Hot carriers Relaxation Dynamics in Perovskite Materials

Mohamed E. Madjet

Max Planck Institute for the Physics of Complex Systems

01187 Dresden

Hybrid organic-inorganic perovskites, such as methylammonium lead iodide CH3NH3PbI3, are attracting great attention as promising new absorber materials for solar power generation. Recently, perovskite-based solar cells reported a conversion efficiency of more than 25%. However, many fundamental processes related to the photophysical properties of these materials remain not fully understood. The excitation of electrons from the valence band to conduction band results in the formation of hot carriers. Right after this photoexcitation an ultrafast thermalization of the hot electron and holes takes place driven by the non-adiabatic electron-phonon interactions. Harvesting the energy of hot carriers before it is converted into heat would enhance the power conversion efficiency. Finding ways to increase the carrier lifetime would provide a path to control the relaxation dynamics, which would be favorable for photovoltaic applications.

Using a mixed quantum-classical approach based on trajectory surface hopping and combined with time dependent method, the dynamics of the generated hot carrier is investigated.

Details about the methods used will be described and the results will be shown for different perovskite materials depending on their structures and compositions.

Using nonadiabatic molecular dynamics simulations (NAMD), we will also show results on photo-induced electron dynamics and charge transfer process in a molecular system (Mg@C60) and at molecule-slab interface (HTM-perovskite slab).
The namd method can be applied to any molecular or bulk system to describe electron dynamics and charge transfer processes.

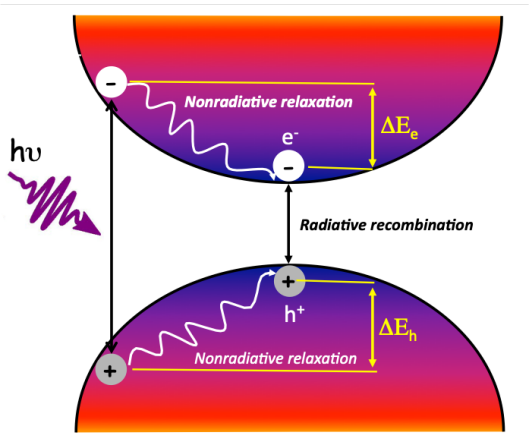

Fig. Schematic diagram representing hot carrier relaxation dynamics.