Ab-initio screening of 3D lead-free hybrid perovskite materials and luminescence recovery of $CH_3NH_3PbBr_3$ by H_2O and O_2 gas

Xiaoyang Che,[1,2] Hong-Hua Fang[3], Maria Antonietta Loi[3], Claudine Katan[1], Mikaël Kepenekian[1], Jacky Even[2]

[1]*ISCR, Université de Rennes 1, CNRS, Rennes, 35042, France.*

[2]*FOTTON, INSA, CNRS, Rennes 35042, France.*

[3] *ZIAM, University of Groningen, Groningen, 9747 AG, The Netherlands.*

E-mail: xiaoyang.che.1@univ-rennes1.fr

The recent revolutionary increase of power conversion efficiency of perovskite-based solar has motivated a growing number of experimental and theoretical studies on 3-dimensional hybrid halide perovskite lights absorbers such us $CH_3NH_3PbI_3$. Nevertheless, there remains toxicity arising from lead and solving instability issues from industrial perspective. In this work, a computational screening of the lead-free materials has been performed.[1] We have investigated the geometrical an electronic structures of different ABX_3 structures(A^+=organic cations, B^{2+} = metallic cations, X^-=halide anion) in orthorhombic *Pnma* phase by means of the ab-initio calculations based on Density Functional Theory (DFT). Furthermore, we have pursued the studies on $CH_3NH_3PbBr_3$, since this material exhibits interesting luminescent properties, so far the surface defect is one of the major factor for the quenching effect.[2] It has been reported that moisture and O_2 gas can recover the luminescent property. In order to elucidate the luminescence quenching-reactivating mechanism, the structural, electronic and optical properties have been inspected both for bulk in orthorhombic phases and (010) surface orientation.

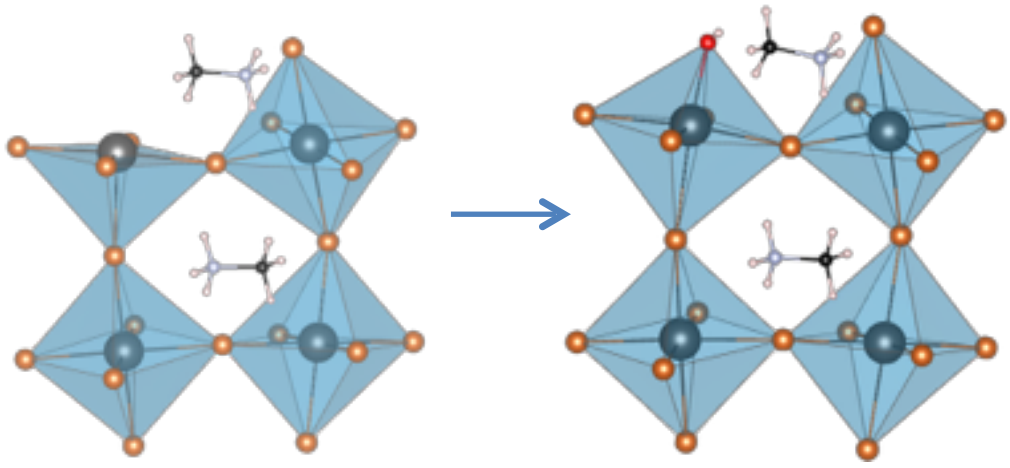

Figure 1 $CH_3NH_3PbBr_3$ (010) surface defects and surface passivation by OH^-

References

1. Filip, M. R. and Giustino, F.**,** *J. Phys. Chem. C* (2015), **120**, 166
2. H. Wei *et al*. *Nature Photonics* (2016), **10**, 333