

## **23g Three-Dimensional Reconstruction of Mesoporous Materials Using Gas Adsorption and Structure Factor Data**

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We report progress towards the reliable three-dimensional reconstruction of amorphous and templated mesoporous materials from experimental gas adsorption data, and, when available, structure factor and other data. The method relies on the rapid evaluation of adsorption isotherms on trial structures using a lattice-gas model similar to that of Kierlik et al (PRL (2001) #055701). A parallel evolutionary strategy is used to generate optimal reconstructions efficiently and in reasonable time. We discuss the efficient implementation of this approach, and analyze its performance by applying it to adsorption data produced by simulation from "known" structures.

This method not only provides a general framework in which to reconstruct material structures from different and unrelated types of experimental data, but also provides an environment in which is possible to determine how much (and of what kind) structural data is present in various experimental measures. We focus particularly on adsorption isotherms, desorption isotherms, and scanning curves in this regard, and consider several classes of amorphous and templated-amorphous silica materials.