BESH2022 Hybrid Perovskites and Non-Adiabatic Dynamics Simulations: Catching Realistic Aspects of the Charge Recombination Process

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Abstract

Dissipation of photon energy to heat and recombination of photogenerated charge carriers are among the main factors limiting the efficiency of solar-light harvesting devices. At the same time, the dynamics of excited electrons and holes depends critically on the microscopic structure of a material, including dopants, defects, grain boundaries, crystallinity and electric order. We summarize recent findings and suggest directions for improvement of hybrid organic-inorganic perovskite materials, established by means of non-adiabatic molecular dynamics (NAMD) simulations. Combined with real-time, time-dependent density functional theory, NAMD provides an ab initio description of the photo-initiated processes, including realistic aspects of material's structure and giving unique atomistic insights into the photo-active material properties.