Computing the Solid-state: Novel Plane-wave DFT Approaches to Hydrogen Bonding

Chick C Wilson[a], Derek S Middlemiss[a], Carole A Morrison[b], [a]*Department of Chemistry, University of Glasgow, Glasgow G12 8QQ.* [b]*School of Chemistry, University of Edinburgh, Edinburgh EH9 3JJ, UK.* E-mail: c.c.wilson@chem.gla.ac.uk

Hydrogen bonding is a critical link between crystallography and many physical, chemical and biological processes in condensed matter systems. Much of our recent work on hydrogen bonds has focused on multi-temperature and pressure X-ray and neutron diffraction, indicating often subtle behaviour of the hydrogen bonding present. Some of these effects challenge the limits of current experimental diffraction, and also our theories of hydrogen bond potentials.

As a complementary approach to this issue, we have been developing methods for studying hydrogen bonds in the solid state. These are based on the application of plane-wave (periodic) density functional theory calculations, which we have shown to be far superior in the study of a variety of hydrogen bonding systems. In addition we have developed advanced MD approaches to these calculations allowing us to examine computationally the temperature evolution of molecular structures in the solid state. This leads to a fuller understanding of the hydrogen bond potential and an improved description of structural evolution as observed in experiments.

These approaches will be illustrated by the results of a range of combined experimental and computational studies. Systems studied molecular complexes with short intermolecular hydrogen bonds, intramolecular hydrogen bonded structures, and dimeric systems containing subtle energy asymmetry leading to structural disorder.

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