Addressing density functional delocalization error in organic crystals

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An organic molecule can often adopt multiple different crystal packing motifs, or polymorphs, with significant impacts on the resulting physical properties. Our ability to predict organic crystal structures has improved tremendously in recent years, thanks in large part to dispersion-corrected planewave density functional theory (DFT). However, we have identified quite a few cases where delocalization error in commonly used generalized gradient approximation and hybrid functionals leads to substantial errors in the predicted crystal energy rankings. Examples ranging from pharmaceuticals to functional organic materials will be presented. The use of dispersion-corrected second-order Moller-Plesset perturbation theory models to correct the problem will be discussed.

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