Nonadiabatic Dynamics Simulations of Organic Materials with Optical Activity

Mario Barbatti

Aix Marseille Univ, CNRS, ICR, Marseille – France
mario.barbatti@univ-amu.fr - *www.barbatti.org*

Organic materials with optical activity (OMOA) are cutting-edge components of advanced electronic and photonic applications. Diversity, plasticity, and low cost make them ideal for a variety of devices, from solar cells, through sensors, to information storage and display.

Photo-electronic processes in OMOA are highly complex, and nonadiabatic dynamics simulations may help by providing insights into physical-chemical phenomena, revealing new reaction pathways, and aiding to deconvolute time-resolved spectroscopic data. The use of nonadiabatic dynamics in this field faces, however, different challenges, including the development of new functionalities, reliable research protocols, efficient computational methods, and better integration with experimental analysis.

In this talk, I will discuss recent investigations by our group on nonadiabatic dynamics of OMOA, dealing with triplet fusion and charge/energy transfer in internal conversion [1,2]. I will also present recent methodological advances we have implemented within the Newton-X platform (www.newtonx.org) for computation of reaction rates [3], spectra [4], couplings [5], and dynamics [6]. Finally, I will deliver a critical appraisal of the status of the field, focused on computational costs and accuracy of the simulations.

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