



UNIVERSITÀ DEGLI STUDI DI MILANO

SEMINARI CHIMICI

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Aula G30, Nuovo Settore Didattico via Golgi

Oratore

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Titolo

Quantum dynamics of ultrafast photochemical processes: from conjugated molecules to semiconducting polymers

Coordinatore

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Non-adiabatic phenomena at avoided crossings and conical intersections are the landmark of photochemical and reactive processes in electronically excited molecular systems. Given that the characteristic time scale of these processes is often ultrafast (i.e., femtoseconds to picoseconds) and quantum coherence plays a prominent role, a quantum mechanical treatment of the nuclear dynamics is generally required. In this talk, we focus on photochemical phenomena in many dimensions, which can be tackled by efficient multiconfigurational techniques in conjunction with recently developed effective-mode models. Examples range from excited-state processes in polyatomic molecules to the photophysics of extended systems like semiconducting polymers. In this latter example, we present a fully quantum analysis of ultrafast exciton dissociation at so-called polymer heterojunctions, using a model Hamiltonian parametrized for three electronic states and 25-30 phonon modes. To conclude, a perspective is given on the development of new hybrid techniques which are tailored to high-dimensional systems and generalized system-bath dynamics.