Some New Applications for Plane−Wave DFT Calculation in Chemistry

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The overwhelming majority of work currently undertaken in quantum mechanical computational chemistry is based on codes that embrace the isolated molecule approach (i.e. Gaussian); that is, the system of interest is alone in an infinite, empty universe. Whilst this style of modelling is clearly relevant to the study of gas−phase systems, it is not nearly applicable to the condensed state. Many interesting questions on structure and bonding could be addressed if a computational approach capable of handling periodic systems were adopted. In our research group we have recently developed two new applications for plane−wave DFT for molecular systems: crystal structure disorder and intermolecular interactions (Hydrogen Bonding). This poster highlights results obtained for the second application from a study of ammonia crystal[1] and BH_3NH_3[2] crystal.

1: *Chem. Eur. J.* **2003**, *9, No. 3*, 628−634.
2: Manuscript in progress.