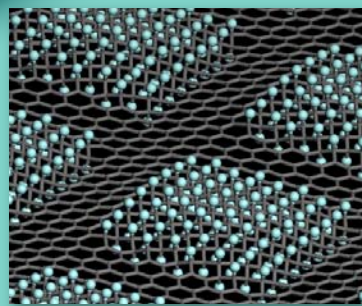


MSC Contact Information:

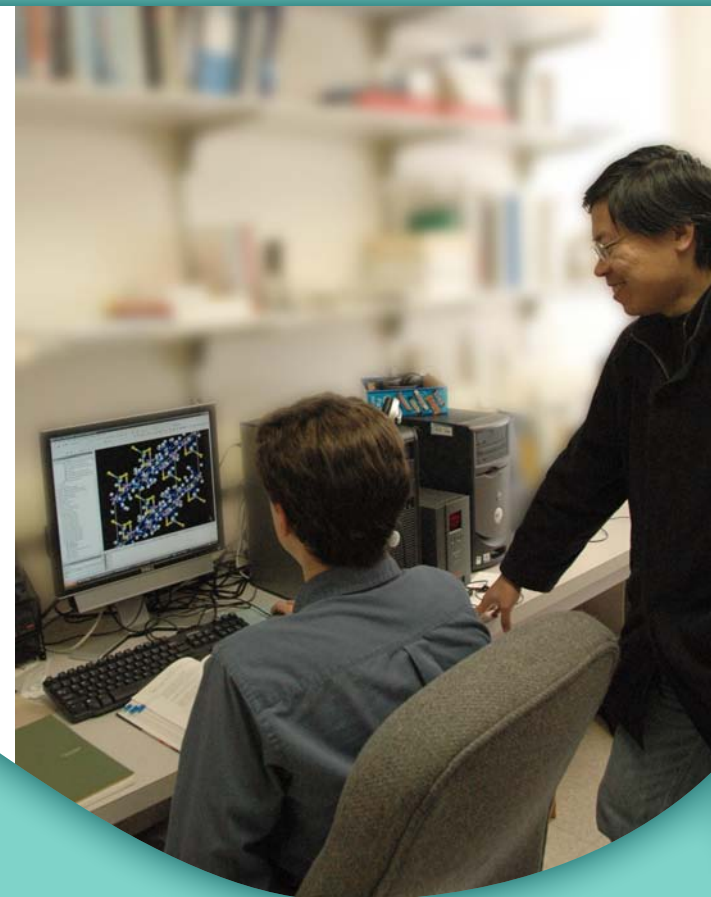
Phone: 814-777-3450
Email: mschelp@psu.edu
Web: www.msc.psu.edu



Junctions
Sofo Group
Penn State



A LEADER IN INTERDISCIPLINARY RESEARCH



MATERIALS SIMULATION CENTER

HPC at Penn State:

The High Performance Computing (HPC) group works with faculty and centers such as the Materials Simulation Center to build and maintain the Lion Clusters, currently approximately 1000 servers with an aggregate capacity of 20 trillion operations per second. The Linux clusters—Lion-XL, Lion-XM, and Lion-XO—provide the core computational capabilities.

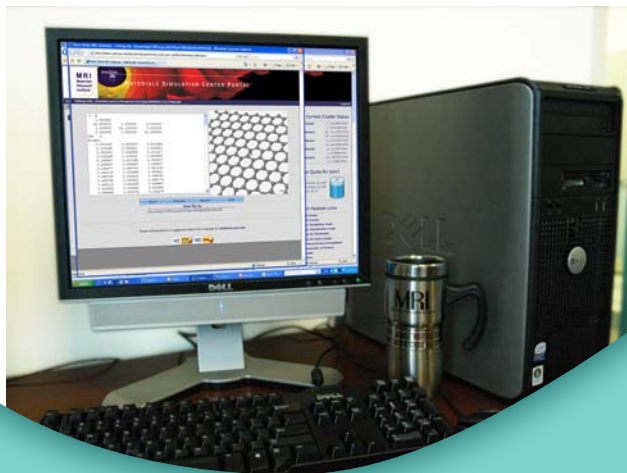
Table with 3 columns: Lion-XL, Lion-XM, Lion-XO. Rows include node counts, processor counts, and RAM capacity.

MATERIALS RESEARCH INSTITUTE
199 MATERIALS RESEARCH INSTITUTE BUILDING
THE PENNSYLVANIA STATE UNIVERSITY
UNIVERSITY PARK, PA 16802
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The Materials Simulation Center is designed to function as a hub to connect experimental and simulation activities through the organization of collaborative projects, short courses, and workshops. For experimentalists, the Center provides the information needed to add a simulation component to their work. For groups already working on materials simulation, the Center is a natural environment for interaction and extension of existing simulation techniques.

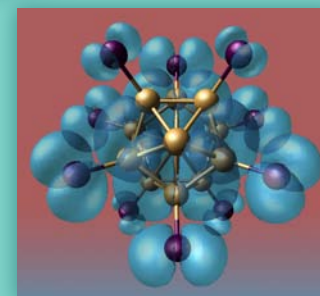


Materials Simulation Codes:

GAMESS
CaChe
CPMD
HyperChem
NWChem
Paratec
VASP
WIEN2k
XMD
Gaussian

Visualization Tools:

Molden
JMOL
XCrysDen
wxDragon
VMD
Molekel
VaspView
GaussView



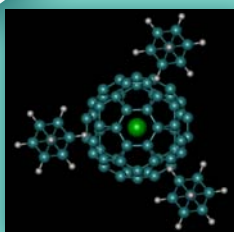
Clusters of atoms called superatoms have properties that mimic the behavior of other atoms on the periodic table.

Castleman Group
Penn State

Model of a solid containing atoms of carbon (blue), potassium (green), and hydrogen (white).

Crespi Group
Penn State

Credit Young-Moo Byun



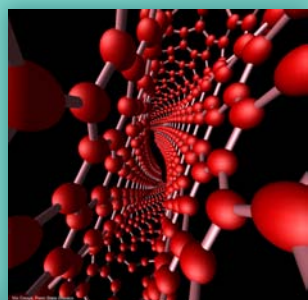
A theoretical new material called graphane. Carbon atoms are shown in gray and hydrogen atoms in white. When synthesized, this stable hydrocarbon might be useful for low-dimensional electronics or possibly hydrogen storage.

Sofa Group
Penn State

Interdisciplinary Cooperation

MSC also promotes the formation of interdisciplinary teams to respond to specially targeted funding opportunities. To achieve these objectives, the Center works closely with the Institute for Computational Sciences (ICS) and the High Performance Computing (HPC) group at Penn State, as well as other research centers and groups.

The Center makes available a range of simulation codes and visualization tools to its users. The Center shares software and hardware with the HPC group, which maintains Penn State's Lion-XE, Lion-XM, and Lion-XL high performance computer clusters. MSC is supported by the Materials Research Institute and the Center for Nanoscale Science (MRSEC).



Flattened, twisted carbon nanotube.

Crespi Group
Penn State

