Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Toward the Design of Alkynylimidazole Fluorophores: Computational and Experimental Characterization of Spectroscopic Features in Solution and in PMMA

Supporting information

Vincenzo Barone[a], Fabio Bellina[b], , Malgorzata Biczysko[c*], Julien Bloino[c], Teresa Fornaro[a], Camille Latouche[a], Marco Lessi[b], Giulia Marianetti[a,b], Pierpaolo Minei[a,b], Alessandro Panattoni[a], AndreaPucci[b]

[a] Scuola Normale Superiore, piazza dei Cavalieri 7, I-56126 Pisa, Italy

[b] Dipartimento di Chimica e Chimica Industriale, Universit di Pisa, via Moruzzi 13, I-56124 Pisa, Italy

[c] Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), UOS di Pisa, Area della Ricerca CNR, Via G. Moruzzi 1, I-56124 Pisa, Italy;

*e-mail: malgorzata.biczysko@pi.iccom.cnr.it

1. **Atomic charges from natural bond orbital analysis for the 1b and 2b chromophores**

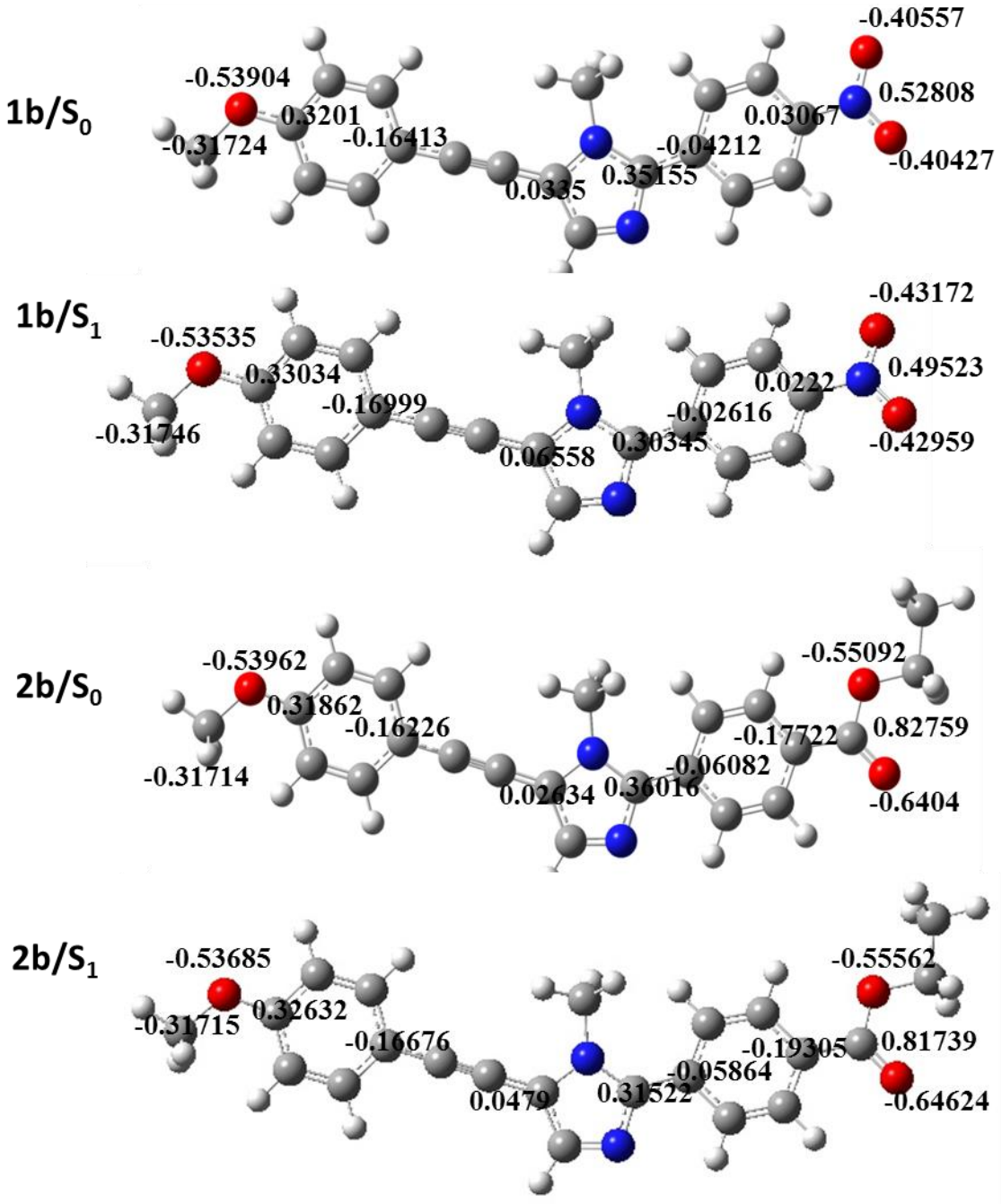

Figure S1. Selected atomic charges from natural bond orbital analysis for the 1b and 2b chromophores. Values computed at CAM-B3LYP/SNSD/PCM(THF) and TD-CAM-B3LYP/SNSD/PCM(THF) levels of theory for the ground and excited states, respectively.

2. Typical responsivity curve of photodiods

The Thorlabs FDS1010 photodiode is ideal for measuring both pulsed and CW light sources, by converting the optical power to an electrical current. The Si detector is mounted on a 0.45”x0.52” ceramic wafer package with an anode and cathode. The photodiode anode produces a current, which is a function of the incident light power and the wavelength (Figure S1)

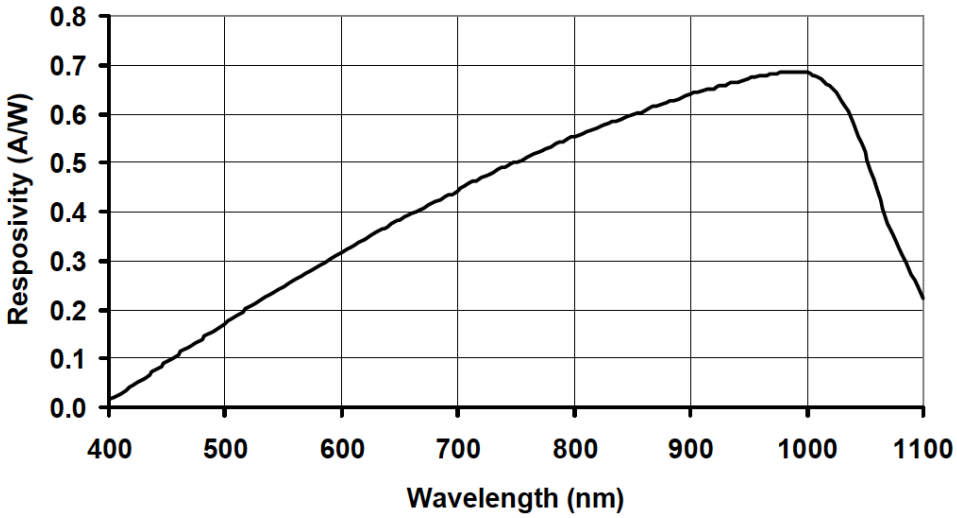

Figure S2. Typical Responsivity curve using Thorlabs calibration services