Low-cost computational models of emission processes in supramolecular crystals

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Computational studies of emissions in fully periodic crystal systems can be challenging without resorting to costly methodologies, which limits their use with the most popular, and fastest, levels of Density Functional Theory. This study seeks to explore a way to include cheap DFT-based schemes in models of emission processes in periodic supramolecular crystals, which could be especially fruitful if introduced into targeted automated computational searches.

To this aim, we present the results of using the DFT+U method to strategically localize excited electron energy levels on a targeted metal complex in the simulation cell. The tactic successfully characterizes the phosphorescence observed in two classes of supramolecular crystals when combined with the ΔSCF approach [1,2]. Furthermore, it is shown to successfully recover both a redshift and a blueshift in supramolecular crystals of structurally related Pt(II)-biaryl emitters.

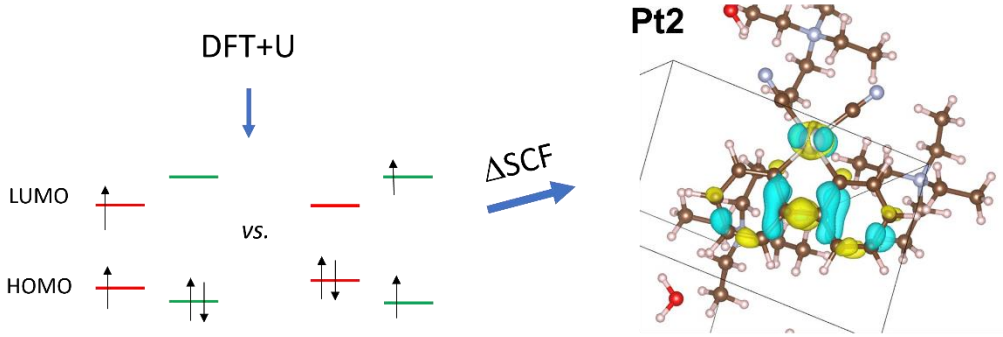

Figure 1: The differential electron density of a Pt(II)-biphenyl emission in its supramolecular crystal environment.

References

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