**Simulating Disorder in Organic LEDs using Large Scale Density Functional Theory**

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Organic semiconductors have favourable properties for use in devices such as organic light emitting diodes (OLEDs), including low cost and light weight. The current generation of OLEDs are based on molecules containing heavy metals, motivating the use of purely organic molecules exhibiting thermally activated delayed fluorescence (TADF) for efficient and environmentally-friendly devices. A key property for TADF is a small singlet-triplet splitting, which is influenced by both internal disorder and the surrounding environment. The computational design of new TADF-based emitters therefore requires a method which can calculate excited states of molecules in large enough systems to account for these effects, while also being able to handle the mixed local/charge transfer excitation character. This has motivated the development of a new method, named transition-based constrained DFT (T-CDFT), which has a computational cost similar to ground state calculations and is able treat both local excitations and charge transfer states. In this talk we will introduce T-CDFT, showing how its implementation in the linear-scaling BigDFT code provides a framework for including explicit environmental and statistical effects on excited state calculations of disordered supramolecular materials, including those used in TADF-based OLEDs.