

**DISIT**

DIPARTIMENTO DI SCIENZE E INNOVAZIONE TECNOLOGICA

SEMINARI RICERCA E FORMAZIONE

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Docenti, Assegnisti, Dottorandi,
Borsisti, StudentiSEMINARIO/CORSO IN LINGUA:
Inglese

Modelling the interplay between structure and energy transfer in biosystems

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Modelling the interplay between electronic energy transfer and structure in biosystems is a considerable challenge due to the multiple space and time scales involved in the process.[1] Depending on the specific case under study, different protocols can be adopted often combining classical simulations with multiscale quantum/classical methods. In this contribution we will overview two challenging cases, the modelling of light harvesting and energy transfer in cryptophyte pigment-protein photosynthetic complexes, and the simulation of Förster resonance energy transfer (FRET) experiments on the partially disordered protein calmodulin.

First, we investigate how protein thermal fluctuations tune exciton states in the phycocyanin PC645 and PC612 antenna complexes of cryptophytes.[2] We adopt a dual molecular dynamics (MD) strategy that combines classical and quantum/classical Born-Oppenheimer simulations, and show that, whereas thermal effects have a small impact on the energy ladder in PC612, they are key to describe the properties of PC645, due to the absence of a hydrogen bond controlling the twist of ring D in PCB β 82 bilins.

Second, we investigate how structure determines the FRET properties of the partially disordered protein calmodulin, with a particular focus on the impact of Förster approximations regarding dielectric screening effects.[3] To characterize the conformational ensemble, we combine extended MD simulations in the microsecond timescale with a rigorous theoretical framework beyond Förster dipole approximation based on electrostatic potential-fitted transition charges coupled to an atomistic polarizable classical environment.[4] Our results indicate that screening effects depend on donor-acceptor separation and solvent exposure, significantly biasing the characterization of the balance between compact and extended conformations in disordered ensembles.

- [1] Cupellini, L. et al.: 'Electronic energy transfer in biomacromolecules' *WIREs Comput. Mol. Sci.* 2019, 9, e1392
[2] Ozaydin, B., Curutchet, C.: 'Unraveling the role of thermal fluctuations on the exciton structure of the cryptophyte PC612 and PC645 photosynthetic antenna complexes' *Front. Mol. Biosci.* 2023, 10, 1268278
[3] Gonzalo, D. et al.: 'On the breakdown of Förster energy transfer theory due to solvent effects: atomistic simulations unveil distance-dependent dielectric screening in calmodulin' *Chem. Sci.* 2025, 16, 3693
[4] Cignoni, E. et al.: 'A fast method for electronic couplings in embedded multichromophoric systems' *J. Phys. Condens. Matter* 2022, 34, 304004

