The University of North Texas is now the home of the Center for Advanced Scientific Computing and Modeling (CASCaM), whose central mission involves research, education, training and outreach in all facets of advanced scientific computing and modeling. The CASCaM facility, supported by the United States Department of Education, affords excellent opportunities for collaboration with UNT computational chemists for students and faculty mentors in Texas and the surrounding states.

There are currently seven faculty involved in CASCaM research pursuing projects ranging from the development of novel modeling techniques to applications in areas such as biology, catalysis, atmospheric chemistry and materials chemistry.

For more information about graduate studies in Chemistry at UNT please contact any of the faculty at the email addresses given below.

Online applications and information can also be found at: http://www.chem.unt.edu

CASCaM at a Glance

- Professor Wes Borden, a leading organic computational chemist and Associate Editor of the Journal of American Chemical Society, joined UNT in 2004 as Welch Professor of Chemistry, and was awarded the ACS' Cope Scholar Award this past year.
- Professors Angela Wilson and Mohammad Omary received CAREER Awards, given by the NSF to the top junior faculty in the U.S.
- Grant support for CASCaM faculty over the past several years is over $2,000,000.
- UNT Chemistry has just taken delivery of its own parallel computational chemistry facility through a grant from the NSF. Additionally, resources dedicated to computational research sit at ~ 500 processors and multiple Terabytes of storage, and are growing almost daily.
- The UNT computational chemistry groups moved into a new, state of the art chemistry-only building in 2004, which include roughly 3,000 sq. ft. for the housing of computer servers and clusters, over four rooms.
- Computational faculty have published >200 refereed scientific publications in the past 5 years.
- Computational faculty have sponsored more than 40 research students in the past 7 years.
- Graduates of our computational chemistry faculty have won competitive fellowships from government and academic institutions. Additionally, our students have won national and regional competitive awards.
- Former students have gone on to positions at places such as PPG, Los Alamos National Laboratory, and Pacific Northwest National Laboratory.

Founded in 1900 The University of North Texas is the largest and most comprehensive of all institutions in the North Texas region and is now related as a Carnegie 2000 Doctoral Research University-Extensive. The University of North Texas offers equal education opportunity to all persons without regard to race, creed, color, national origin or disability.

Martin Schwartz, Regent Professor
- Conducting polymers
- Transition metal bonding
- Hypervalent metal complexes

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- Homoaromaticity

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CASCaM Expertise

- Applications Areas of Chemistry  
  - Inorganic/organometallic chemistry  
  - Organics  
  - Solids & surfaces  
  - Biological chemistry  
  - Physical chemistry

- Methodology  
  - Molecular Mechanics  
  - Semiempirical Quantum Mechanics  
  - Ab initio & Density Functional Theory  
  - Bioinformatics  
  - Artificial Intelligence  
  - Molecular Dynamics