

Nanomaterials Theory Institute (NTI)



■ Vision

- To be a leading nanomaterials modeling Center in the world, addressing the most outstanding problems in theoretical and computational nanoscience
- To capitalize on the human resources in national labs, universities and industry to achieve this goal
- To perform frontier research in nanoscience that is strongly integrated with the CNMS experimental programs
- To advance the theory and computational methodologies needed for understanding nanoscale science and exploiting nanotechnology

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■ Scope

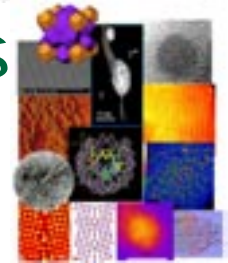
➤ Engage four classes of problems

- ✓ Experiment drives theory agenda
 - Many problems in this class - e.g., neutron scattering
- ✓ Equal partner with experiment
 - E.g., molecular electronics
- ✓ Theory drives experiment
 - E.g., quantum computing
- ✓ New theory paradigm or methods developed to underpin understanding
 - E.g., multiscale methods development

➤ NTI approach to each focus area

- ✓ Build multi-institutional multi-disciplinary team consisting of lab, university and industrial partners
- ✓ Utilize ORNL high-performance computing facilities and expertise (Center for Computational Sciences)

Science-Driven Design and Synthesis

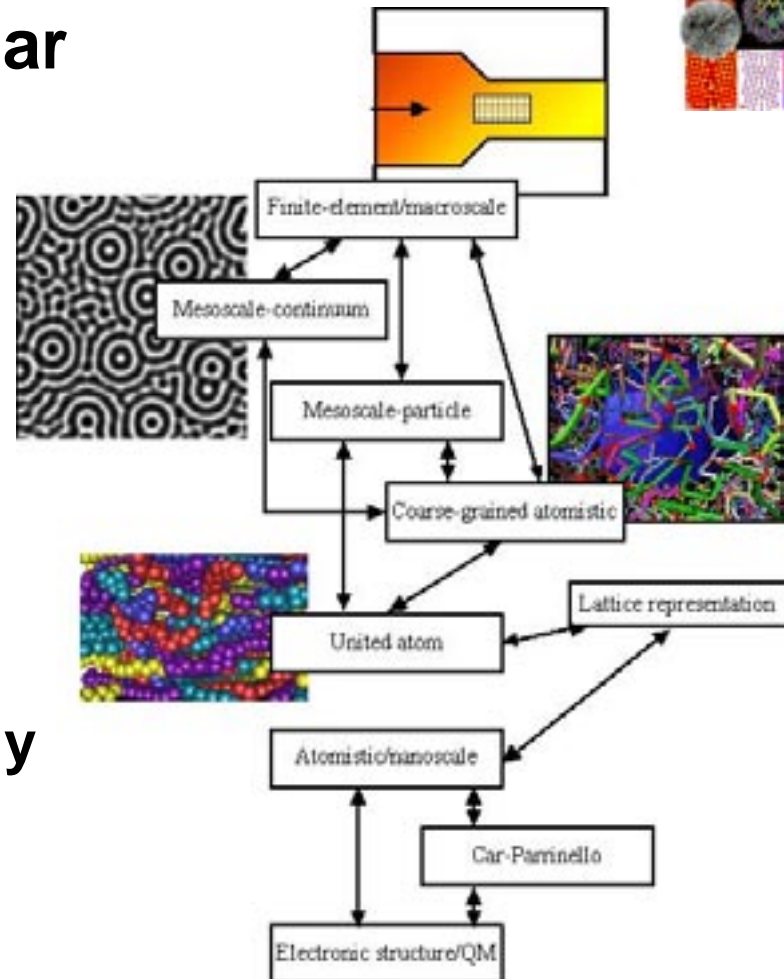


■ Pervasive use of molecular modeling

- Electronic structure calculations
- Atomistic simulation
- Mesoscale methods

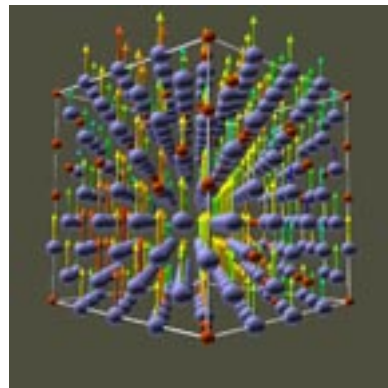
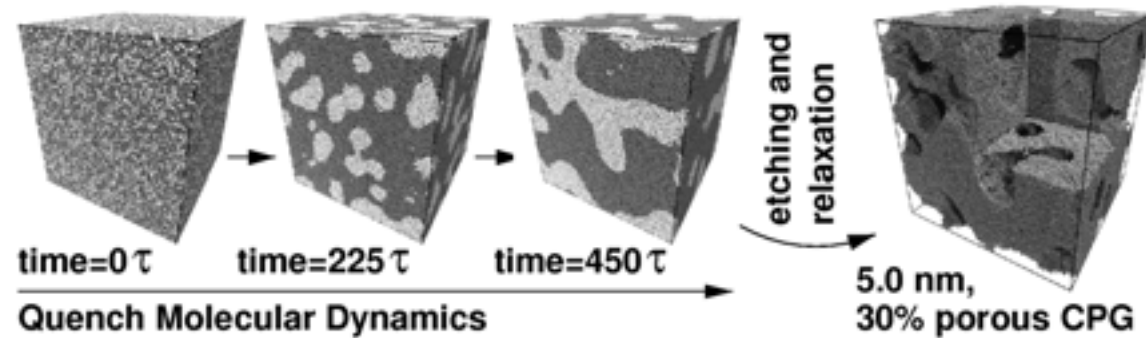
■ Roles

- Identify target materials
- Characterize targets virtually
- Develop and optimize synthesis paths
- Virtual experiments



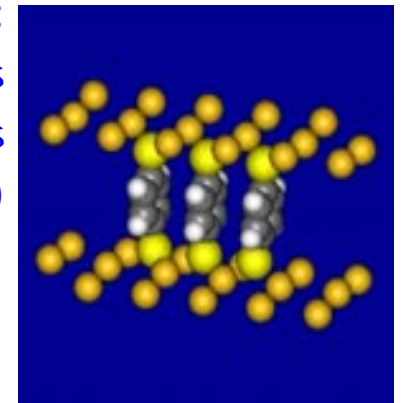
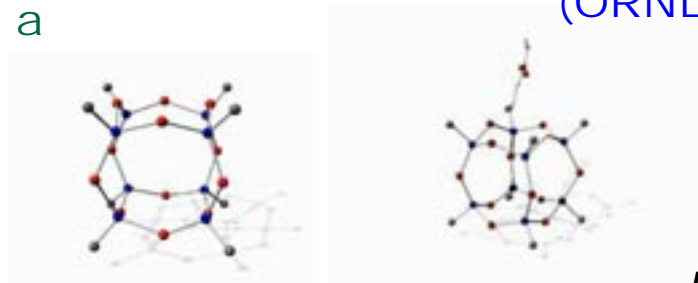
Science-Driven Design and Synthesis

Templated nanoporous materials
(NCSU/ORNL/UTK)

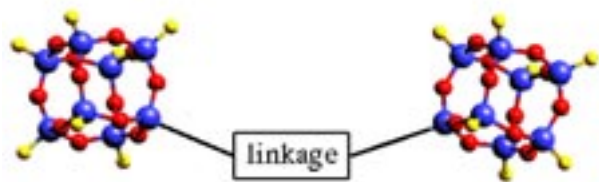


Inhomogeneous distribution of magnetic moment in a CuNi alloy (ORNL)

Molecular electronics: benzene-dithiol molecules attached to gold atoms (ORNL/UTK)



Images at left courtesy of Hybrid Plastics



Polymer nanocomposites with cross-linked polymer-functionalized polyhedral oligomeric silsesquioxanes molecules (NSF NIRT UTK/Mich/UVA)