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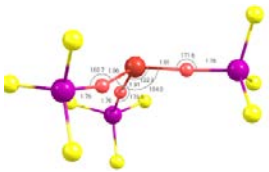
The University of North Texas is the home of the Center for Advanced Scientific Computing and Modeling (CASCaM, http://cascam.unt.edu/), a center of excellence whose mission involves research, education, training, and outreach in all facets of advanced scientific computing and modeling.

There are currently 16 faculty involved in CASCaM pursuing research projects that range from development of novel modeling techniques to applications in biology, chemistry, engineering, material science and physics. 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 mentioned within.



Founded in 1890, The University of North Texas is the largest and most comprehensive of all institutions in the North Texas region and is rated as a Carnegie 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.
- Professors Wilson and Srivilliputhur have received the CAREER award, given by the NSF to top junior faculty.
- Grant support for CASCaM faculty over the past several years is over $24,000,000.
- Resources dedicated to computational research are approximately 4,000 cores.
- The UNT computational chemistry groups occupy a 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 more than 200 refereed scientific publications in the past 7 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 of 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, Lockheed-Martin, and Pacific Northwest National Laboratory.

UNIVERSITY OF NORTH TEXAS
CASCaM
CENTER FOR ADVANCED SCIENTIFIC COMPUTING AND MODELING

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- Pandey, R. S.; Sayres, M. A. W.; Azad, R. K., Detecting evolutionary strata on the human X chromosome in the absence of gametologous Y-linked sequences. *Genome Biol. Evol.* **2013,** *5*, 1863-1871.

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- Nelin, C. J.; Bagus, P. S.; Ilton, E. S., Theoretical analysis of the U L_3-edge NEXAFS in U oxides. *RCS Advances* **2014,** *4*, 7148-7153.

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- Chen, B.; Hrovat, D. A.; West, R.; Deng, S. H. M.; Wang, X.-B.; Borden, W. T., The Negative Ion Photoelectron Spectrum of Cyclopropane-1,2,3-Trione Radical Anion, (CO)3•- - A Joint Experimental and Computational Study. *J. Am. Chem. Soc.* **2014**, *136*, 12345-12354.

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- Dong, R.; Calzolari, A.; di Felice, R.; El-Shafei, A.; Hussain, M.; Buongiorno Nardelli, M., Optical enhancement in heteroleptic Ru(II) polypyridyl complexes using electron-donor ancillary ligands. *J. Phys. Chem. C* **2014**, *118*, 8747-8755.

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- Jones, A. M.; Xuan, Y.; Xu, M.; Wang, R.-S.; Ho, C.-H.; Lalonde, S; et al., Border control: a membrane-linked interactome of Arabidopsis. *Science* **2014,** *344* (6185), 711-716.

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- Huang, S.-H.; Nesterov, V. N.; Richmond, M. G., New azido-substituted tantalum compounds: syntheses and DFT examination of nitrogen-rich mono-, di-, and trinuclear tantalum(v) compounds. *Dalton T.* **2014,** *43*, 3453-3461.

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- Sariyanni, Z.-E.; Sun, D.; Rostovtsev, Y. V., Stimulated Raman spectroscopy with 0π pulses. *Optical Society of America* **2014**, *39*, 766-768.

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- Srinivas, G. N.; Schwartz, M., μ- and μ_4–η^2 coordination of A_2H_2 (A = C, Si, Ge, Sn and Pb) ligands with transition metals. *Inorg. Chim. Acta* **2009,** *362*, 2172-2176.

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- Karewar, S. V.; Gupta, N.; Caro, A.; Srinivasan, S. G., A concentration dependent embedded atom method potential for the Mg-Li system. *Comput. Mater. Sci.* **2014**, *85*, 172-178.

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- Zhang, L.; Niu, J.; Li, M.; Xia, Z., Catalytic Mechanisms of Sulfur-Doped Graphene as Efficient Oxygen Reduction Reaction Catalysts for Fuel Cells. *J. Phys. Chem. C* **2014,** *118*, 3545-3553.

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