

Complexing the Atomic Pair Distribution Function and Small-angle Scattering for Determining the Structure of Nanoparticles: Challenges and Prospects

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The fine structural details of nanoparticles are an ever-elusive challenge to crystallographic structure determination techniques. A promising approach to this challenge is atomic pair distribution function (PDF) analysis, which gives the internal arrangement of atoms from nanoparticle ensembles. Another widely used approach is small-angle x-ray or neutron scattering (SAS), which gives information about the morphology of nanoparticles, but not their internal arrangement. For complex disordered, distorted capped, and multi-phase nanoparticles, a single technique is not enough to determine a robust and quantitative structure solution. To reliably model these systems, we need all the information we can get.

In this talk we describe Complex Modeling, a computational method for complexing experimental and theoretical information from multiple sources to obtain a reliable and coherent structural view of a material. We demonstrate how the PDF and SAS can be complexed to give a more detailed picture of nanoparticle systems. We discuss the challenges of obtaining a “complete” picture of these systems and the prospects of complexing other structural information and theory to approach this goal.