Computational optical and X-ray spectroscopy studies for crystals & 2D materials

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I will present our recent computational spectroscopy studies for crystals and 2D materials. We simulated UV absorption, and vibrationally-resolved fluorescence and phosphorescence spectra for co-crystals of organic molecules[1] as well as metal-organic framework crystals to help elucidate the details of thermally-activated delayed fluorescence (TADF) photophysics. We simulated X-ray photoelectron (XPS) and absorption (XAS) spectra for crystals study the proton transfer reactions, and a series of carbon-based 2D materials, including graphene,[2] N-doped[3] and BN-codoped[4] graphene, graphdyine,[5] N-doped graphdyine,[6] and g-C_3N_4,[7] to understand effects of size, defect, doping, stacking. Calculations provide basic refence of representative local structures in such materials that can help clear assignments of experimental spectroscopies, and some general conclusions will be summarized.

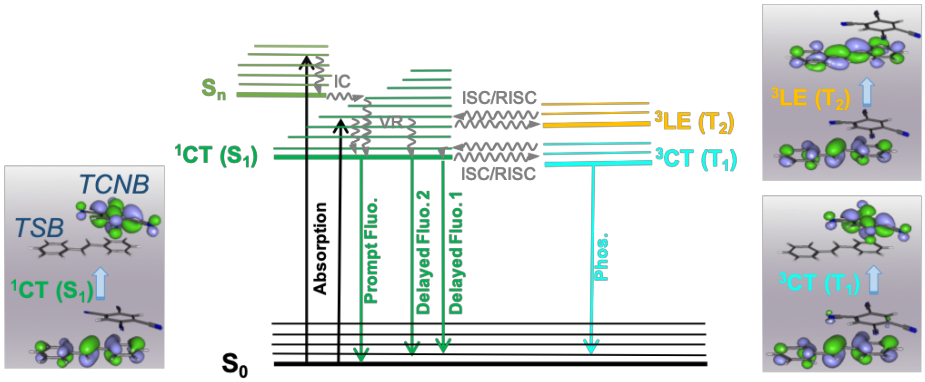

Figure 1: Jablonski diagram for the TSB-TCNB cocrystal. ISC/RISC via two channels S_1-T_1 and S_1-T_2 are responsible for the TADF. [1].

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