Computational design of organic materials in optoelectronic applications

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Abstract:

Organic materials have been widely used in various optoelectronic applications, such as organic light-emitting diodes (OLEDs) and solar cells, owing to their low cost, flexibility and low-temperature and solution processability. In addition, the versatility of synthetic organic chemistry offers possibilities for tailoring organic materials for specific applications. In this context, computational modeling allows us to truly exploit the power of organic synthesis by providing us (i) low-cost and reliable prediction of target properties and (ii) better understanding of the structure-packing-property relationship (SPPR). In this talk, I will present how computations can help in accelerating the discovery pace of organic materials in three applications: (i) hole transport materials in perovskite solar cells, (ii) thermally activated delayed fluorescence (TADF) emitters for single-layer OLEDs, and (iii) non-fullerene acceptors for organic photovoltaics.