TOPOLOGIES OF SURFACE ELECTRONIC STATES OF NANOCRISTALLINE MATERIALS

Research Challenge
Engineered nanocrystals have promise in new functional electronic and optical materials. The team uses computational electronic structure investigations to explore the properties of unconventional nanomaterials, such as nanocrystals of Hg_{x}Cd_{1-x}Se alloys. In particular, the team uses Blue Waters to answer the question whether topologically-protected surface states can exist on the surfaces of small nanocrystals and, if not, are there new topologies associated with surface electronic states of nanocrystals.

Methods & Codes
For electronic structure calculations, the team uses the open-source Quantum Espresso software suite and the plain-wave density-functional theory method. For studying the effect of nanocrystal size, the team uses projected density of states, charge density maps, surface and bulk band structures obtained from calculations of whole nanocrystals. The computations will reveal whether there is a crystal size regime wherein quantum confinement enhances the band gap while retaining topologically-protected surface states.

Why Blue Waters
The effort required Blue Waters resources due to the scale of bulk slab and full-atom nanocrystal simulations. Numerous calculations, each requiring tens of nodes with a fast interconnect, were required for current investigations, with larger models potentially required in the future. Simulations greatly benefitted from the Blue Waters fast communications hardware.

Results & Impact
While the team is still a few calculations away from completing this ambitious project, this study has the potential to identify nanostructures with unconventional electronic transport properties of utility in energy storage and information technology. Understanding of the surface states will set the stage for new discoveries about unique electronic behavior on the nanoscale.