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CHESS X-rays show how to grow crystals from crystals

By *Anne Ju*

Way too small to see, nanocrystals – tiny crystals that are at least 1,000 times smaller than the diameter of a human hair – exhibit unprecedented properties that intrigue scientists and engineers. To apply these materials in emerging nanotechnologies, scientists need to better understand their structure, their corresponding functions and how they pack together.

A collaboration between Cornell High Energy Synchrotron Source (CHESS) and materials scientists has yielded greater understanding of what particular nanocrystals look like individually and how they fit together as they form larger structures called supercrystals. Such knowledge could lead to effective bottom-up engineering of new materials for applications ranging from solar cells to electronic components. The work was published by Journal of the American Chemical Society.

The collaboration used innovative X-ray crystallography methods at the B1 CHESS beamline led by CHESS staff scientist Zhongwu Wang. It involved the simultaneous collection of data on the ordering and orientation of lead sulfide nanocrystals and supercrystals using both wide-angle (WAXS) and small-angle (SAXS) X-ray scattering, which typically are done one at the time.

Wide-angle X-ray scattering is used for relatively smaller-scale characterization, revealing information on how atomic planes within individual nanocrystals are oriented. Small-angle scattering goes a step further by yielding data on how nanocrystals, approximately 100 atoms in diameter, are arranged relative to each other, when they join together as a supercrystal.

Wang and his collaborators worked with Tobias Hanrath, associate professor of chemical and biomolecular engineering, who studies lead sulfide and other nanocrystals for photovoltaic materials, to prepare the samples and conduct the experiments.

The new combined method at CHESS provided insights into the unexpected complexity of the arrangement of nanocrystals within the supercrystal. The discovery could inform new methods for growing supercrystals and how to optimize their properties.

"You can think of an individual nanoparticle as a designer atom," Hanrath said. "We want to figure out how you can take the particles and put them together in different configurations in which the particles can interact in purposeful and programmable ways. And we need to use tools like at CHESS in order to look at the actual structures, which are far more complex than when you just treat them as little spheres."

Wang said the WAXS/SAXS X-ray techniques will help them and other scientists understand how nanocrystals change, and how they interact with different solvents and in different environments. He and other collaborators plan to look at increasingly complex nanocrystal assemblies.

"We will combine in-situ spectroscopic techniques with our X-ray techniques to build a series of structure-property relations of confined nanocrystals with different sizes, shapes and compositions," Wang said.

The paper, "Decoding the Superlattice and Interface Structure of Truncate PbS Nanocrystal-Assembled Supercrystal

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STORY CONTACTS

Cornell Chronicle
Anne Ju
607- 255-9735
amj8@cornell.edu

Media Contact
Syl Kacapyr
607-255-7701
vpk6@cornell.edu

and Associated Interaction Forces," includes co-authorship by postdoctoral associate Ruipeng Li, graduate student Kaifu Bian, and William Bassett, professor in earth and atmospheric sciences. It was supported by the National Science Foundation, which supports CHESS.

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