Abstract Submitted
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Ab initio modeling of the optical properties in organometallic halide perovskites for photovoltaic applications[1] AMANDA NEUKIRCH, WANYI NEI, Los Alamos National Laboratory, LAURENT PEDESSEAU, JACKY EVEN, Universite Europeennne de Bretagne, CLAUDINE KATAN, CNRS, Institut des Sciences Chimiques de Rennes, ADITYA MOHITE, SEGREI TRETIAK, Los Alamos National Laboratory — The need for an inexpensive, clean, and plentiful source of energy has generated large amounts of research in an assortment of solution processed organic and hybrid organic-inorganic solar cells. A relative newcomer to the field of solution processed photovoltaics is the lead halide perovskite solar cell. In the past 5 years, the efficiencies of devices made from this material have increased from 3.5% to nearly 20%. Despite the rapid development of organic-inorganic perovskite solar cells, a thorough understanding of the fundamental photophysical processes driving the high performance of these devices is not well understood. I am using state-of-the-art ab initio computational techniques in order to characterize the properties at the interface of perovskite devices in order to aide in materials design and device engineering. I will present an in-depth analysis of the electronic and optical properties of bulk and surface states of pure and mixed halide systems. The high-level static quantum mechanical calculations, including spin-orbit-coupling and the many body GW approach, identify the key electronic states involved in photoinduced dynamics. This knowledge provides important information on how the optical properties change with variations to the system.

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