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Excited state dynamics in nanoscale materials: time-domain ab initio studies

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Photo-induced processes at interfaces are key to photovoltaic and photo-catalytic applications. They require understanding of dynamical response of novel materials on atomic and nanometer scales. Our non-adiabatic molecular dynamics techniques, implemented within time-dependent density functional theory, allow us to model such non-equilibrium response in real time. The talk will focus on photo-initiated charge and energy transfer in several classes of nanoscale materials. Examples include semiconductor surfaces sensitized with organic molecules, water, semiconductor quantum dots, graphene and perovskites, carbon nanotube bundles, mixtures of C60 with inorganic particles, etc. Photo-induced charge separation and recombination across such interfaces creates many challenges due to stark differences between molecular and periodic, and organic and inorganic systems. Our simulations provide a unifying description of quantum dynamics on nanoscale, characterize the rates and branching ratios of competing processes, resolve debated issues, and generate theoretical guidelines for development of novel systems for solar energy harvesting, electronics and other applications.