

Non-radiative decay paths in optoelectronic materials: A TDDFT and CASPT2 study

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In the framework of optoelectronics, non-radiative decay paths are relevant to interpret efficiency losses [1] or to help in the design of molecular rotors [2]. Here, the distyrylbenzene cyano functionalized family of molecules (DCS) are studied in attempts to interpret the distinct fluorescence quantum yields and to understand the non-radiative mechanisms in optoelectronics. Time dependent density functional theory (TDDFT) and the complete active space self-consistent field method (CASSCF) followed by the complete-active-space second-order perturbation theory (CASPT2), are used to determine the radiationless decay routes. The vertical absorption energy, in line with experiments, turns to be an important descriptor for the interpretation of the experimental quantum yields [3]. The region of the conical intersection (CI) further contributes to explain the distinct yields.

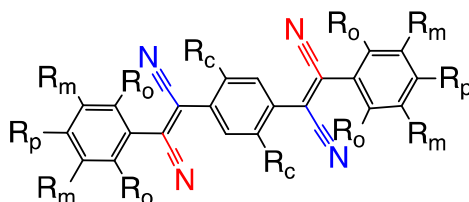


Figure 1. Chemical structure of α and β DCS molecules, where R_x represents a functional group substitution in the position o, m, p: orto, meta and para, respectively.

References

[1] *J. Phys. Chem. C* 119, 2249 (2015).

[2] *Phys. Chem. Chem. Phys.* 18(48), 32786 (2016).

[3] *J. Phys. Chem. C* 121, 23166 (2017).