Poster Presentation

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Quantum mechanical synthon interaction energies

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The notion of a supramolecular synthons has dominated thinking in the field of crystal engineering for some time. However, there have been concerns expressed about whether the synthon concept is appropriate or even predictive.

In a recent paper [1] Turner et. al have presented a novel method for calculating molecular interaction energies, quickly and accurately, to within 2 kJ/mol relative to e.g. accurate basis set superposition error corrected CCSD values. By summing these interaction energies in shells, it is also possible to obtain lattice energies accurate to the best periodic DFT calculations.

Here we present an atom-atom breakdown of the demonstrably accurate interaction energies described by Turner et al [1]. This allows for the first time to quantitatively associate a quantum mechanical interaction energy with the concept of a synthon defined as a group of atoms.

We calculate and present interaction energies, and summary statistics (mean, standard deviation) associated with different synthons. We comment to what extent the results validate the supramolecular synthon concept. We describe strategies for finding synthons from the atom-atom energies without the preconceived notions of atom proximity.

[1] Turner M. J., Thomas S. P., Shi M. W., Jayatilaka D., Spackman M. A. (2015), Chem. Commun., 51, 3735

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