Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Nanoscale charge localization induced by random orientations of organic molecules in hybrid perovskite CH3NH3PbI3 JIE MA, LIN-WANG WANG, Lawrence Berkeley National Lab — Perovskite-based solar cells have achieved high solar-energy conversion efficiencies and attracted wide attentions nowadays. Despite the rapid progress in solar-cell devices, many fundamental issues of the hybrid perovskites have not been fully understood. Experimentally, it is well known that in CH3NH3PbI3, the organic molecules CH3NH3 are randomly orientated at the room temperature, but the impact of the random molecular orientation has not been investigated. Using linear-scaling *ab-initio* methods, we have calculated the electronic structures of the tetragonal phase of CH3NH3PbI3 with randomly orientated organic molecules in large supercells up to $\sim$ 20,000 atoms. Due to the dipole moment of the organic molecule, the random orientation creates a novel system with long-range potential fluctuations unlike alloys or other conventional disordered systems. We find that the charge densities of the conduction-band minimum and the valence-band maximum are localized separately in nanoscales due to the potential fluctuations. The charge localization causes electron-hole separation and reduces carrier recombination rates, which may contribute to the long carrier lifetime observed in experiments. We have also proposed a model to explain the charge localization.

Jie Ma
Lawrence Berkeley National Lab

Date submitted: 13 Nov 2014 Electronic form version 1.4