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Numerical Methods

Solving Structures Without Crystals

Method provides structural solutions to materials lacking long-range order

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Synthesize a new solidstate compound, and modern crystallography methods usually can help solve the material's atomic structure, provided that samples of the material are available in the form of bulk crystals, even small ones. But for nanoparticles and other materials that lack long-range order, determining structures is challenging because crystallography methods aren't applicable.

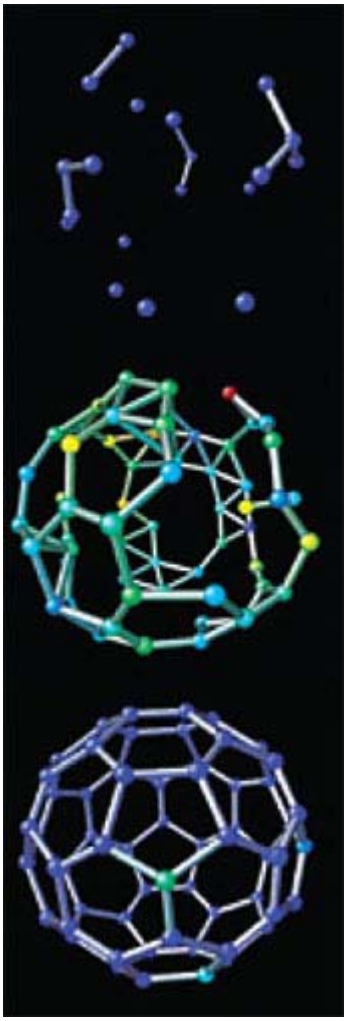

Image courtesy of Pavol Juhás

Under Construction

A new method builds up structures of crystallographically inaccessible clusters (C_{60} in this example) through an iterative process that's based on ranking the agreement between experimental and theoretical

structure data. Light-colored atoms indicate large error.

A new computational method, though, is poised to help with the problem. Researchers have developed a numerical procedure for determining the atomic structures of aperiodic materials using the type of data measured in X-ray and neutron-diffraction studies of powders and other noncrystalline samples. According to the researchers, the method may enable structures to be solved with subangstrom resolution even when crystallographic methods fail.

"Knowing the structure of a material is a prerequisite to understanding its properties," says Simon J. L. Billinge, a professor of physics at Michigan State University, East Lansing. Yet for certain types of solids, such as nanometer-sized chunks of semiconductors, the absence of long-range order rules out the possibility of solving the structure via crystallography.

So Billinge, Pavol Juhás, Phillip M. Duxbury, and their coworkers in computer science at Michigan State developed a computational technique for building up cluster structures one atom at a time using readily available high-resolution diffraction data. The data, which are known as atomic pair distribution functions (PDFs), consist of lists of interatomic spacings and a histogram that indicates how many atom pairs share a particular spacing.

To build up structures, the algorithm "positions" a small number of atoms in a cluster and then compares the distance list derived from the computer-generated cluster with an experimentally measured list. Distance values obtained from other computer-generated clusters of the same size are also compared with the experimental data. The theoretical cluster that matches the experimental data most closely "wins" that round and is promoted to the next level, where structures of clusters with one additional atom are once again ranked according to the closeness of the match with experimental data (*Nature* **2006,** *440*, 655).

Billinge explains that the procedure was inspired by the rules of

promotion and relegation (downgrading) that are used to rank teams in European soccer leagues, such as La Liga in Spain.

Named accordingly, the Liga method was used to deduce the structure of C_{60}, using PDF data obtained from neutron-scattering measurements on a solid-phase sample of buckeyballs. The team reports that the calculated data set matches the experimentally measured results quite closely, yet the computed structure deviates slightly from the ideal structure of C_{60} due to noise in the data and experimental limitations.

In a commentary in the same issue of *Nature*, John J. Rehr, a physics professor at the University of Washington, remarks that "aperiodic materials are among the technologically most interesting nanoscale materials currently under study. The new approach to solving these materials' structures could be widely applicable."

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