

Using density functional theory to understand molecular solids - and vice versa

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Molecular crystals are crystalline solids composed of molecules bound together by relatively weak intermolecular interactions, typically consisting of van der Waals interactions and/or hydrogen bonds. Such crystals play an important role in many areas of science and engineering, ranging from biology and medicine to mechanics and electronics. Therefore, much effort has been dedicated to understanding their structure and properties.

Predicting the behavior of such solids from first principles is highly desired for understanding their unique properties and for allowing rational design of novel materials and structures. Preferably, we would like to obtain such understanding from density functional theory (DFT), because the relative computational simplicity afforded by DFT allows us to attack realistic, experimentally accessible problems. Unfortunately, despite many other successes, DFT has traditionally struggled with useful prediction of properties of crystals that contain weakly-bound units, as well as with electron and optical spectroscopy in general.

Here, I will show how the use of dispersion-corrected DFT and optimally-tuned screened range-separated hybrid functionals allows us to overcome these limitations, quantitatively, with a focus on predicting collective effects, i.e., phenomena that the individual units comprising the crystal do not exhibit, but arise through their interaction. Finally, I will show that lessons learned from molecular solids contribute to progress in DFT of general solids.