Reverse Monte Carlo for magic-size metal chalcogenide nanoclusters

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Metal chalcogenide semiconductor nanoclusters, which form as quantum dots (QDs), have been used in biomedical labelling, solar cells, light emitting diodes.

The quantum dots are found either as regular quantum dots (RQDs) or magic-size clusters (MSCs), which are normally in the size range up to around 30˚A. MSCs contain a well-defined number of atoms and thus a single size.

As a class of truly monodisperse nanomaterials, the properties of MSCs with such extremely small size are very sensitive to structure. However, the effect of detailed atomic structure has been less well understood, and normally the pair distribution function is defined for a continuous homogeneous material, for nanoscale ordering especially for these ultra-small nanoclusters presents some new challenges.

So we are writing a new RMC code to perform the structure analysis on the X-ray total scattering PDF data to predict the atomic structure for nanoclusters. Some preliminary results will be shown and more work for the code are in progress. Besides some ab initio random structure searching results will also be used as a compare to the RMC results.