

CASCaM
University of North Texas
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The University of North Texas is the home of the Center for Advanced Scientific Computing and Modeling (CASCaM, <http://cascam.unt.edu/>), a center of excellence whose mission involves research, education, training, and outreach in all facets of advanced scientific computing and modeling.

There are currently 13 faculty involved in CASCaM pursuing research projects that range from development of novel modeling techniques to applications in biology, chemistry, engineering, and material science. The CASCaM center, initiated with support from the U.S. Department of Education, affords excellent opportunities for interdisciplinary graduate studies in computational research. Faculty expertise covers a spectrum of modern materials modeling found few other places: from theory to applications to code development; from the atomic to continuum scale; applications ranging from gas-phase chemistry of atoms to life-cycle prediction for aerospace structures.

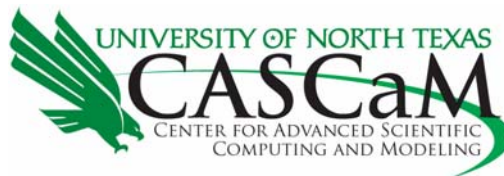
For more information about graduate studies at UNT please contact any of the faculty at the email addresses given below.

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.

CASCaM at a Glance

- CASCaM is distinguished from similar groups in that it is a student-centered research effort.
- Professor Wes Borden, a leading organic computational chemist and Associate Editor of the *Journal of American Chemical Society*, is Welch Professor of Chemistry.
- Professor Angela Wilson received the CAREER award, given by the NSF to top junior faculty.
- Grant support for CASCaM faculty over the past several years is over \$10,000,000.
- Resources dedicated to computational chemistry are ~2000 cores, numerous Tb of storage, and roughly 5 Tflops of computing power.
- The UNT computational chemistry groups occupy a new, state of the art chemistry building, which include roughly 3,000 sq. ft. for the housing of computer servers and clusters.
- CASCaM faculty have published >200 refereed scientific publications in the past 5 years.
- CASCaM faculty have sponsored more than 50 research students in the past 7 years.
- CASCaM has a dedicated facilities manager, Dr. David Hrovat, with over 20 years experience in system maintenance and computational chemistry research.
- 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 of CASCaM faculty have gone on to positions at places such as PPG, Los Alamos National Laboratory, and Pacific Northwest National Laboratory.



CASCaM Faculty

Paul Bagus, Research Professor

Ph.D. 1965, University of Chicago
Editorial Board, Journal of Electron Spectroscopy

- Surface and cluster chemistry
- X-Ray photoelectron spectroscopy

<http://chem.unt.edu/people/Bagus.htm>

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- Mintz, B.; Wilson, A. K.; Bagus, P. S. Basis set requirements for interactions in ionic systems: LiCl. *Chem. Phys. Letters*. **2009**, 468, 286-289.

Sandra Boetcher, Assistant Professor

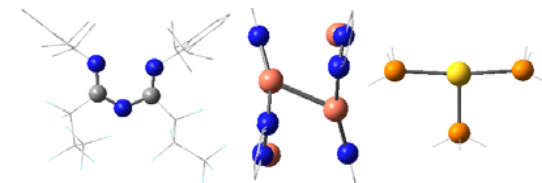
Ph.D. 2006, University of Minnesota

- Computational Fluid Dynamics
- Biomedical Modeling

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- Boetcher, S. K. S.; Sparrow, E. M.; Dugay, M. V. Characteristics of direct-contact, skin-surface temperature sensors, *International Journal of Heat and Mass Transfer*; **2009**, 52, 3799-3804.



Wes Borden, Welch Professor

Ph.D. 1968, Harvard University
Associate Editor, J. Am. Chem. Soc.

- Organic and organometallic chemistry
- Radicals and diradicals

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- Zhou, X.; Hrovat, D. A.; Borden, W. T. Annulated derivatives of cyclooctatene in which $\sigma \rightarrow \pi^*$ electron transfer is energetically favorable. *238th ACS National Meeting*, **2009**, COMP-211.

Thomas Cundari, Regents Professor

Ph.D. 1990, University of Florida

Co-Editor, Reviews in Computational Chemistry

- Computer-aided catalyst design
- Materials chemistry

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- Cundari, T. R.; Morello, G. R. A Computational Study of Metal-Mediated Decomposition of Nitrene Transfer Reagents. *Journal of Organic Chemistry*, **2009**, *74*, 15 5711-5714

Jincheng Du, Assistant Professor

Ph.D. 2004, Alfred University

- Heterogeneous catalysis
- Ceramics

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- Du, J.; Benmore, C. J.; Corrales, L. R.; Hart, R. T.; Weber, J. K. R. A molecular dynamics simulation interpretation of neutron and X-ray diffraction measurements on single phase Y2O3-Al2O3 glasses. *Journal of Physics: Condensed Matter*, **2007**, *21*, 20, 205102/1-205102/9.

Zhi-Gang Feng, Assistant Professor

Ph.D. 1997, Tulane University

- Computational fluid dynamics
- Particulate flow

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- Feng, Z-G.; Michaelides, E. E. Inclusion of Heat Transfer Computations for Particle Laden Flows. *Physics of Fluids* **2008**, *20*, 040604/1-10.

Paul Marshall, Regents Professor

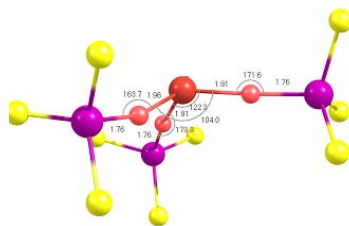
Ph.D. 1985, Cambridge University

- Gas-phase kinetics
- Atmospheric and combustion chemistry

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- Gao, Y.; DeYonker, N. J.; Garret, E.; Chauncey, III.; Wilson, A. K.; Cundari, T. R.; Marshall, P. Enthalpy of Formation of the Cyclohexadienyl Radical and the C-H Bond Enthalpy of 1,4-Cyclohexadiene: An Experimental and Computational Re-Evaluation. *Journal of Phys. Chem. A*, **2009**, *25*, 6955-6963



Alan Needleman, Visiting Professor

Ph.D. 1971, Harvard University

- Deformation/fracture in structural materials
- Continuum modeling of metals

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- Diercks, D.; Kaufman, M.; Needleman, A. Convergent beam electron diffraction measurements of relaxation in strained silicon using higher order Laue zone line splitting. *J. Applied Phys.* **2009**, *6*, 063526/1-063526/4.

Yuri Rostovtsev, Assistant Professor

Ph.D. Institute of Applied Physics, Russia

- Quantum and Nonlinear Optics
- Quantum Nucleonics

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- Sautenkov, V.A.; Li, H.; Welch, G.R.; Davis, J. P.; Narducci, F. A.; Scully, M. O. Using phase dynamics in EIT to probe ground state relaxation in rubidium vapor. *Journal of Modern Optics*. **2009**

Martin Schwartz, Regents Professor

Ph.D. 1972, The University of Wisconsin

- Conducting polymers
- Transition metal bonding

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- Schwartz, M.; Berry, R. J.; Dudis, D. S.; Yeates, A. T. Effects of Substituents on the Electronic Properties of Polyacetylenes. *THEOCHEM* **2008**, *859*, 37-45.

Srinivasan Srivilliputhur, Assistant Professor

Ph.D. 1998, University of Washington

- Corrosion and oxidation
- Nuclear materials and processes

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- Watanbe, T.; Srivilliputhur, S. G.; Schelling, P. K.; Tulenko, J. S.; Sinott, S. B.; Phillpot, S. R. Thermal transport in off-stoichiometric uranium dioxide by atomic level simulation. *J. American Ceramic Society* **2009**, *92*, 4, 850-856.

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- Material Deformation
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- Wang, Z. Q.; Beyerlein, I.J.; LeSar, R. Plastic anisotropy in fcc single crystals in high rate deformation. *International Journal of Plasticity*, **2009**, *25*, 26-28

Angela Wilson, Associate Professor

Ph.D. 1995, University of Minnesota

NSF CAREER Awardee

- Basis set development
- Atmospheric chemistry

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- Prascher, B. P.; Lucente-Schultz, R. M.; Wilson, A.K. A CCSD(T) and ccCA study of mixed silicon hydrides and halides: Structures and thermochemistry. *Chemical Phys.* **2009**, *359*, 1-3, 1-13.

Current Research Sponsors

