

## Materials Modeling

Materials Modeling uses advanced computer modeling and simulations to predict the behavior and improve the design and performance of new and existing man made and biological materials. UNT researchers conduct fully integrated, multi-scale research using cutting-edge technology and collaborative expertise in chemistry, mechanical and energy engineering, materials science and engineering, physics, and biology. Computational approaches yield accurate, rapid predictions for materials and processes that are often too difficult to address in a traditional laboratory setting. Materials can be studied under extreme conditions of temperature and stress to assess durability and performance. Analyzing materials in both the virtual and physical domains and from the vantage of multiple disciplines gives a thorough, understanding of material integrity that distinguishes this program from others in the nation and puts UNT at the forefront of materials research to expedite solutions in medicine, energy, the environment, and industrial technologies.

- **New university research facility features high performance computing clusters unique to the region, with high-speed networks and advanced software**
- **Close interactions between modelers and experimentalists yield novel approaches and solutions supported by fully integrated, in-house, multi-scale modeling research facilities with instruments for true 3-D characterization of materials and devices down to atomic length scales**
- **Facilities are supported by the U.S. Department of Education, the U.S. Department of Energy, the Air Force Research Laboratory, and other sponsors**
- **Affiliated national centers include a National Science Foundation Chemical Bonding Center and a Department of Energy, Energy Frontier Research Center**

### Representative Faculty

**Paul Bagus**, Research Professor of Chemistry: *spectroscopic properties and the modeling of nanomaterials; and origin of surface and interface materials properties and processes*

**Thomas Cundari**, Co-Director of the Center for Advanced Scientific Computing and Modeling; and Regents Professor of Chemistry: *high-accuracy methods for modeling transition metals; metal-based catalysts, sensors, optics and materials; and multiple bonding of metals*

**Qunfeng Dong**, Assistant Professor of Biological Sciences and Computer Science: *bioinformatics*

**Jincheng Du**, Assistant Professor of Materials Science and Engineering: *atomistic simulations to understand the structure of complex materials and systems*

**Alan Needleman**, Professor of Materials Science and Engineering: *continuum mechanics and the computational modeling of deformation and fracture processes in structural materials, including metals*

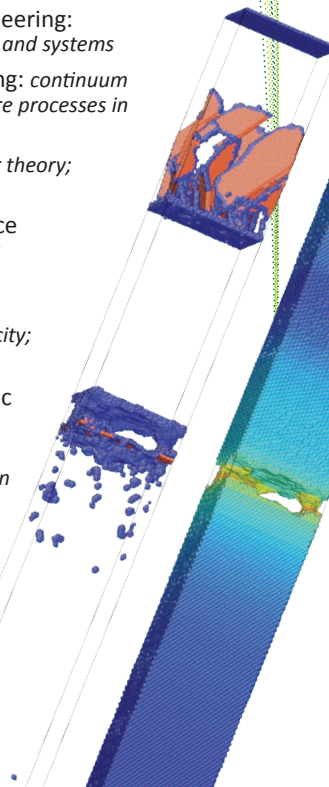
**Yuri Rostovtsev**, Assistant Professor of Physics: *condensed matter theory; and quantum coherence and interference*

**Srinivasan Srivilliputhur**, Assistant Professor of Materials Science and Engineering: *large scale molecular dynamics; atomistic modeling of deformation behavior and defect physics; and metals and alloys*

**Zhiqiang Wang**, Assistant Professor of Materials Science and Engineering: *molecular dynamics; dislocation dynamics; crystal plasticity; mesoscale modeling; and mesoscopic microstructure evolution*

**Angela Wilson**, Co-Director of the Center for Advanced Scientific Computing and Modeling; and Regents Professor of Chemistry: *development and understanding of computational chemistry methodology and its applications, including materials science, transition metal chemistry, and environmental chemistry*

**Zhenhai Xia**, Associate Professor of Materials Science and Engineering: *mechanical properties and behaviors of metallic and ceramic composites; thin film forms; peripheral nerves; and materials mimicking biological materials*



## Select Research Resources

### **TALON: High-Performance Computing System**

[citc.unt.edu/hpc/content/talon](http://citc.unt.edu/hpc/content/talon)

Unique to the region, the TALON supercomputer features high performance computing clusters supported by high-speed networks, high performance storage, and advanced software. Availability of the Talon HPC system greatly increases the computation resources available to UNT researchers.

### **RAVE: Research and Visualization Environment**

[citc.unt.edu/rave](http://citc.unt.edu/rave)

The RAVE offers excellent computer resources to help scholars visually analyze large amounts of complex data for graphically intensive research, simulations, statistics, and design. The state-of-the-art space features high-powered workstations, visualization software, and a large-scale, video display wall for analysis with superior graphical output to enhance and explain research.

### **ISES: Institute for Science and Engineering Simulation**

[research.unt.edu/ises](http://research.unt.edu/ises)

At the forefront of jet engine research and experimentation, ISES uses advanced characterization, simulation and modeling of aerospace components and materials to maintain and extend the life of aging U.S. Air Force aircraft, prevent catastrophic engine failure, and aid the Air Force in developing better materials for the next generation of aircraft.

### **CASCaM: Center for Advanced Scientific Computing and Modeling**

[cascam.unt.edu](http://cascam.unt.edu)

The CASCaM facility, supported by the United States Department of Energy, and the United States Air Force Research Laboratory, provides research, education, training and outreach in all facets of advanced scientific computing and modeling and provides excellent opportunities for collaboration with UNT's world-class research group in computational chemistry.

### **Computational Materials Modeling Group**

[www.mtse.unt.edu/CMM](http://www.mtse.unt.edu/CMM)

This consortium of top-level materials science engineers use modeling to study diverse properties of a wide range of materials such as metals, ceramics, and ordered and disordered alloys; research experiments provide the basis for novel materials design and include performance assessments of aerospace materials, catalysis and alternate energy generation, the behavior of nanostructured materials, and interaction of radiation with materials.

### **CART: Center for Advanced Research and Technology**

[research.unt.edu/cart](http://research.unt.edu/cart)

CART is one of the most advanced university research facilities in the nation for materials synthesis and analysis, from atomic to macro scales. The facility offers a suite of sophisticated instruments used for true 3-D characterization and processing with an adjoining clean room so that materials can be synthesized, tested and controlled in close proximity, creating a powerful combination of capabilities in one location. UNT is among an elite group of public institutions nationwide to offer these open access resources.

### **Contributing Research Clusters:**

#### **Materials Modeling**

[mmrc.unt.edu](http://mmrc.unt.edu)

#### **Multi-scale Surface Science and Engineering**

[surfaces.unt.edu](http://surfaces.unt.edu)