Merging Theoretical Spectroscopy & Computational Chemistry: Thermally Activated Delayed Fluorescence (TADF) as a new light-emitting mechanism for OLEDs

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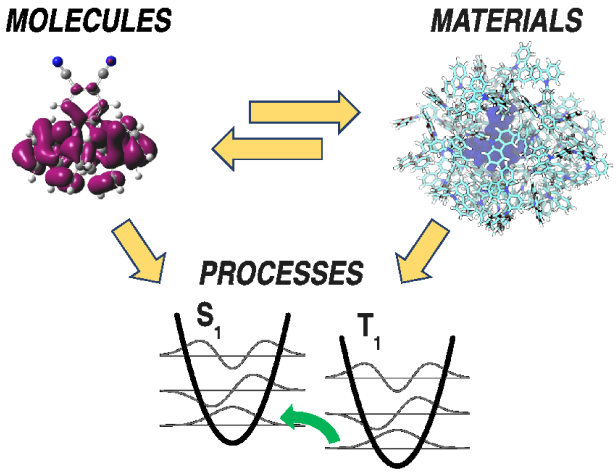
We present recent advances and investigations related with a new mechanism for light-emission in conjugated molecules, Thermally Activated Delayed Fluorescence (TADF), seeking to harvest both the singlet and triplet excitons generated under electrical excitation ideally achieveing a 100% of efficiency. The new strategy may fuel the use and manufacturing of 3rd generation OLEDs, although a complete understanding of the molecular mechanism is not fully uncovered yet. Therefore, we will review our recent efforts to address some challenging issues using quantum and atomistic models [1-6]. Among them, we will remark how the mixed nature of the excited-states involved (charge-transfer or locally-excited) ultimately control the singlet-triplet energy difference, and how this is a dynamic process mediated by conformational fluctuations and spin-orbit coupling.



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