Ab Initio Quantum Dynamics in Nanoscale Materials

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Excited state dynamics play key roles in numerous novel nanoscale, condensed matter and materials designed for energy, optoelectronics and other applications. Controlling these far-from-equilibrium processes and steering them in desired directions require understanding of material's dynamical response on the nanometer scale and with fine time resolution. We couple real-time time-dependent density functional theory for the evolution of electrons with non-adiabatic molecular dynamics for atomic motions to model such non-equilibrium response in the time-domain and at the atomistic level. The talk will describe the basics of the simulation methodology [1-3] and will discuss several exciting applications [??] among the broad variety of systems and processes studied in our group, including metal halide perovskites, transition metal dichalcogenides, plasmonic systems, quantum dots, molecular crystals, etc. Photo-induced charge and energy transfer, Auger-type processes, energy losses and charge recombination create many challenges due to large differences between molecular and periodic, and organic and inorganic matter. Our simulations provide a unifying description of quantum dynamics on the nanoscale, characterize the timescales and branching ratios of competing processes, resolve debated issues, and generate theoretical guidelines for development of novel systems.

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