Poster Presentation

MS55.P02

Intermolecular interactions in molecular crystals and glasses

E. Beake[1], M. Dove[1], A. Phillips[1]
[1]*Queen Mary, University of London, School of Physics and Astronomy, London, UK*

The local structure of materials may not be apparent from Bragg crystallography, but emerges naturally from refinement against a pair distribution function (PDF). In molecular systems, the most prominent features in the PDF are the low-r peaks corresponding to the intramolecular interactions, yet these features are often the least interesting. The domination of the PDF by intramolecular interactions makes it difficult in the case of molecular materials to investigate the more interesting intermolecular interactions. In particular, few amorphous framework materials or molecular glasses have been characterized in any detail. Using reverse Monte Carlo (RMC) refinement against total neutron and x-ray scattering data we have studied the intermolecular interactions in two families of molecular materials, each including both crystalline and glassy phases. To overcome the problem posed by intramolecular interactions prior chemical knowledge of the molecular structure is incorporated into the refinement using empirical intramolecular potentials. One family consists of three phases of ZIF-4, a metal-organic framework consisting of tetrahedrally coordinated Zn2+ ions connected by imidazolate rings. In this material, we identify the molecular motion responsible for the greater flexibility shown by the amorphous phase compared to two crystalline phases [1]. The other family consists of the isomeric molecules para- and ortho-terphenyl (PTP/OTP). OTP is a paradigmatic glass-former, with a critical cooling rate of less than 0.1 K/min. PTP, on the other hand, is a crystalline material that undergoes an order-disorder phase transition at 178 K. We have characterized these materials' flexibility with the aid of molecular dynamics simulations. Our results demonstrate that RMC refinement with appropriate intramolecular potentials is capable of elucidating the intermolecular interactions of molecular systems, revealing new structural details in glassy and amorphous structures.

[1] E O R Beake, M T Dove, A E Phillips, et al. (2013) J. Phys.: Condens. Matter, 25, 395403

Keywords: Pair Distribution Function, Reverse Monte Carlo