Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A1]Poster Session 1

Symposium A

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-03]Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations

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Hybrid organic/inorganic perovskites(HOIPs) have drawn significant research interests due to the incomparable rapid rise in energy conversion efficiency seen in photovoltaic devices based on $CH_3NH_3PbI_3$. Current research attempts in this field have concentrated on searching for similar perovskites with better properties, especially stability under a humid condition and/or irradiation [1]. In this work, employing first-principles calculations based on the density functional theory, we have investigated effects of vacancy on the optimized structures, bandgap, total and partial density of state, effective on-site and bond charge, by comparing with relevant experimental and/or theoretical data [2]. These analyses reveal that a Pb vacancy induces an asymmetric distortion of the lattice, which leads to a local volume expansion at low temperature [3]. The degenerate states at the conduction band minimum(CMB) are split each other due to the defect and it promotes broadening of the light absorption spectra. Possible effects of interstitial impurity, such as a water molecule, will also discussed in the presentation.

[1] A. K. Chauhan and P. Kumar, J. Phys. D: Appl. Phys. 50 (2017) 325105.
[2] Y. Wang et al., Phys. Chem. Chem. Phys. 16 (2014)1424.
[3] A. Walsh et al., Angewandte Chemie 2 (2015) 1791.