Molecular and electron dynamics of perovskites for PV applications

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The conversion of solar energy into electricity is a common theme among researchers in several scientific fields. Recently, attention has been turned to the use of lead-halide organic-inorganic perovskite materials, which provide a high efficiency among photovoltaic (PV) cells. For my new research direction, I will be focusing on the computational analysis of photo-induced processes in perovskite materials. Organic-inorganic perovskites exhibit properties of both ionic liquids and solid semiconductors, thus demonstrating intriguing and unusual properties, but, the connection between structure and property are not well understood. Computational modeling of electronic structure and dynamics in organic-inorganic lead halide perovskites will provide insight into this problem.

Ab initio molecular dynamics (AIMD) calculations will aid in examination of the methylammonium ion that exists within the perovskite cage. This is a freely-rotating ion that can be easily polarized. It has been postulated that this methylammonium cation is likely responsible for charge separation and reduces carrier recombination, which can be calculated, starting with on-the-fly non-adiabatic couplings. Additional observables that can be calculated and compared to experiment are absorption and Raman spectra. Optoelectronic spectral properties can be evaluated in the excited state as well.

In addition to an examination of how electrons behave internally, photo-induced dynamics at an interface is equally important, as PV cells contain several useful interfaces. Charge transfer dynamics at interfaces could be mapped with relation to spatial position. Structures of perovskite materials could then be modified according to results and improved with relatively little cost, compared to experimental approaches requiring expensive instrumentation and materials.