

Theoretical studies on fluorescence properties of 5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine

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1,3,4-thiadiazole derivatives have been shown to reveal a broad spectrum of biological activities such as antitumor, antibacterial and antifungal, along with numerous interesting spectroscopic, crystallographic and biophysical properties [1]. One of their commonly observed feature is a dual fluorescence emission, usually explained in literature by coexistence of multiple emissive states with different electronic and/or molecular structures associated with e.g. excited-state intramolecular proton transfer (ESIPT) or by aggregation effects related to the formation of excimer systems and aggregation-induced emission (AIE) or aggregation-induced emission enhancement (AIEE).

In this contribution, results of (time-dependent) density functional theory ((TD)DFT) calculations are presented aiming at providing a conclusive assignment of dual fluorescence signal that has been recently demonstrated experimentally for 5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine in foil, gel, and in isopropanol solution upon increasing sample concentration. The (TD)DFT studies included both monomeric and aggregated models built based on the motifs found in the X-ray crystal structure of the compound (Fig. 1), and their computed photophysical properties clearly confirm AIE-origin of the dual emission feature.

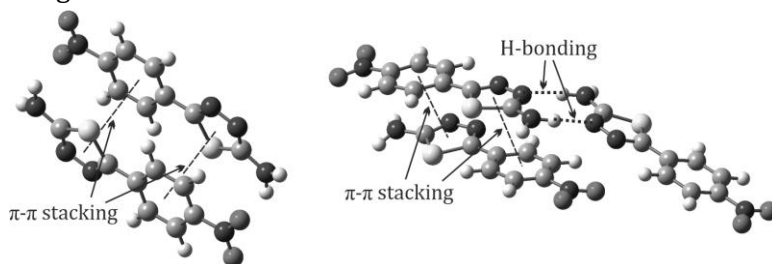


Fig. 1. Selected DFT-optimized dimer and trimer forms of 5-(4-nitrophenyl)-1,3,4-thiadiazol-2-amine.

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[1] Hu Y., Li C.-Y, Wang X.-M., Yang Y.-H. and Zhu H.-L. (2014) Chem. Rev., 114, 5572–5610.

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