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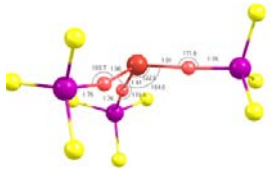
The University of North Texas is the home of the Center for Advanced Scientific Computing and Modeling (CASCaM, http://cascam.unt.edu/), a center of excellence whose mission involves research, education, training, and outreach in all facets of advanced scientific computing and modeling.

There are currently 18 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 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.
- 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 approximately 2000 cores, numerous Tb of storage, and roughly 5 Tflops of computing power.
- 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 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

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- Bioinformatics and Computational Biology
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- Azad, R.K.; Lawrence, J.G.; Towards more robust methods of alien gene detection; *Nucleic Acids Res.*, **2011**, 39(9), e56.

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- Bagus, P.S.; Wieckowski, A.; Freund, H.; The contribution of lattice strain to core-level binding energy shifts in metal nanoparticles: Generality and origin of the shifts; *Comput. Theor. Chem.*, **2012**, 987, 22-24.

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- Organic and organometallic chemistry
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- Bao, X.; Hrovat, D.A.; Borden, W.T.; Calculations of the Effects of Methyl Groups on the Energy Differences between Cyclooctatetraene and Bicyclo[4.2.0]octa-2,4,7-triene and between Their Iron Tricarbonyl Complexes; *J. Org. Chem.*, **2012**, 77(2), 956-965.

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- Revanna, K.V.; Chiu, C.-C.; Bierschank, E.; Dong, Q.; GSV: a web-based Genome Synteny Viewer for customized data**;** *BMC Bioinf.*, **2011**, 12, 316.

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- Du, J.; Devanathan, R.; Rene Corrales, L.; Weber, W.J.; First-principles calculations of the electronic structure, phase transition and properties of ZrSiO4 polymorphs; *Comput. Theor. Chem.*, **2012**, 987, 62-70.

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- Environmental sustainability

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- Karnae, S.; John, K.; Source apportionment of fine particulate matter measured in an industrialized coastal urban area of South Texas; *Atmos. Environ.*, **2011**, 45(23), 3769-3776.

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- Thompson, K.M.; Gao, Y.; Marshall, P.; Kinetic and theoretical investigations of the S + NO2 reaction; *Int. J. Chem. Kinet.*, **2012**, 44(1), 90-99.

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- Karton, A.; Martin, J.M.L.; Explicitly correlated Wn theory: W1-F12 and W2-F12; *J. Chem. Phys.*, **2012**, 136(12), 124114/1-124114/12.

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- Hutchens, S.B.; Needleman, A.; Greer, J.R.; A microstructurally motivated description of the deformation of vertically aligned carbon nanotube structures; *Appl. Phys. Lett.*, **2012**, 100(12), 121910/1-121910/4.

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- Nesterov, V.V.; Nesterov, V.N.; Richmond, M.G.; Structural characterization of cis-2,6-(E,E)-bis(ferrocenylidene)-N-methyl-4-piperidone and DFT evaluation of alternative polymorphic modifications via ferrocene rotation; *Polyhedron*, **2012**, 35(1), 124-129.

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- O'Brien, C.; Anisimov, P.M.; Rostovtsev, Y.; Kocharovskaya, O.; Coherent control of refractive index in far-detuned Λ systems; *Phys. Rev. A: At., Mol., Opt. Phys.*, **2011**, 84(6, Pt. B), 063835/1-063835/8.

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- Wang, Z.Q.; Beyerlein, I.J.; An atomistically-informed dislocation dynamics model for the plastic anisotropy and tension-compression asymmetry of BCC metals; *Int. J. Plast.*, **2011**, 27(10), 1471-1484.

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- Zhang, L.; Xia, Z.; Mechanisms of Oxygen Reduction Reaction on Nitrogen-Doped Graphene for Fuel Cells; *J. Phys. Chem. C*, **2011**, 115(22), 11170-11176.

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