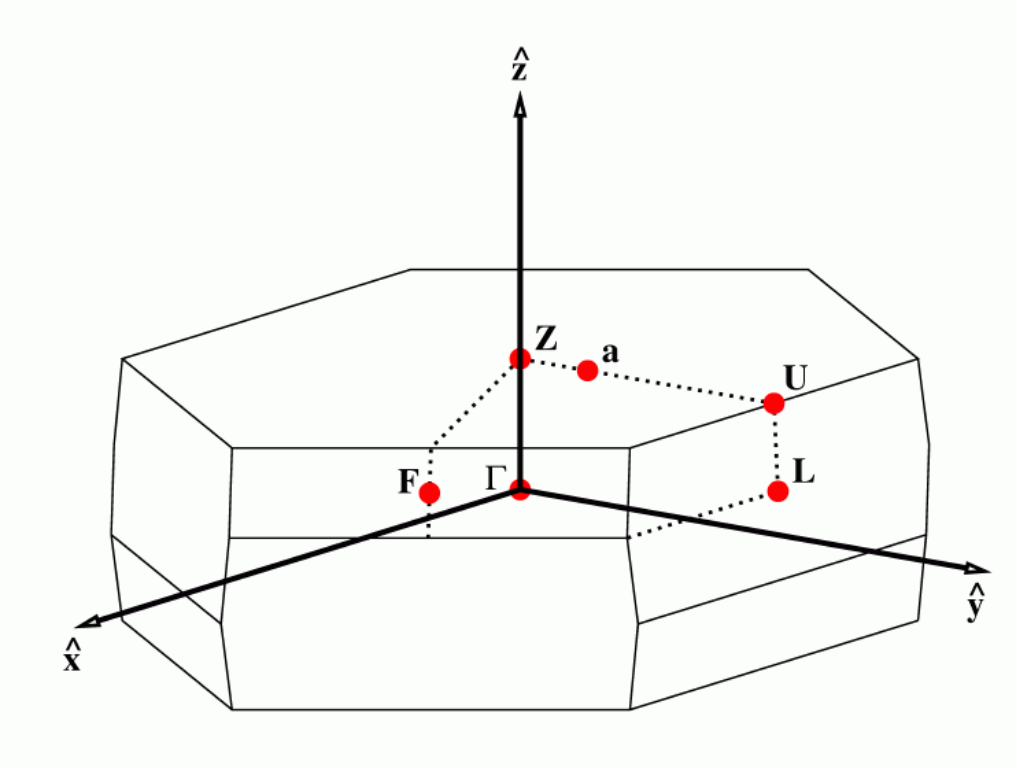
1. **Piezoelectric-Ferroelectric materials with controllable Tunability (fractional variance of capacitance; and Loss tangent (ratio of imaginary and real part of dielectric constant)**
   Material Systems under study are
   $BaTiO_3$, $SrTiO_3$; $Ba_xSr_{(1-x)}TiO_3$, $AgTa_xNb_{(1-x)}O_3$

2. **Thermoelectric materials with ZT ~ 4**
   Controlling the electrical conductivity (increasing) and (decreasing) the thermal conductivity and increasing Seeback Coefficient through varying materials composition and structure, many candidates…

Using Density Functional Theory, Tight Binding Theory, Molecular Dynamics, Non-equilibrium Molecular Dynamics and Solution to Boltzmann Transport Equation for Complex Geometries.

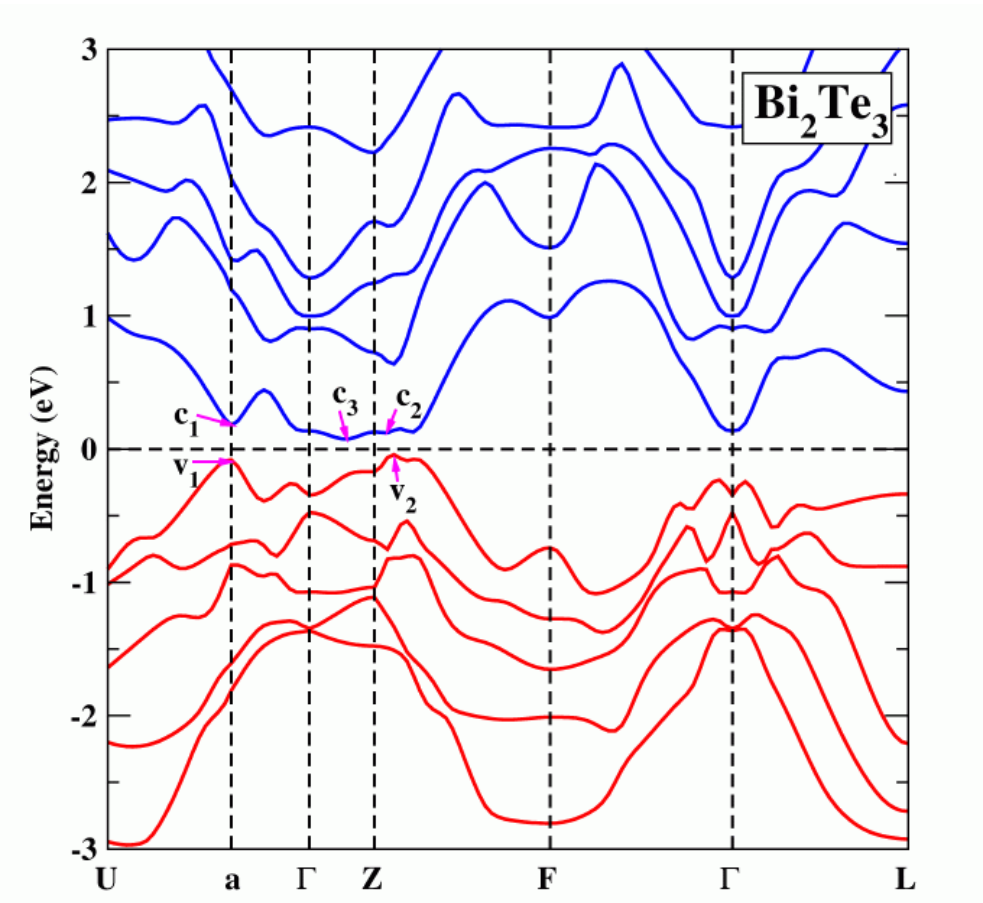
First-Principles Calculations

We performed electronic structure calculations using the self-consistent full-potential linearized augmented plane-wave method (FLAPW) within density functional theory (DFT), using the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof for the exchange and correlation potential. We used 60 k points for the k-space integration and plot the band structure of Bi2Te3 along those high-symmetry lines.



Brillouin zone of Bi_2Te_3 (corresponding to the rhombohedral unit cell). High-symmetry k-points are marked with the red points.

Electronic Band Structure of Bi_2Te_3

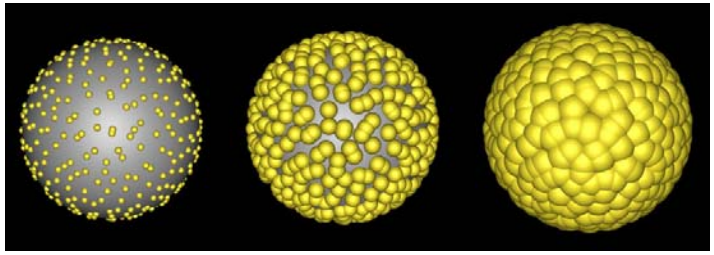


1. We found an indirect band gap of 0.12 eV and a direct band gap of 0.18 eV for bulk Bi2Te3 semiconductor, agreeing excellently with the optical measurements for Bi-doped Bi2Te3 that find an indirect gap of 0.15±0.02 eV and a direct gap of 0.22±0.02 eV.
2. The two maxima (v1 and v2) in the highest valence band have six-fold degeneracy.
3. The two minima (c1 and c2) in the lowest conduction band have six-fold degeneracy.
4. The lowest manimnum (c3) in the lowest conduction band have two-fold degeneracy

Project on Nano Particles and Composites for IR defeat

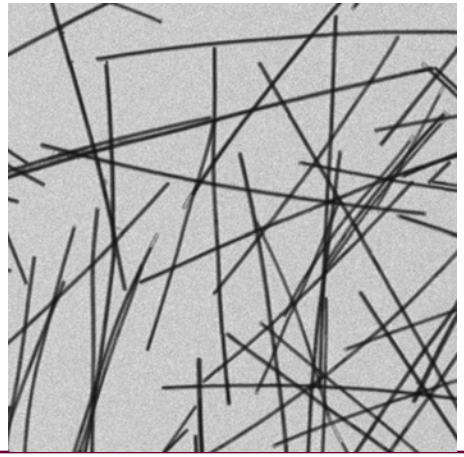
Resonant nanoparticles are predicted to have infrared extinction (scattering and absorption) cross sections that are as much as 100 times larger than conventional materials.

Could lead to tunable optical response – possible light-weight materials with high IR shielding capability, incorporating to paints, fabrics, and plastic coatings.

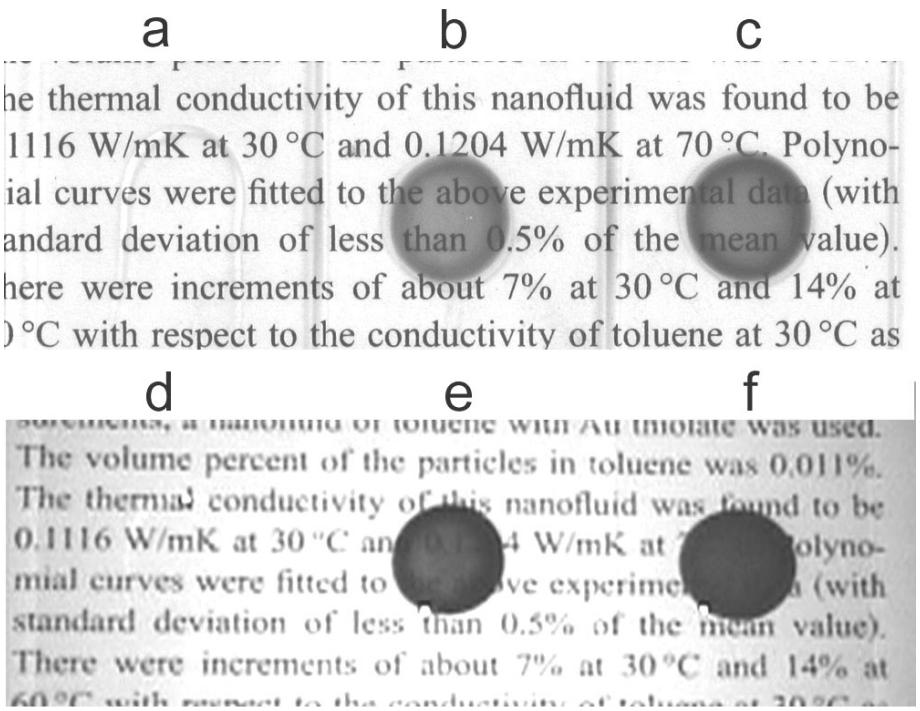


Potential defense, security and consumer applications

Nano-particles, anisotropic metallic nano-rods and nano-platelets



IR Block with Visible Transparency



Visible Image

Near IR Image (820 nm)

PVA **7 nm Shell** **15 nm Shell**

Modeling

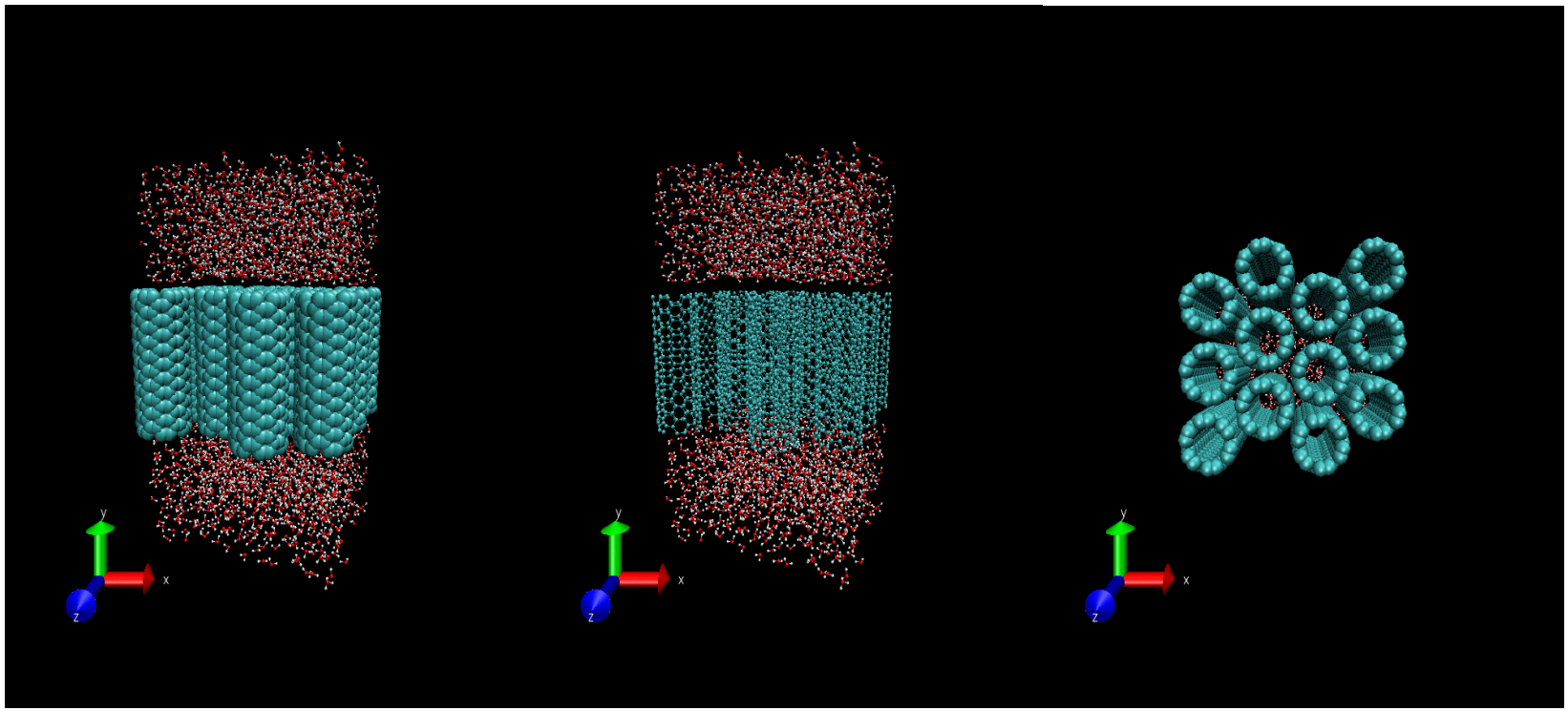
- Metal nano particles, shell structures, thermal, mechanical stability, compatibility with matrix
  - ⇒ ***Processing issues… growth mechanisms***
  - ⇒ ***Fabrication***
  - ⇒ ***Scale up***

- Metal rods and platelets, structure, stability
  - ⇒ ***Surface functionalization for compatibility***

- Optical characterization – calculation of spectra as a function of structure

Behavior of Water in nanotube

- Used classical MD package (NAMD)



- Sandwich model – nanotube membrane separate two layers of water and serves as the transport channel.

Dr. Cagin is interested in collaboration.

- Perhaps someone can connect us with potential ORNL collaborators?

- Dr. Cagin believes that significant new results could be obtained with:
  - ⇒ ***leadership-class computing***
  - ⇒ ***comp-sci help with large data sets***

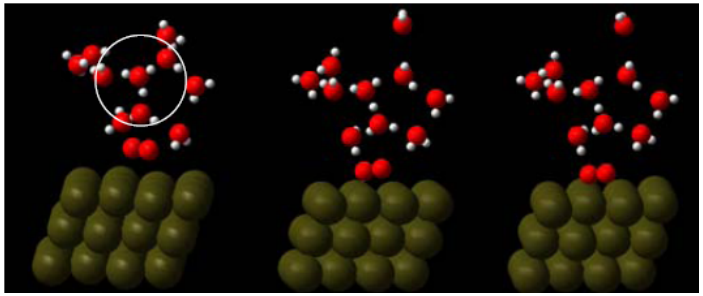
Much activity in simulation of catalysts, leading to improved catalysts for many applications.

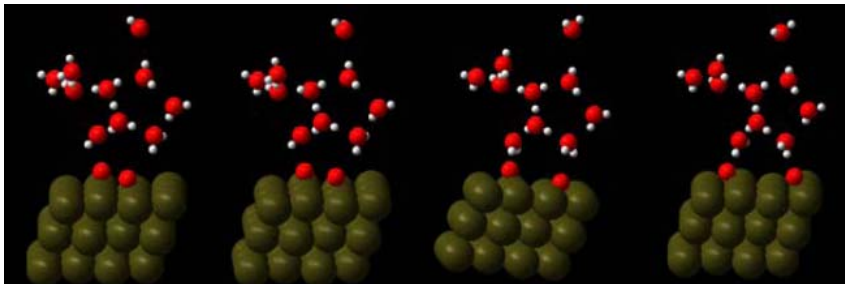
- Perla Balbuena (also in Chem E) and co-workers use “state-of-the-art first-principles” computational chemistry and physics in various applications.

- A few examples follow ...

Catalysis on metal nanoparticles

- Metal nanoparticles provide catalytic sites for O reduction in low-T fuel cells. Important because of slow kinetics and high cost of today's Pt catalysts.
- Our research focuses on :
  - ⇒ ***understanding reduction mechanism on Pt clusters and surfaces using DFT and ab initio molecular dynamics***
  - ⇒ ***determining adsorption of intermediate species such as O, OH, H2O and H2O2 on clusters and surfaces made of Pt and Pt alloys***
  - ⇒ ***DFT analyses of free energies of elementary steps and elaboration of thermodynamics guidelines for design of alternative bimetallic catalysts***
  - ⇒ ***proton transport at the catalyst-membrane interface.***





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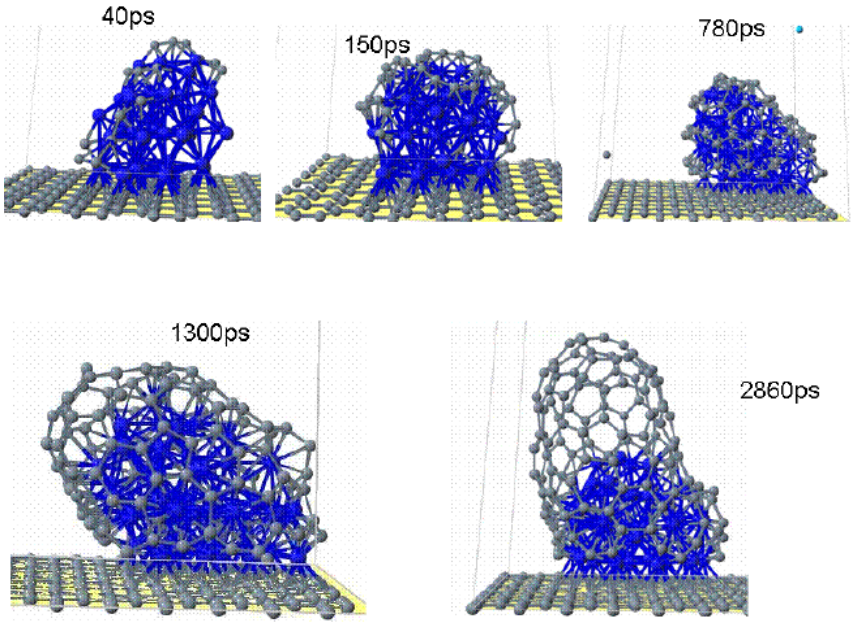
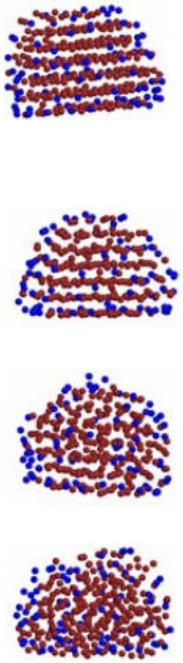
Catalyzed growth of single-wall carbon nanotubes

- Developed reactive force fields to investigate chemical vapor deposition in which a precursor gas (CO) is catalyzed on surface of metal nanoparticles.
- Carbon atoms combine and eventually grow into a SWCNT.
- Classical MD techniques were coordinated with experiments on model catalysts; main findings have been reported in four journal articles.
- Obtained force field parameters for metal-C interactions from DFT simulations of small clusters.
- Initial stages of growth are very sensitive to the strength of the metal-substrate interactions.



Physical properties of metal nanoparticles

- Metal nanoclusters exhibit unusual chemical and physical properties – different from bulk material or of atoms. (Example: they melt at much lower temp.)
- Lots of potential applications, but need to understand properties.
- When nanoclusters are deposited on surfaces, their properties strongly depend not only on their particle size and chemical composition, but also on the structure of the surface and metal/substrate interface.
- Employ MD simulations to study the structure and dynamics of several mono and bimetallic systems, including Cu-Ni and Pt-Au nanoclusters with various compositions and cluster sizes, both in vacuum and deposited on a graphite surface.



There's much more …

- Simulation to understand ion complexation inside macromolecules
  - ⇒ ***precedes formation of embedded metallic nanonclusters, which have many potential applications***
  - ⇒ ***team uses classical MD and DFT to simulate process***
  - ⇒ ***results are motivating experimental tests***
- Polymerization reactions in benign solvents
  - ⇒ ***Used Møller-Plesset perturbation theory and DFT to study decomposition mechanisms of polymerization initiators***
  - ⇒ ***Found that decomposition of initiators with electron-donating R groups follows two pathways:***
    - two-bond mechanism – the O-O single bond and one R-C bond break simultaneously, followed by decomposition of R-C(O)O• radical;
    - one-bond mechanism – the single O-O bond cleavage produces a carboxyl radical pair and a subsequent decomposition of the carboxyl radicals.
  - ⇒ ***Geometrical and energetic analyses indicate that despite the similar structures of the peroxydicarbonates, quite different decomposition energy barriers are determined by the nature of the R groups.***
- Investigating storage of H2 and CH4 in C-containing self-assembled structures
- Working to identify biomaterials that can be emulated for ion carrier and oxygen reduction functions

Dr. Balbeuna is interested in collaboration.

- Perhaps someone can connect us with potential ORNL collaborators?

- Dr. Balbuena is interested in:
  - ⇒ ***Using higher levels of theory to make models more realistic (but more CPU-hungry)***
  - ⇒ ***Going well beyond current resolution (also incurs CPU demands)***
  - ⇒ ***Investigating catalyst dissolution in nanoscale catalysts using DFT:***
    - "hot" problem in catalysts for fuel cells
    - knows how but lacks the computational power

- This would have significant impact on first-principles design and would allow extension of ideas on design of bimetallic catalysts.

- Note: Simulation-based idea in

  Y. Wang and P. B. Balbuena, "Design of Oxygen Reduction Bimetallic Catalysts: Ab initio-Derived Thermodynamic Guidelines," J. Phys. Chem. B., 109, 18902-18906, (2005)

  has been tested at BNL and found to work.

STAPL: Standard Template Adaptive Parallel Library

- STAPL is a superset of STL (Standard Template Library)
  - ⇒ ***STL provides containers, ways to access data in containers, and algorithms that operate on the data, for C++ codes.***
  - ⇒ ***STL is serial only.***
  - ⇒ ***STAPL provides all of these services in parallel, and also more.***
- STAPL is not:
  - ⇒ ***A rigid framework***
  - ⇒ ***A sealed black box***
- STAPL is:
  - ⇒ ***a library***
  - ⇒ ***open-source (eventually) and extendable***
  - ⇒ ***portable and flexible***
  - ⇒ ***committed to working nicely with other parallel code (like solver libraries)***
- STAPL can make it much easier to develop parallel code (especially C++ code) or to parallelize existing C++ code
- Main developers: L. Rauchwerger, N. Amato, B. Stroustrup

STAPL has been exercised as it has been built.

- Parallel discrete-ordinates project
  - ⇒ ***Originally funded as NNSA ASCI Level 2 project***
  - ⇒ ***Funding continued by LANL, LLNL, and SNL***
  - ⇒ ***3D parallel code built using STAPL***
  - ⇒ ***Testimonial: STAPL can save an application coder a lot of time!***
  - ⇒ ***We run mostly on LLNL computers (1024 CPUs is fairly routine)***
  - ⇒ ***Code is becoming a very useful methods testbed***
- Protein-folding project
  - ⇒ ***algorithm inspired by motion-planning for robots!***
  - ⇒ ***also built using STAPL***
- Seismic ray-tracing

Next step: "domain-specific" libraries

- STAPL is a general-purpose library with very basic services.
- Specific application "domains" (such as particle transport) could use more advanced services.
- Idea:
  - ⇒ ***Build advanced library from (basic) STAPL***
  - ⇒ ***For example, a transport-specific library could have:***
    - quadrature objects
    - partitioning algorithms suitable for efficient "sweeps"
    - scheduling algorithms for full or partial sweeps
    - support for nested preconditioned-Krylov solves
    - ray-tracing methods
    - input and output, etc.
- We are now designing such a library. ***I am convinced that this will make it much faster to build new transport codes and test new solution ideas!***

Bottom line: We seek to start a few good TAMU/ORNL collaborations.

- I've talked mostly about high-end computational work, but other areas may be better
  - ⇒ ***bio and/or rad-bio?***
  - ⇒ ***nanotech?***
  - ⇒ ***materials?***

- We are open to suggestions!