Modeling Finite Nano Systems

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Abstract

Modeling the nanoscale can occur within a single element or by limiting the large-scale nature of arrays and nano systems to a finite size. We consider measuring the order in finite nanoporous arrays via the pair distribution function and by reciprocal space parameters. Porous arrays have been made in triangular, hexagonal and square geometries, and we compare the experimental versions with ideal models. An order parameter derived from the pair distribution function takes values from zero to one; whereas a reciprocal space parameter has nominal values from zero to ten. We also look at modeling nano systems from a theoretical graph network view, where a graph has atoms at a vertex and bonds represent links. In this way, we can calculate standard statistical mechanics functions (entropy, enthalpy, and free energy) and matrix indices (Wiener Index) of finite nano structures, such as fullerenes, carbon nanotubes, and graphene nanoflakes. For many of these parameters, the data have power law behavior, especially when plotted versus the number of bonds or the number of atoms. We conclude with a summary and indications for future work.