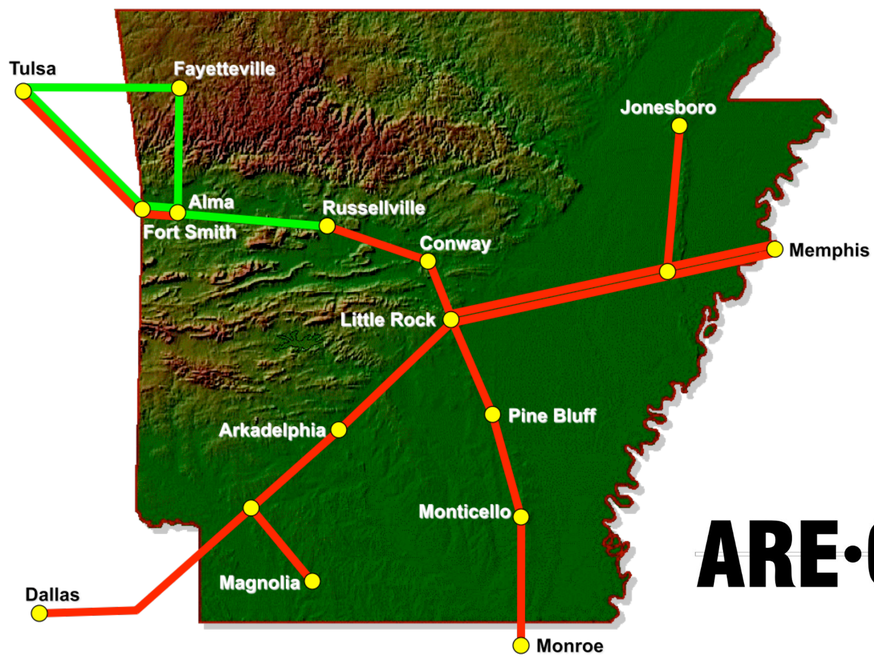
Arkansas High Performance Computing Center

CI-TRAIN

Cyberinfrastructure for Transformational Scientific Discovery

Faculty and staff *Campus Cyberinfrastructure Champions* serve as **liaisons** between researchers and resources, both local and national, *using shared large-scale computational and visualization resources* and high-speed network access to participating institutions to SUPPORT RESEARCH in a wide spectrum of computational and visualization domains.

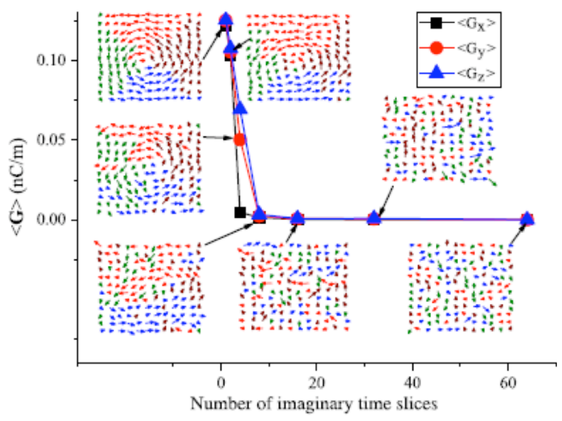
Arkansas Research and Education Optical Network

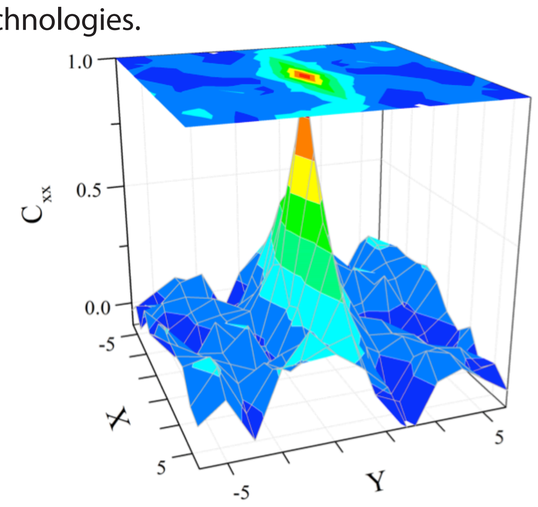


ARE·ON

Computational Nanotechnology

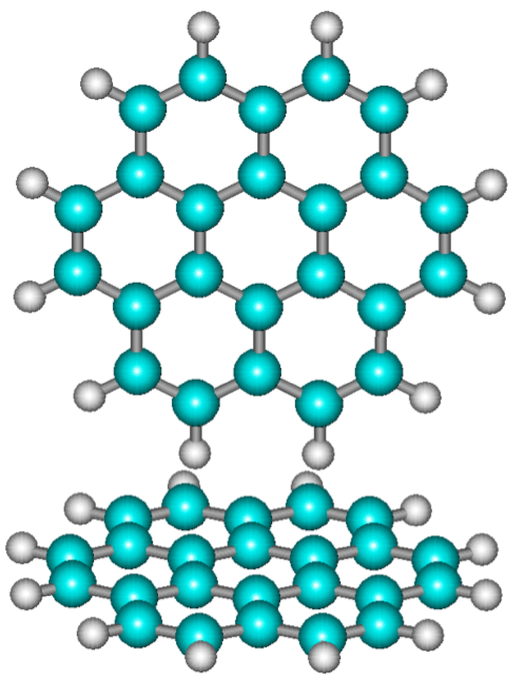
Research by Laurent Bellaiche, Professor of Physics, Sergey Prosandeev, and his colleagues use effective Hamiltonian techniques to investigate the effects of quantum vibrations on materials at the nanoscale level. They have discovered that these vibrations suppress the paraelectric-to-ferrotoroidic transition, or equivalently, wash out the formation of vortex states. These materials have application to the development of new computer memory technology that is 10,000 times more dense than current technologies.





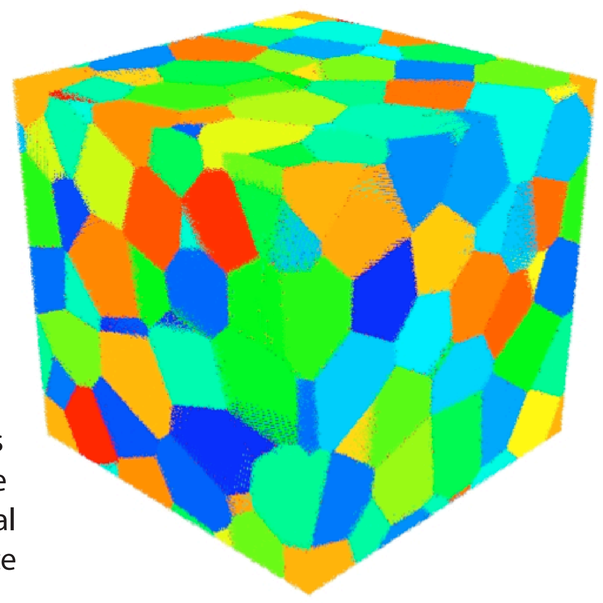
Computational Chemistry

Peter Pulay, Distinguished Professor of Chemistry, Tomasz Janowski, and colleagues use Arkansas high performance computing resources to compute fundamental properties of chemicals. This illustration shows the T-shape configuration of the coronene molecule used in high level *ab initio* calculations that determine the binding energy of the coronene dimer. Calculations by the Pulay group have application to the development of formulas for new drugs. Bigger systems under investigation involve the study of DNA intercalation and DNA base pair interactions.



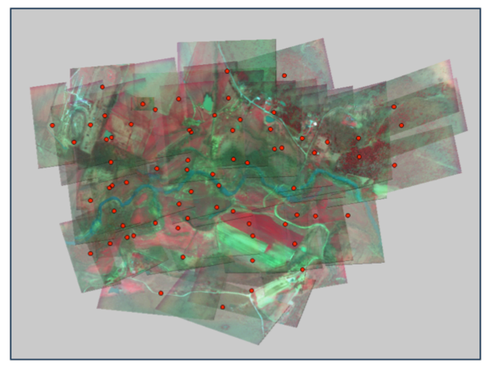
Computational Materials Science

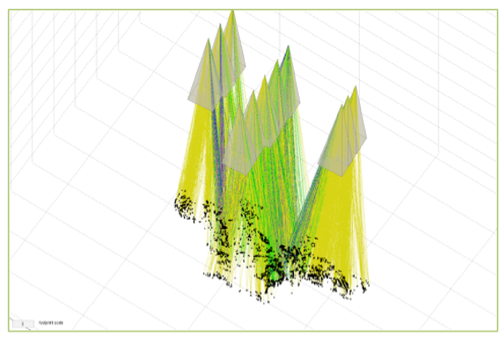
Douglas Spearot, Assistant Professor Mechanical Engineering, studies properties of materials under a range of extreme conditions. This figure shows a simulation model of nanocrystalline Cu-0.5at.%Sb containing 135 grains with average grain diameter of 15 nm. The different colors represent individual grains and the Sb atoms are colored red and placed at the grain boundaries. This research leads to new formulas for alloys that can be used in the manufacture of new metal products such as extra light aerospace components that can withstand extreme temperature and force.

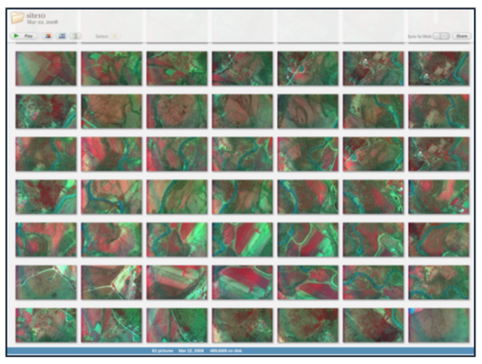


Geospatial Science

Jackson Cothren, Director of the Center for Advanced Spatial Technologies, Fred Limp, and colleagues develop new techniques for processing very complex sets of spatial data. Features are extracted from images and matched with features from a variety of sources. Arkansas high performance computing resources will be used to stitch a set of unorganized images into a much larger mosaic.







http://hpc.uark.edu