A baby crystal is born

January 17 2012

Lead sulfide (PbS) forms when an equal number of lead and sulfur atoms exchange electrons and bond together in cubic crystals. Now scientists have determined that a structure comprising 32 lead-sulfur pairs is the smallest possible cubic arrangement that exhibits the same coordination as bulk lead sulfide. (The coordination number is the number of nearest neighbors each atom in the crystal has.)

Researchers from McNeese State University in Louisiana, John Hopkins University in Maryland, and the University of Konstanz in Germany identified the "baby crystal" by running computer simulations that calculated the energy and geometry of different structures containing different numbers of atoms. They found that (PbS)32 is the smallest stable unit that possesses both the same cubic structure and coordination number as the bulk crystal. The researchers also experimentally tested their theoretical findings by gently depositing (PbS)32 clusters on a graphite surface where they could easily migrate and merge together to form larger nanoscale structures.

By using scanning tunneling microscope images to measure the dimensions of the resultant lead sulfide nano-blocks, the researchers confirmed that the (PbS)32 "baby crystals" had indeed stacked together as theoretically predicted.

The results, published in the AIP's Journal of Chemical Physics, show how small lead sulfide crystals come together to form larger units and could help provide a better understanding of the mechanisms involved in the formation of solids.

More information: B. Kiran et al. "(PbS)32: A Baby Crystal", *Journal of Chemical Physics.*

Provided by American Institute of Physics