SEAGrid Science Exemplars

In this presentation 3 examples of SEAGrid gateway usage will be elaborated focusing on the science derived as well as implementation providing a comprehensive view of the capabilities and utility of gateways such as SEAGrid.

**Diffraction Workflows**

The research of Coleman and Spearot (Coleman, 2014; Coleman, 2015)  provided the diffraction characteristics of alumina polymorphs using an efficient implementation of diffraction compute as part of LAMMPS software. The polymorphs are otherwise difficult to distinguish by methods such  as centrosymmetry analysis or radial distribution functions (Coleman, 2015) while the current diffraction based methods work very well. This research involved the extension of the LAMMPS package to support diffraction simulations, which we integrated into the SEAGrid gateway. To further enable the research, we also developed infrastructure in the SEAGrid gateway to distribute the computing and the visualization tasks on multiple resources available in XSEDE to exploit specialized hardware and software available on different systems.

**Calcium Carbonate Hydration**

In a bio-mineralization simulation work Espinoza-Marzal and co-workers involved multiple software tools and techniques to ascertain the free energies of hydration of calcium carbonate for various hydration models. The computation involved Monte Carlo searches using classical force fields followed by semi-empirical quantum chemical calculations using DFTB+ software and subsequently ab initio and DFT computations for energetics.  This study clarified the hydration environment for calciun carbonate and defined the energetics of hydration in first and second shells around the central calcium carbonate moiety (Lopez-Barganza, 2015).

**Topological Insulators of the HgTe/HgCdTe Ternary System**.

Topological insulators (TIs) represent a novel state of matter: the bulk (3D) of a TI is electrically insulating, but the surface (2D) contains topologically protected conductive states.1,2 TI materials are receiving surging interest as platforms for discovery of exotic condensed matter phenomena, e.g., Majorana fermions,3–5 and for the utility of the spin-protected surface conduction in spintronics and quantum computing.6–9 Most materials that are intrinsically 3D topological insulators are Bi-or Sb-based, in particular selenides and tellurides of these metals.

our DFT simulations reveal that the wurtzite polymorph of HgSe has a remarkably different electronic structure from the naturally known zincblende phase of HgSe. While zincblende HgSe is a semimetal, the wurtzite polymorph has the attributes of a 3D TI insulator including band inversion and a non-zero band-gap. Motivated by the calculations, we successfully realize this non-natural wurtzite phase by topotactic exchange of Cd2+ in wurtzite CdSe NCs with Hg2+. Measured band-gaps of the synthesized wurtzite HgxCd1-xSe alloy NCs show a trend in agreement with our simulations. Systematic electronic structure investigations of the HgxCd1-xSe alloys elucidate the physical principles underlying 3D TI behavior. Band inversion is a result of the scalar relativistic effect of Hg 6s electrons on the Г6 band, while band gap opening is the result of symmetry breaking due to the crystalline anisotropy of the wurtzite structure. The relativistic contribution of Hg is sufficient for alloys with *x* ≥ 0.33 to demonstrate attributes of 3D TIs at room temperature. Thus, we introduce crystal anisotropy as a new handle for tuning band topology, elucidate the important role of scalar relativistic effects, and expand of the class of materials with 3D TI attributes to include mercury chalcogenides.