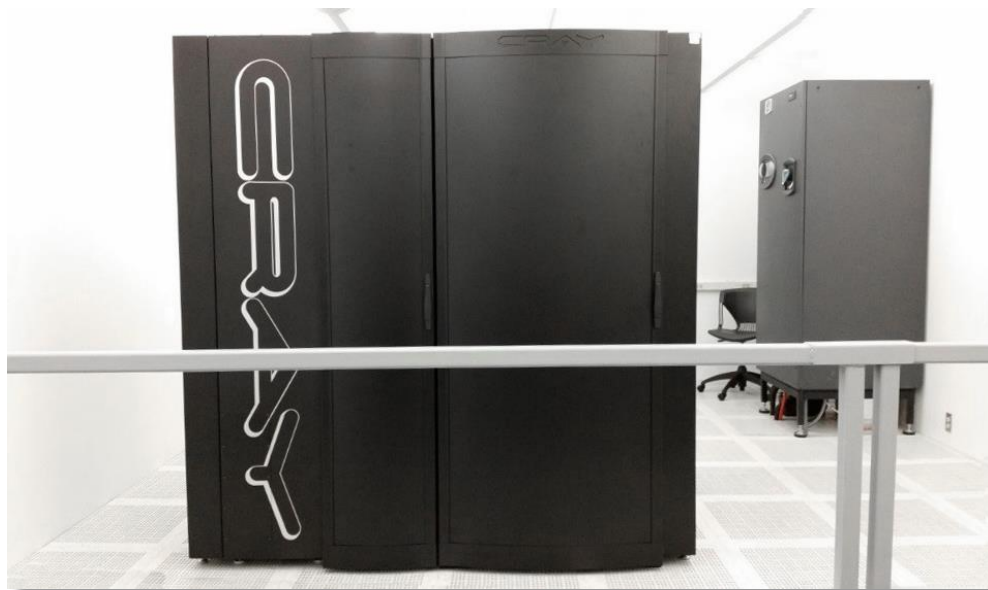


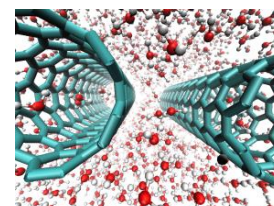
# Computational Modeling Core

*Excellence in Computational Nanomaterials, Chemistry and Biology*

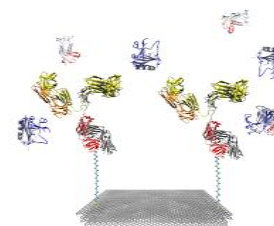


## Advance your research with computational models

Whether you want to analyze biomolecules, determine nanomaterial properties, or understand nano-bio interactions, the Joint School of Nanoscience and Nanoengineering (JSNN) offers 24/7 access to a host of computational resources with training, workshops, research collaborations, and project consultations. JSNN provides state-of-the-art facilities with skilled research staff to address the needs of academic, industry and government users. For access to the core user facility and professional staff, join the JSNN's Nanomanufacturing Innovation Consortium (NIC), administrated by Gateway University Research Park ([www.gatewayurp.com/pages/The\\_Nanoschool](http://www.gatewayurp.com/pages/The_Nanoschool)).



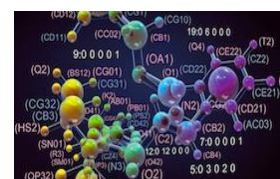
Nanomaterial Modeling



Computational Biology



Bioinformatics



Computational Chemistry

### EXPERT TRAINING

Experienced staff can provide high-quality training in one-on-one, classroom or small group sessions.

### DEDICATED RESOURCES

Utilize our state-of-art computational and software packages to solve today's material, physical, chemical and biological challenges

### NEW METHOD DEVELOPMENT

Work with our skilled staff to develop new computational methods to solve today's material, physical, chemical and biological problems

## COMPUTATIONAL RESOURCES AND SOFTWARE PACKAGES

- Cray XC30 Supercomputer with GPU and CPU
- Cave Automatic Virtual Environment - 3D Visualization Suite
- Dell Quad Core Computers – Multiple
- Software packages include
  - Accelrys, Material Studio, ANSYS, GROMACS, Lammps, MATLAB
- Training available on:
  - I-Tasser, NAMD, VMD, Rasmol, QT/XMGrace, Material Studio, ANSYS, GROMACS, Lammps, MATLAB, SYBYL-X, Autodock



For questions regarding computational resources, please contact –

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