Computational Chemistry

Computational chemistry makes use of results generated from computer algorithms to help scientists model and predict the behavior of chemicals in experiments that might otherwise be impossible, too dangerous, or too expensive to perform in a laboratory environment. UNT offers one of the largest and well recognized computational chemistry research programs in the world, with specific expertise in the electronic structure domain. Drawing talent from both the modeling and experimental communities, its unique, interdisciplinary focus generates innovative applications in chemistry, biology, engineering and materials science. Diverse areas of research — from the atomic to the continuum scale — include organic and materials chemistry, inorganic/ organometallics, biological chemistry, physical chemistry, multi-scale and mesoscale modeling, computational fluid dynamics, and surface and cluster modeling. Methodologies span molecular mechanics and semiempirical quantum mechanics, *ab initio* and density functional theory, bioinformatics, artificial intelligence, and molecular dynamics.

- **One of the largest and well respected programs of its kind in the world**
- **Unique, interdisciplinary focus integrates chemistry with cutting-edge theory and simulation, and experiment and characterization**
- **High performance computing clusters and a wide selection of visualization software advance all aspects of computational research**
- **Funded research projects include catalysis, photonics, flexible electronics, combustion chemistry and materials fatigue**
- **Innovative research collaborations with engineers and scientists from other disciplines to advance modeling across length and time scales**

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*

Wes Borden, Welch Chair; and Distinguished Research Professor of Chemistry: *electronic structure calculations and the reactions of organic and organometallic compounds*

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*

Paul Marshall, Regents Professor of Chemistry: *bond formation and chemical kinetics using laser spectroscopy and* ab initio *computational chemistry, with interests in atmospheric and combustion chemistry, short-lived radicals, and transient species*

Jan Martin, Distinguished Research Professor of Chemistry: *computational thermochemistry and spectroscopy; the design of more universally applicable density functional methods; and applications in catalysis and renewable energy*

Martin Schwartz, Professor of Chemistry: *molecular dynamics simulations of polymer composites; and quantum mechanical modeling of bonding and thermochemistry*

Srinivasan Srivilliputhur, Assistant Professor of Materials Science and Engineering: *large scale molecular dynamics; atomistic modeling of deformation behavior and defect physics; structure property-relations in metals and alloys; and parallel computing and visualization*

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*
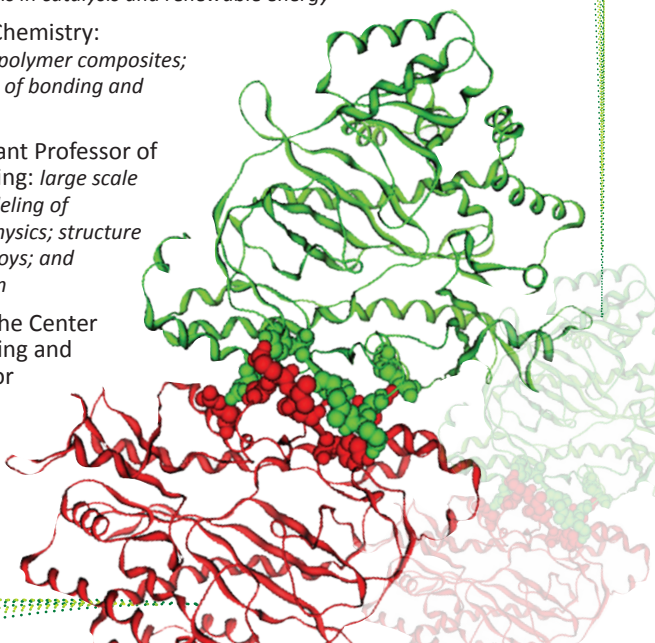
Select Research Resources

CASCaM: Center for Advanced Scientific Computing and Modeling
cascam.unt.edu

This UNT-based facility is a vital hub for research, education, training and outreach in all facets of advanced scientific computing and modeling. CASCaM provides excellent opportunities for mentorship and collaboration with UNT computational chemists, researchers and external partners working in multiple areas of science and engineering, with project support from the National Science Foundation, the United States Department of Energy, and the Air Force Research Laboratory.

Computational Chemistry Laboratory

This research and teaching lab offers advanced computing technology and extensive hardware, with a wide selection of visualization software resources designed to express and analyze diverse computational problems, including Spartan, GaussView, AbInit, Crystal, Gamess, Guassian, Molcas, Molpro and NWChem.

RAVE: Research and Visualization Environment
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.

TALON: High-Performance Computing System
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 has greatly increased the computation resources available to UNT researchers.

ISES: Institute for Science and Engineering Simulation
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 with critical experimentation to maintain and extend the life of aging U.S. Air Force aircraft, prevent catastrophic engine failure, and develop better materials for next generation aircraft. Researchers from chemistry and materials science/engineering share expertise and findings with a team of international collaborators representing universities, industries, and government.

Contributing Research Clusters:

Computational Chemical Biology
c3b.unt.edu

Materials Modeling
mmrc.unt.edu