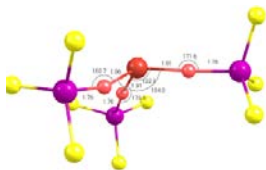


The University of North Texas is the home of the Center for Advanced Scientific Computing and Modeling (CASCaM, <http://cascam.unt.edu/>), a center of excellence whose mission involves research, education, training, and outreach in all facets of advanced scientific computing and modeling.

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 Srivilliputhur has received the CAREER award, given by the NSF to top junior faculty
- Professor Bagus Received the Alexander von Humboldt Foundation U.S. Senior Scientist Award
- Professor Buongiorno Nardelli is a Fellow of the American Physics Society.
- Professor Du has received the UNT Early Career Award of Research & Creativity.
- Grant support for CASCaM faculty over the past several years is over \$25,000,000.
- Resources dedicated to computational research are approximately 5,500 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 700 refereed scientific publications in the past 8 years.
- CASCaM faculty have sponsored more than 60 research students in the past 8 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.



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- Tobin, J. G.; Yu, S.-W.; Booth, C. H.; Tyliszczak, T.; Shuh, D. K.; van der Laan, G.; Sokaras, D.; Nordlund, D.; Weng, T.-C.; Bagus, P. S., Oxidation and crystal field effects in uranium. *Phys. Rev. B Condens. Matter Mater. Phys.* **2015**, *92*, 1-12.

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- Liu, J.; Bao, X.; Hrovat, D. A.; Borden, W. T., Theoretical Analysis of the Fragmentation of (CO)<sub>5</sub>: A Symmetry-Allowed Highly Exothermic Reaction that Follows a Stepwise Pathway. *J. Org. Chem.* **2015**, *80*, 11788-11793.

### Marco Buongiorno Nardelli, Professor

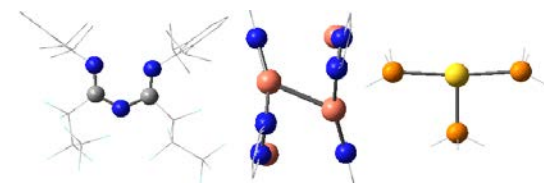
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- Olatunji-Ojo, O.; Cundari, T. R., Effect of Ligand Connectivity and Charge State on the Amination of C-H Bonds by Copper Amide Complexes. *Organometallics* **2015**, *34*, 5045-5050.

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- Horne, K.; Ban, H., Sensitivity analysis of the transient torque viscosity measurement method. *Metrologia*, **2015**, *52*, 1-7.

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- Ahmadi, M.; John, K., Statistical evaluation of the impact of shale gas activities on ozone pollution in North Texas. *Sci. Total Environ.*, **2015**, *536*, 457-467.

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