Physics Colloquium

Thursday, January 28th at 3:30 pm in SC 234

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Clathrate Materials: Novel, Open Framework, Crystalline Materials Based on Si, Ge, and Sn

The Column IV elements Si, Ge, and Sn usually crystallize in the diamond lattice structure. It is less well-known that these elements can also form novel crystalline solids, called clathrates because of their structural similarities to clathrate hydrates. Column IV clathrates are metastable, expanded volume phases. As in the diamond structure, in the clathrates, the atoms are tetrahedrally coordinated in sp^3 covalent bonding configurations with their near-neighbors. In contrast to the diamond lattice, however, the clathrates contain pentagonal rings of atoms and their lattices are open frameworks containing large (20-, 24-, 28-atom) "cages". The two common clathrate varieties are **Type I**, a simple cubic lattice with 46 atoms per unit cell and **Type II**, a face centered cubic lattice with 34 atoms per unit cell. The cages can contain weakly bound impurities ("guests"), usually alkali or alkaline earth atoms. A reason that the clathrates are interesting is that the choice of guest may be used to tune the material properties. The guests act as electron donors, but because of their weak bonding, they have only small effects on the host electronic structures. However, they can vibrate with low frequency modes, which can strongly affect the material vibrational properties. Some laboratory-synthesized, guest-containing clathrates show great promise for thermoelectric applications **precisely because** the guests only weakly perturb the electronic properties, while strongly affecting the vibrational properties.

This talk will begin with a tutorial on the clathrates and their lattices. Some results of our calculations of the properties of some Si, Ge and Sn-based **Type I** and **Type II** clathrates will then be presented. Where data is available, some of these results will be compared with experiments. Our calculations are motivated by experiments performed by the G.S. Nolas group at the University of South Florida. The calculations use a density-functional based, planewave, pseudopotential method. The results include equations of state, structural parameters, electronic bands, vibrational spectra, mean-square atomic displacements, and thermodynamic properties. Calculations of some of the transport properties of some of these materials are planned as part of my student Dong Xue's PhD dissertation project.

Refreshments 3:00-3:20 pm in SC 103