Abstract for "3rd RMC Conference, 28-30 September, Hotel Normafa, Budapest"

Empirical potential structure refinement: where it came from, what it does, and why.

A K Soper

ISIS Facility, Rutherford Appleton Laboratory,
Chilton, Didcot, Oxfordshire, OX11 0QX
UK

Abstract

Empirical potential structure refinement (EPSR) – originally called EPMC[1] - evolved from Reverse Monte Carlo (RMC) simulation 10 years ago. Subsequently there have been several examinations of the methodology of EPSR,[2] the most recent being a full appraisal of using EPSR to extract partial structure factors from diffraction data.[3] There is a growing literature of applications of the EPSR method to the study of (mostly) molecular systems. Although EPSR and RMC are closely analogous in many regards, there are some technical but important distinctions between the two tools. Fundamentally RMC attempts to build a structural model of the scattering system with the minimum of prior information. It therefore has the ability to explore a very wide range of possible structures which are consistent with the scattering data. EPSR on the other hand attempts to restrict the structural phase space that can be explored by imposing harmonic constraints on the structure of any molecules present in the system under study, and by assuming an initial guess for any interatomic forces (repulsive, dispersive, Coulombic) which are likely to be present. The difference between the scattering data and the simulated data is then used to develop a perturbation to those forces so that the simulation reproduces as close as possible the diffraction data. The need for supplying these additional constraints arises because there are usually far fewer X-ray and neutron isotope data sets available compared to the number of partial structure factors needed to define the structure for most of the systems that are investigated with EPSR. Moreover, due to the systematic error that creeps into all diffraction measurements, it is never safe to rely solely on the diffraction data to supply all the necessary structural constraints. The talk will be illustrated with some recent applications of EPSR to both atomic and molecular systems.

---

[1] *Empirical potential Monte Carlo simulation of fluid structure*, A K Soper, *Chem. Phys*. **202**, 295-306 (1996)

[2] *The radial distribution functions of water and ice from 220K to 673K and at pressures up to 400MPa.* A K Soper, *Chem. Phys.*, **258**, 121-137 (2000); *Tests of the empirical potential structure refinement method and a new method of application to neutron diffraction data on water*, A K Soper, *Mol. Phys.*, **99**, 1503-1516 (2001); *Obtaining distribution functions for water from diffraction data*, F Bruni, M A Ricci, and A K Soper, in Conference Proceedings Vol 76, *Francesco Paolo Ricci: His Legacy and Future Perspectives of Neutron Scattering*, M Nardone and M A Ricci (Eds.) (Società Italiana di Fisica, Bologna, 2001)

[3] *Partial structure factors from disordered materials diffraction data: an approach using Empirical Potential Structure Refinement.* A K Soper, *Physical Review B*, **72**, 104204 (2005)