

Investigation of Ion Migration in Methyl ammonium Lead Iodide Perovskites by Molecular Dynamics.

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Abstract

Studies on perovskites have shown an upward trend over the past decade due to the encouraging power conversion efficiency of more than 23.3% that has been achieved in perovskites solar cells. Large scale commercialization of Methyl Ammonium Lead Iodide (MAPbI₃) perovskite can be realized if its stability is improved and current – voltage hysteresis is mitigated. From the recent literature, it is obvious that researchers have different views concerning the origin of hysteresis ranging from migration of mobile MA⁺ ions, iodide ions and the formation of iodide Frenkel defects. For example, some scientists recently found that doping the MAPbI₃ perovskite with potassium iodide (KI) eliminates the hysteresis since the K⁺ ions energetically prefer and occupy the interstitial sites thus, preventing the iodide ions from forming Frenkel defects by migrating to occupy the interstitials. This study is centered on investigating ion migration by molecular dynamics in which the diffusion coefficients of migrating species is determined in order to establish whether hysteresis is caused by iodide Frankel defects, iodine migration, MA⁺ migration or migration of other species in MAPbI₃. The Large-scale Atomic Molecular Massively Parallel Simulator (LAMMPS) program is being used for Molecular Dynamics simulation and the diffusion coefficients of the different species are determined from the slopes of the mean squared displacement (MSD) as a function of time. The work is in the exploratory stages and we will only present some preliminary results.