How Can We Use Intermolecular Interactions in Crystals? Lattice Energies, Predicting Crystal Growth and More…

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Accurate and fast models for intermolecular interactions provide quantitative insight into crystal packing, but their value can extend beyond neighbouring interactions into the prediction of lattice energies [1], and when combined with solvation models yield sensible estimates for solubilities for crystals in different solvents. We present both a new and improved CrystalExplorer interaction energy model [2,3], along with its application for predicting lattice energies, solubilities and the underlying thermodynamics guiding crystal growth from solution.

We also discuss state-of-the-art Density Functional Tight Binding methods like GFN2-xTB [4], general purpose force-field methods like GFN-FF, [5,6] and machine learning methods to compute intermolecular interactions, and how they might be used by theorists and experimentalists alike. Such energies may be visualised through energy frameworks [7], as in the attached image, which provide qualitative insight into the underlying energetic structure in crystals, and often correlate with the elastic and mechanical properties of molecular crystals.

References:

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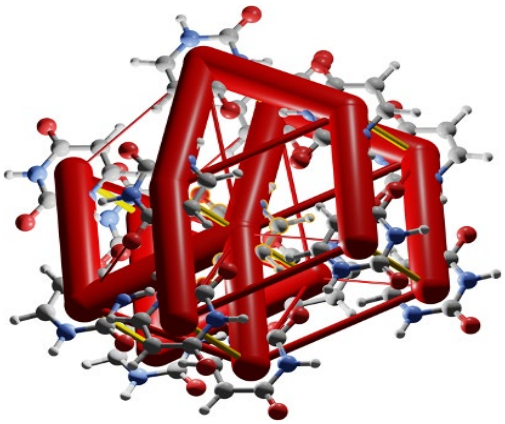

Figure 1