Influence of organic molecules on the performance of hybrid perovskites for solar energy harvesting

Dhara J. Trivedi

Department of Physics, Clarkson University

Perovskites are unmatched in their ability to realize finely tunable optoelectronic properties through simple changes such as cation substitution, pressure modification, variable layered arrangements, and dimensionality induced confinement effects associated with an electronic decoupling of adjacent inorganic layers. This flexibility has led to their successful application as efficient light emitters, photodetectors, and hybrid photovoltaic (PV) and thermoelectric (TE) materials. Recent studies have pointed towards an underestimation of the impact both organic A-site cations and spacer molecules may have on the electronic structure of the host perovskite. The atomistic description obtained using ab initio electronic structure calculations provides a unique and comprehensive understanding of the influence of these molecules on the performance of the perovskite-based photovoltaics. This talk will highlight some of our recent work geared towards understanding the influence of organic molecules on the efficiency of perovskites as a hybrid PV-TE material for perovskite-based solar energy-harvesting device.