#ICMolTalks

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Abstract

AB INITIO MODELLING OF PHOTOLUMINESCENCE

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In this contribution I present computational protocols to model photoluminescence in molecular systems which go beyond the nowadays routine modelling of emission energies. Our protocols merge state-of-the-art quantum chemical calculations, excited state decay rate theories (i.e., Fermi-golden rule based)[1] along with semi-classical nonadiabatic excited state dynamics to enable the quantitative determination of fluorescence lifetimes and quantum yields. In particular, I present an extensive analysis of the parameters influencing the excited state decay rate calculations.[2] Further, protocols to model anti-Kasha fluorescence in molecular systems (i.e., fluorescence from higher-lying excited states),[3] to model complex excited state dynamics in thermally activated delayed fluorescence (TADF) materials,[4] and the first attempts to capturing fluorescence events in molecular systems within a semi-classical NonAdiabatic Molecular Dynamics framework,[5] are presented. Finally, I present our recent efforts to expand our protocols from molecular systems to the solid state. In particular I present protocols allowing modeling the photophysical properties of organic molecular crystals. The objective is to evaluate the effect of various sources of disorder resulting in the shape and broadening of UV-vis spectra.[6] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photophysics and photochemistry at the first principles level.

References

[1] Z. Shuai, Q. Peng, Phys. Rep., 537, 123 (2014).

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[3] K. Veys, D. Escudero, Acc. Chem. Res., 55, 2698 (2022).

[4] a) M. T. do Casal, Y. Badawy, D. Escudero, J. Phys. Chem. C, 128, 18170 (2024); b) Y. He, D. Escudero, https://doi.org/10.48550/arXiv.2508.16436 (2025)

[5] M. Pérez-Escribano, J. Jankowska, G. Granucci, D. Escudero, J. Chem. Phys., 158, 124104 (2023)

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Biography

Prof. Escudero is currently Associate BOFZAP Professor in the Department of Chemistry, at the KU Leuven and he leads the “Computational Photochemistry” Lab (https://chem.kuleuven.be/en/research/qcpc/cpc). Born in 1984 in Palma de Mallorca, he graduated in Chemistry at the Universitat de les Illes Balears, Spain, and obtained his PhD with honors in Chemistry at the Friedrich-Schiller-Universität Jena, Germany, in 2011. Following his PhD, he spent three years (2011-2014) at the Max-Planck Institut für Kohlenforschung, Germany and four years (2014-2018) at the Université de Nantes as a postdoctoral researcher. In his research group they work at the interface between photochemistry and theoretical chemistry. Their research comprises both methodological developments and fundamental theoretical investigations; and their applications in the field of molecular light-to-energy conversions. He has published more than 115 publications, with more than 5000 citations and a h-index of 40. He is ranked among the 2% top researchers in several chemical-related fields in the standardized citation metrics author database (DOI: 10.17632/btchxktzyw.3), and he serves since 2024 as an Associate Editor of the Dyes&Pigments journal.