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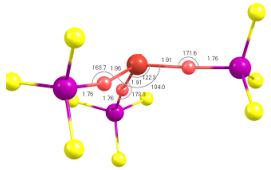
The University of North Texas is the home of the Center for Advanced Scientific Computing and Modeling (CASCaM, http://cascam.unt.edu/), a center of excellence whose mission involves research, education, training, and outreach in all facets of advanced scientific computing and modeling.

There are currently 15 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 Bagus Received the 2016 AVS Gaede-Langmuir Award
- Professor Buongiorno Nardelli is a Fellow of the American Physics Society.
- Professor Buongiorno Nardelli has received the 2017 UNT Office of Research and Innovation's Research Leadership Award.
- Professor Cundari has received the UNT Foundation Eminent Faculty Award.
- 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 1, 000 refereed scientific publications in the past 9 years.
- CASCaM faculty have sponsored more than 70 research students in the past 9 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.

UNT CENTER FOR ADVANCED SCIENTIFIC COMPUTING & MODELING

CASCaM Faculty

Oliviero Andreussi, Assistant Professor
Ph.D. 2008, Eidgenössische Technische Hochschule (ETHZ), Zurich, Switzerland
- Development of computational models in the fields of chemistry, biophysics and materials

http://www.materialab.org/
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- Bononi, F.C.; Chen, Z.; Rocca, D.; Andreussi, O.; Hullar, T.; Anastasio, C.; Donadio, D., Bathochromic Shift in the UV-Visible Absorption Spectra of Phenols at Ice Surfaces: Insights from First-Principles Calculations. *J. Phys. Chem. A* **2020**, *124*, 9288-9298.

Rajeev Azad, Associate Professor
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- Bioinformatics and Computational Biology
- Gene prediction, Genomic structural variations

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- Sturtevant, D.; Lu, S.; Zhou, Z.-W.; Shen, Y.; Wang, S.; Song, J.-M.; Zhong, J.; Burks, D.J.; Yang, Z.-Q.; Yang, Q.-Y.; Cannon, A.E.; Herrfurth, C.; Feussner, I.; Borisjuk, L.; Munz, E.; Verbeck, G.F.; Wang, X.; Azad, R.K.; Singleton, B.; Dyer, J.M.; Chen, L.-L.; Chapman, K.D.; Guo, L., The genome of jojoba (Simmondsia chinensis): a taxonomically isolated species that directs wax ester accumulation in its seeds. *Sci. Adv.* **2020**, *6*, eaay3240.

Paul Bagus, Research Professor
Ph.D. 1965, University of Chicago
- Surface and cluster chemistry
- X-Ray photoelectron spectroscopy

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- Bagus, P. S.; Sassi, M. J.; Rosso, K. M., Cluster embedding of ionic systems: Point charges and extended ions. *J. Chem. Phys.* **2019,** *151*, 044107/1-044107/7.

Marco Buongiorno Nardelli, Distinguished Research Professor
Ph.D. 1993, International School for Advanced Studies
- Electronic structure theory, computational materials

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- Nath, P.; Usanmaz, D.; Hicks, D.; Oses, C.; Fornari, M.; Buongiorno Nardelli, M.; Toher, C.; Curtarolo, S., AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids. *Phys. Rev. Mater.* **2019,** *3*, 073801.

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- Development and application of methods for the computational investigation of chemical and biochemical systems

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- Hix, M. A.; Wong, L.; Flath, B.; Chelico, L.; Cisneros, G. A., Single-nucleotide polymorphism of the DNA cytosine deaminase APOBEC3H haplotype I leads to enzyme destabilization and correlates with lung cancer. *NAR Cancer* **2020**, *2*.

Thomas Cundari, Regents Professor
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- Computer-aided catalyst design

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- Anderson, M. E.; Braïda, B.; Hiberty, P.C. ; Cundari, T. R. Revealing a Decisive Role for Secondary Coordination Sphere Nucleophiles on Methane Activation. *J. Am. Chem. Soc.* **2020**, *142*, 3125-3131.

Jincheng Du, Professor
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- Heterogeneous catalysis, Ceramics

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- Kerisit, S.; Du, J., Monte Carlo simulation of borosilicate glass dissolution using molecular dynamics-generated glass structures. *J. Non-Cryst. Solids* **2019,** *522*, 119601.

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- Environmental sustainability

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- Karnae, S.; John, K., Source apportionment of PM2.5 measured in South Texas near U.S.A. - Mexico border. *Atmos. Pollut. Res.* **2019,** *10*, 1663-1676.

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- Gas-phase kinetics
- Atmospheric and combustion chemistry

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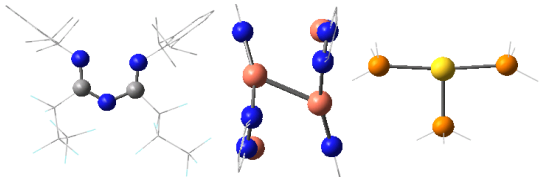
- Marshall, P.; Papadimitriou, V. C.; Papanastasiou, D. K.; Roberts, J. M.; Burkholder, J. B., UV and infrared absorption spectra and 248 nm photolysis of maleic anhydride (C4H2O3). *J. Photochem. Photobiol., A* **2019,** *382*, 111953.



Michael Richmond, Professor
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- Fluxional properties of cluster coordinated ligands
- Organometallic redox reactions

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- Pinky, T.; Rahman, M. M.; Ghosh, S.; Azam, K. A.; Mia, M. J.; Alam, M. M.; Tocher, D. A.; Richmond, M. G.; Kabir, S. E., Activation of thiosaccharin at a polynuclear osmium cluster. *J. Organomet. Chem.* **2019,** *880*, 223-231.

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- Quantum and Nonlinear Optics, Nucleonics

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- Zorica Brankovic, Yuri Rostovtsev, A resonant single frequency molecular detector with high sensitivity and selectivity for gas mixtures, *Sci. Rep.* **2020**, *10*, 1-10.

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- Corrosion and oxidation
- Nuclear materials and processes

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- Gwalani, B.; Salloom, R.; Alam, T.; Valentin, S. G.; Zhou, X.; Thompson, G.; Srinivasan, S. G.; Banerjee, R., Composition-dependent apparent activation-energy and sluggish grain-growth in high entropy alloys. *Mater. Res. Lett.* **2019,** *7*, 267-274.

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- Materials for clean energy (fuel cells)
- Multiscale/multi-physics modeling and simulation

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- Wan, Y.; Gao, Y.; Wang, J.; Yang, Y.; Xia, Z., Rapid water harvesting and nonthermal drying in humid air by N-doped graphene micropads. *Langmuir* **2019,** *35* (38), 12389-12399.

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