FACOLTÀ DI SCIENZE MATEMATICHE, FISICHE E NATURALI
DIPARTIMENTO DI MATEMATICA E FISICA "NICCOLÒ TARTAGLIA"

ULTRAFAST ELECTRONIC AND NUCLEAR DYNAMICS IN PHOTOVOLTAIC MATERIALS

Introduce: Stefania PAGLIARA, Università Cattolica del Sacro Cuore

Interviene: Dr. Carlo Andrea ROZZI, CNR - Istituto Nanoscienze, Modena, Italia

Abstract:
I will report on recent studies of sub-ps dynamics of photoinduced charge separation in several prototypical photovoltaic materials. The simulations, performed by combining Time-dependent Density-Functional Theory and Ehrenfest molecular dynamics were validated against high time resolution pump-probe spectroscopy and ultrafast electron diffraction. I will discuss the role of the coherent coupling between electronic and nuclear degrees of freedom in triggering charge delocalization and charge transfer both for covalently bonded molecules, non-bonded bulk heterojunctions, polymer-copolymer aggregates and Methylammonium Lead Iodide perovskites. I will further discuss the possible exploitation of our findings in order to design and synthesize novel molecular scaffolds for photovoltaic applications.

Webinar

Venerdì 22 gennaio 2021, ore 11.00

Clicca qui per partecipare su Microsoft Teams

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