Università degli Studi di Padova

DiSC

Giovedì **13 Novembre 2025** alle ore **14:00** presso l'aula L2

il **Dr. Marco Romanelli**

Institute of Theoretical Chemistry, Faculty of Chemistry,
University of Vienna, Austria

terrà il seminario dal titolo:

Modelling light-induced dynamics in periodic systems: a SHARC-VASP surface hopping interface.

Light-induced excited-state dynamics in molecules and materials comprises a broad range of distinct relevant phenomena, ranging from charge-carrier transfer and recombination in photovoltaic systems down to molecular photochemistry. Accurate modelling of such processes is still to date a challenging task even for standalone molecules, making it even more arduous when extended heterogeneous systems are targeted for photocatalytic applications. In this framework, Tully's surface hopping[1,2] is one of the simplest-yet-successful approaches that have been historically used to model excited-state dynamics in molecular systems. Nevertheless, its application to extended periodic materials is far less explored, mostly due to the intrinsic difficulty of properly describing excited states of matter in the solid state. In this talk, after giving an overview of such method and its state-of-the-art applications to deal with solid-state systems [3–5], I will discuss our current progress and outlook for setting up an appropriate modelling framework to investigate light-induced processes in periodic materials. Our approach practically builds on interfacing the SHARC code[6], originally designed for excited-state molecular dynamics, with the Vienna Ab Initio Simulation Package[7] (VASP) for simulating periodic materials within a Density Functional theory framework.

(1) Tully, J. C.; Pkeston, R. K. *J Chem Phys* 1971, *55* (2), 562–572.
(2)Tully, J. C.. *J Chem Phys* 1990, *93* (2), 1061–
(3)Smith, B.; Akimov, A. V. *Journal of Physics: Condensed Matter* 2020, *32* (7), 073001.
(4)Prezhdo, O. V. *Acc Chem Res* 2021, *54* (23), 4239–4249.
(5)Akimov, A. V.; Prezhdo, O. V. *J Chem Theory Comput* 2013, *9* (11), 4959–4972.
(6)Mai, S.; Marquetand, P.; González, L. *WIREs Computational Molecular Science* 2018, *8* (6), e1370.
(7)Kresse, G.; Furthmüller, J. *Phys Rev B* 1996, *54* (16), 11169–11186.

La presenza della S. V. sarà molto gradita

Il Direttore del Dipartimento
Stefano Mammi

Stefano Corni