Poster

Parameterization of an intermolecular forcefield for halogen bonded molecular crystals

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Over the past two decades, there has been an increased interest in halogen-bonded molecular crystals due to their potential use in a variety of applications such as luminescent materials, magnetic materials, soft materials, and pharmaceutical solids [1]. The physicochemical properties of these solids are driven by their crystal packing. Understanding the packing of molecules within the crystal and the intermolecular interactions present within it can help in designing materials with specific properties. Theoretical modelling of these molecular solids allows for a better understanding of key material properties such as lattice energy,[2] polymorphism [3], solubility [4], and mechanical properties [5]. It can be performed both by employing periodic-DFT and force field methods. However, the cases where one has to deal with thousands of crystal structures, particularly during crystal structure prediction (CSP), due to high computational cost of the periodic DFT calculations, forcefield methods are generally preferred. The W99 potential developed by D.E. Williams is widely used in crystal structure prediction of organic molecular crystals containing elements down to the 3rd row of the Periodic table [6-7], with the latest modifications to improve the description of hydrogen bonding interactions [8]. The lattice energy calculations, however, become more challenging for structures, containing heavy elements, including those containing halogen bonding interactions.

In this presentation, the latest Williams forcefields (W99) will be reparametrized for the halogen atom, particularly iodine (I), being most prone to halogen bond formation. The parameterization will be performed against a set of 180 low temperature, high quality (low R-factor and disorder) crystal structures of halogen bonded binary cocrystals chosen from the crystallographic database. Additionally, the experimental sublimation data collected for some of these cocrystals will be used for this purpose. The re-parameterization of the repulsion-dispersion parameters will be carried out using the distributed multipoles obtained separately from the gas phase and the polarizable continuum model (PCM) model. Finally, the re-parameterized forcefields will be validated against a set of cocrystals by obtaining the standard deviation of cell parameters and halogen bond lengths upon lattice energy minimization.

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