Kolokvij Zavoda za teorijsku fiziku i Zavoda za fizičku kemiju

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RBI Ivan Supek Wing Lecture Hall
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Resonant-energy transfer in real time

Intramolecular charge transfer (CT) is the key phenomenon in a variety of dyes that find use in OLED, organic solar cells and whose large nonlinear optical responses are exploited in bioimaging, nanofabrication, etc. The large nonlinearity of the responses of these materials shows up with a large and nontrivial sensitivity to the local environment. The relevant physics of CT dyes is well captured by so-called essential state models that quantitatively reproduce their steady-state and time-resolved linear and non-linear optical, accounting for vibrational coupling and polar solvation and its dynamics [1,2]. Intermolecular interactions can also quite naturally be accounted for in essential state models to address energy transfer phenomena [3] and excitonic effects in molecular aggregates [4].
Recently, essential state model have been applied to define a dynamical, non-adiabatic model for Resonance Energy Transfer (RET) [5]. Specifically, we consider two dyes, an energy donor (D) and an energy acceptor (A). Each dye corresponds to a push-pull chromophore, described in terms of two
electronic states coupled to a single effective vibration. Accounting for dissipation phenomena within the Redfield approach, we follow the real time dynamics of RET from the excited D towards A. Moreover, a newly derived multistate Redfield-Smoluchowski equation is used to investigate how the dynamical disorder, induced by polar solvation, affects RET.

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[2]S. A. Kurhuzenkau, et al. Phys.Chem.Chem.Phys., 2016, 18, 12839, and references therein.
[3] C. Sissa, et al. Phys. Chem. Chem. Phys., 2011, 13, 12734–12744
[4] S. Sanyal, et al. Phys.Chem.Chem.Phys., 2017, 19, 24979
[5] F. Di Maiolo, A. Painelli, J. Chem. Theory Comput. 2018, 14, 5339−5349