Photophysical properties of a dual emitter: a TD-DFT study

Romain Paulino Neto\textsuperscript{*†}, Gilles Lemercier\textsuperscript{2}, and Ilaria Ciofini\textsuperscript{1}

\textsuperscript{1}Institut de Recherche de Chimie Paris (IRCP) – Ecole Nationale Supérieure de Chimie de Paris – ENSCP 11, rue Pierre et Marie Curie 75005 PARIS, France
\textsuperscript{2}Institut de Chimie Moléculaire de Reims (ICMR) – Université de Reims - Champagne Ardenne, CNRS : UMR7312 – UFR Sciences, BP1039, 51687 Reims Cedex 2, France

RÉSUMÉ

Optical properties of 5-(4-dimethylaminophenylethynyl)-1,10-phenanthroline (Phen-PENMe\textsubscript{2})\textsuperscript{[1]} in aprotic solvents were studied. Phen-PENMe\textsubscript{2} displays a dual emission, which is stemming from the presence of two distinct emissive excited states: an intramolecular charge-transfer (ICT) state and a locally excited (LE) state. The dual emission of Phen-PENMe\textsubscript{2} was studied using a combined experimental and theoretical approach. TD-DFT calculations were performed to give more insights to the optical behavior of the compound, linking the two excited states to two different conformations of the molecule. In view of the experimental and theoretical results, the Phen-PENMe\textsubscript{2} compound can be seen as a potential local ratio-metric probe for medium polarity.

Guérin, J.; Aronica, C.; Boeuf, G.; Chauvin, J.; Moreau, J.; Lemercier, G.; J. Lumin. 2011, 131, 2668

MOTS-CLÉS: DFT, TD, DFT, emission, absorption

\textsuperscript{*}Intervenant

\textsuperscript{†}Auteur correspondant: romain.paulino.neto@etu.upmc.fr