MS31-O3 Organic crystal polymorphism: A benchmark for dispersion corrected mean field electronic structure methods

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We analyze the energy landscape of the 6th crystal structure prediction blind test targets with various ab inito and semiempirical methodologies. A new benchmark set of 59 crystal structures (termed POLY59) for testing quantum chemical methods based on the blind test target crystals is presented.

We focus on different means to include London dispersion interactions within the density functional theory (DFT) framework. We show the impact of pair-wise dispersion corrections like the semi-empirical D2 scheme, the Tkatchenko-Scheffler TS method, and the density dependent dispersion correction dDsC.

Recent methodological progress includes higher order contributions in both the many-body and multipole sense. We use the D3 correction with Axilrod-Teller-Muto type three-body contribution, the many body dispersion MBD, and the nonlocal van der Waals density functional vdW-DF2. The density functionals with D3 and MBD correction provide an energy ranking of the blind test polymorphs in excellent agreement with the experimentally found structures. As computationally less demanding method, we test our recently presented minimal basis Hartree-Fock method (HF-3c) and a density functional tight binding Hamiltonian (DFTB). Considering the speed-up of three to four orders of magnitudes, the energy ranking provided by the low-cost methods is very reasonable. We compare the computed geometries with the corresponding X-ray data where TPSS-D3 performs best. The importance of zero-point vibrational energy and thermal effects on crystal densities is highlighted.

Related references:

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MS31-O4 Generation of crystal structure landscapes using known crystal structures

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We have developed an algorithm whereby a target molecule is shape matched to molecules in known crystal structures, which are then used as starting analogues for optimising putative crystal structures of the target molecule with a simple force field. Remarkably, this process generates the experimentally-observed crystal structure for over 90% of the molecules in a test set of around 300 $Z' = 1$ crystal structures of drug-like molecules. Many of the target molecules require fewer than 1000 analogues to generate the experimental crystal structure. While challenges remain for $Z' > 1$ structures, conformational flexibility and ranking, this procedure shows promise for fast crystal-structure landscape generation and should complement existing structural-informatics tools for assessing organic solid forms.

This presentation will discuss how over 800,000 known crystal structures in the Cambridge Structural Database (CSD) can be used to predict the crystal structures of unknown systems.

Keywords: Crystal structure prediction; shape searching; Cambridge Structural Database