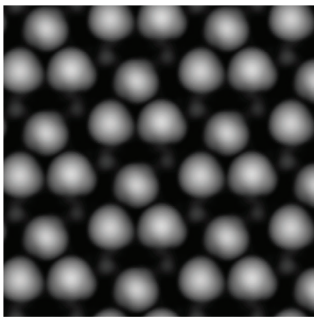
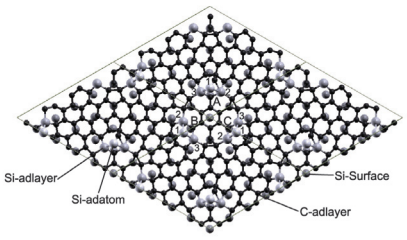
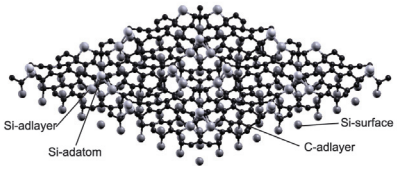




Top view



Perspective view

Calculating surfaces for graphene growth

The understanding of surface reconstructions has become essential as scientists seek to develop materials with tailored properties. For instance, researchers over the past few years have been searching for a process to mass-produce circuits using a material called graphene – a one-atom-thick layer of graphite – which displays unique electronic properties.

Nancy Sandler, Ph.D., an assistant professor in the Physics and Astronomy Department at Ohio University, is investigating models for surface reconstructions of silicon carbide (SiC), a substrate material used to produce graphene. Her modeling was generated with the density functional theory-based code SIESTA on the IBM Glenn Cluster at the Ohio Supercomputer Center.

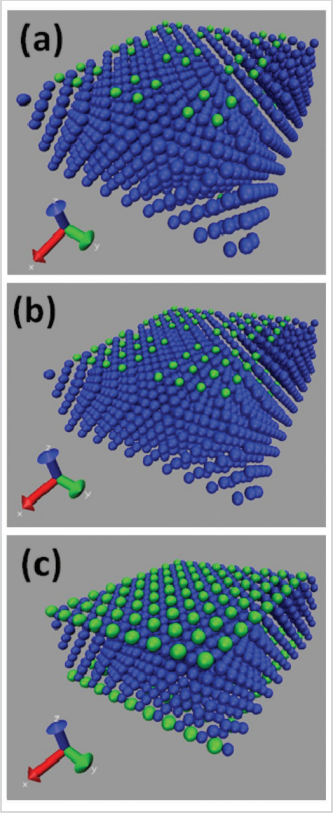
"Despite the success in the fabrication of high-quality films of graphene, there is little knowledge on the mechanisms of nucleation and growth of these films on the underlying SiC material," said Sandler. "Many of the properties of the film obtained are strongly determined by the substrate that remains after graphene separation."

Sandler and her team studied three models, each with the addition of carbon-rich layers of different coverage and electronic properties similar to that existing before graphitization. They analyzed corresponding band structures and density-of-states, comparing them to experimental scanning tunneling microscope measurements.

The model that best described the experimental observations featured an intermediate-coverage carbon-rich layer, on top of which a complex network of three-atom products, called trimers, is formed. This trimer network produces electronic properties common to both reconstructions and provides insight into graphene formation at higher temperatures. ■

Project lead: Nancy Sandler, Ohio University
Research title: Model calculations for surface reconstructions of semiconductor materials
Funding source: National Science Foundation

below: Atomic models of (a) a 2x2 island, (b) a 4x4 island, and (c) a monolayer of N atoms on Cu [001].



Controlling nanometer-scale structures

Surprising behaviors often arise when small numbers of atoms and molecules are brought into close proximity. Such small aggregates offer a window into an intermediate state of matter between isolated atoms and bulk materials. An improved understanding and control of these nanometer-scale structures may contribute to new paradigms for technologies such as molecular circuits, spin-based electronics and quantum computation.

A research team led by Ohio State University's Jay A. Gupta, assistant professor of physics, and David G. Stroud, professor of physics, is using scanning tunneling microscopes (STM) to better measure the properties of nanoscale structures, whose size can vary from a few atoms to thousands of atoms.

Quantum confinement of electrons in the cluster leads to a discrete spectrum of states with a level spacing that depends on the size. By isolating the nanocluster from the underlying metal substrate by using an ultrathin insulating film of only a few atomic layers (e.g., Cu2N islands), scientists can measure this spectrum with STM. They seek to understand how these electronic structure properties depend on the dimensions of nitrogen islands.

"We have studied the electronic structure of nanoscale islands of Cu2N on the Cu [001] surface," said Gupta. "We leverage hundreds of processors on Ohio Supercomputer Center systems to perform ab-initio calculations using density functional theory. Those results are compared with our scanning tunneling microscopy measurements, and we find that our tunneling spectroscopy results are in good agreement with our computational predictions." ■

Project lead: Jay Gupta, The Ohio State University
Research title: Emergence of band structure in nitrogen islands on copper [001]: Comparison of density functional theory and scanning tunneling microscopy
Funding source: Center for Emergent Materials - The Ohio State University