



Center for Simulation and Modeling (CSM)

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Key Interests

Quantum Models | Biomolecular Simulations | Polymers | High Performance Computing |
Smart Materials | Magnetics | Nanotechnology | Pharmaceuticals

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FACILITIES & EQUIPMENT

- › High Performance Computing (HPC) Cluster

SELECT PUBLICATIONS

- › G. Gogovi *et al.*, Modeling the Tertiary Structure of the Rift Valley Fever Virus L protein. *Molecules* 24, 1768 (2019).
- › D. Reitz & E. Blaisten-Barojas, Simulating the NaK eutectic alloy with Monte Carlo and Machine Learning. *Scientific Reports* 9, 704 (2019).
- › S. Silayi *et al.*, A tight-binding molecular dynamics study of the noble metals Cu, Ag and Au. *Comp Mater Sci.* 146, 278-286 (2018).
- › N. Lebedev *et al.*, Effect of iron doping on protein molecular conductance. *Phys. Chem. Chem. Phys.* 20, 14072-14081 (2018).
- › C. Lockhart *et al.*, Cholesterol changes the mechanism of Abeta peptide binding to the DMPC bilayer. *J Chem Inform Model.* 57, 2554-2565 (2017).

Research Focus

The Center for Simulation and Modeling (CSM) focuses on modeling, discovery, prediction, and analysis of the interactions between atoms and molecules in condensed phases of matter and beyond. The Center also emphasizes the development of the next generation of atomistic and quantum models for simulation of soft and hard materials and biomolecules. We believe that the ability to predict properties of matter is a fundamental requirement for technological and biomedical advances and economic competitiveness.

More specifically, the CSM develops new capabilities for simulation of materials using innovative algorithmic methods for high performance computing. A key component of our industrial development is the ability to invent and design novel materials, such as smart materials, pharmaceuticals, nano-structures, ceramics, magnetic crystals, and materials for the recording industry. Another key component is large-scale biomolecular simulations, which address fundamental biological questions such as Alzheimer's disease, activity of anti-microbial peptides, and permeability of blood-brain barriers.

Current research thrusts at the CSM include:

- Monte Carlo and Machine Learning studies of binary eutectic alloys that phase segregate upon solidification
- Optimization algorithms for multiple length scale atomistic approaches such as the Adaptive Tempering Monte Carlo method currently applied for detecting high density explosive materials.
- Magnetic frustration and nematic bond ordering in crystals from a density functional theory perspective
- Molecular Dynamics studies of the structural and thermodynamic properties of polymers in a variety of solvents and their self-aggregation into nanoparticles for drug delivery
- Application of replica exchange molecular dynamics simulations for studying the mechanisms of binding of A β peptides to neuronal membranes and for investigating ion permeation through lipid bilayers
- Probing the physicochemical properties of multicomponent lipid bilayers via novel all-atom molecular dynamics