Abstract

The melting point is one of the most fundamental and practically important properties of a compound. In addition, melting-related properties (e.g. solubility) are important in many fields of research. Although the melting point is the most commonly reported property of organic compounds and often the first property measured after a new compound is synthesized, it is one of the most difficult physical properties to predict (Lennard-Jones & Devonshire, 1939)(Luo, Strachan, & Swift, 2004). For this reason molecular simulation methods have been developed aiming towards accurate computation of melting points. Knowledge of the melting point before a compound has been synthesized could significantly accelerate the design of new materials. Theoretical predictions of the melting point have a long history, and have been based on a wide variety of calculation approaches. The molecular simulation methods developed for the computation of melting points achieve different levels of accuracy in their predictions. What they have in common is that generally most of them are not fully predictive, since they require experimental information on the most stable crystal structure that is adopted by the compound. An interesting and challenging task is the prediction of the melting point of a compound from first principles- given just the molecular diagram.

In this work, the idea of predicting the melting point of a given organic compound using as an input a computationally obtained crystal structure is investigated. To ensure reliable predictions, it is essential to develop an understanding of how the level of detail of the force fields in terms of crystal structure prediction (CSP) as well as in melting point prediction affects the accuracy of the calculations. To explore these requirements the proposed approach in this work combines the application of a CSP multistage methodology (Kazantsev, Karamertzanis, Adjiman, & Pantelides, 2011) developed by the Molecular Systems Engineering group at Imperial College and the freeze method (Ramrattan, 2014) which was recently developed in the group.

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