Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A Computational View on the Change of Geometric and Electronic Properties of Perovskites Arisen by the Partial Substitution of Pb by Sn

Ming-Gang Ju[1], Guangxu Sun[1], Yi Zhao[2] and WanZhen Liang[2*]
[1] *Department of Chemical Physics, University of Science and Technology of China, Hefei 230026, P. R. China*
[2] *State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China*
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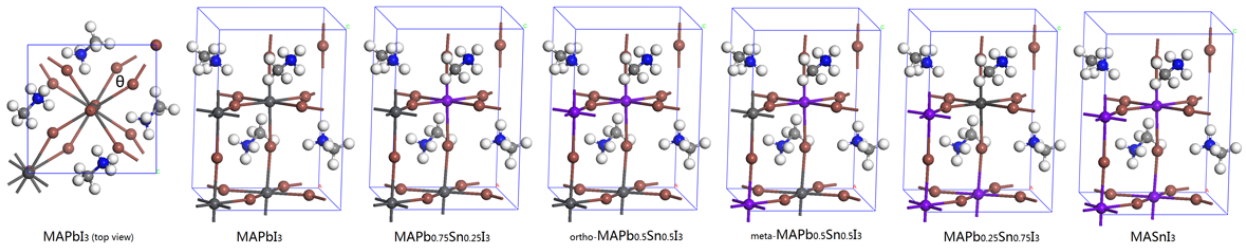

Fig. 1: Optimized structures of $MAPb_xSn_{1-x}I_3$ with symmetry *I4cm*. Blue=N, gray=C, white=H, brown=I, dark=Pb and purple=Sn.

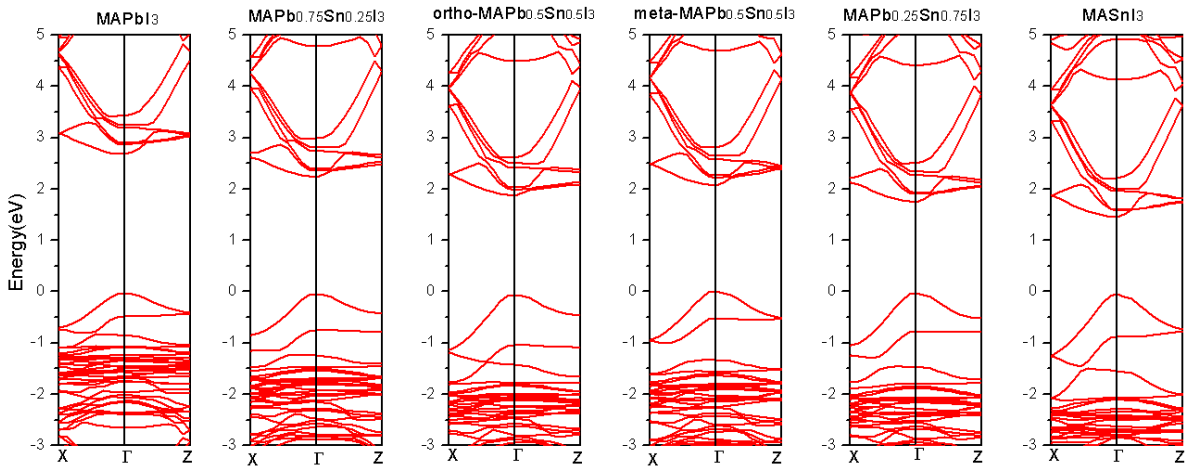

Fig. 2: Band diagram of the compounds $MAPb_xSn_{1-x}I_3$ with symmetry *I4cm* computed by PBE0 functional without SO coupling. The valence band top is set to zero.

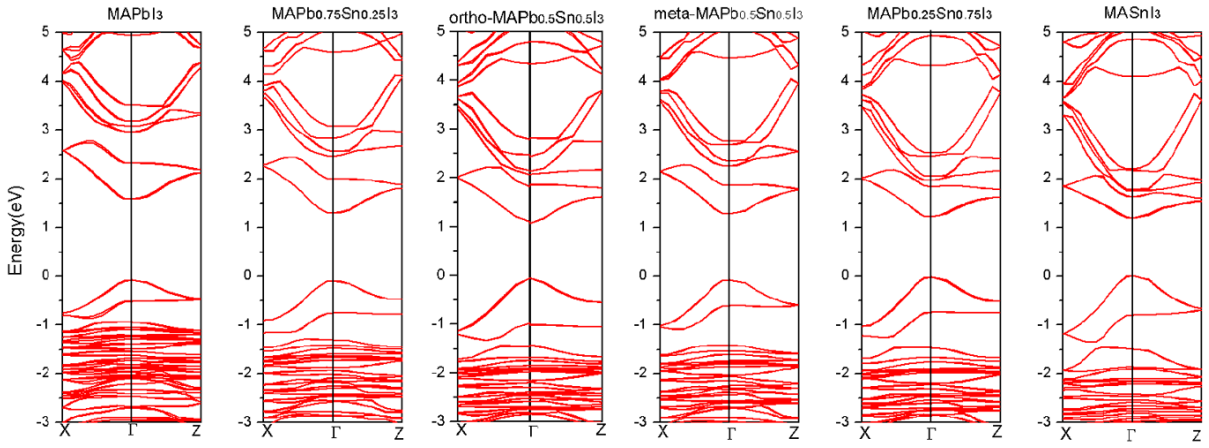

Fig. 3: Band diagram of the compounds $MAPb_xSn_{1-x}I_3$ with symmetry *I4cm* computed by PBE0 functional with SO coupling. The valence band top is set to zero.

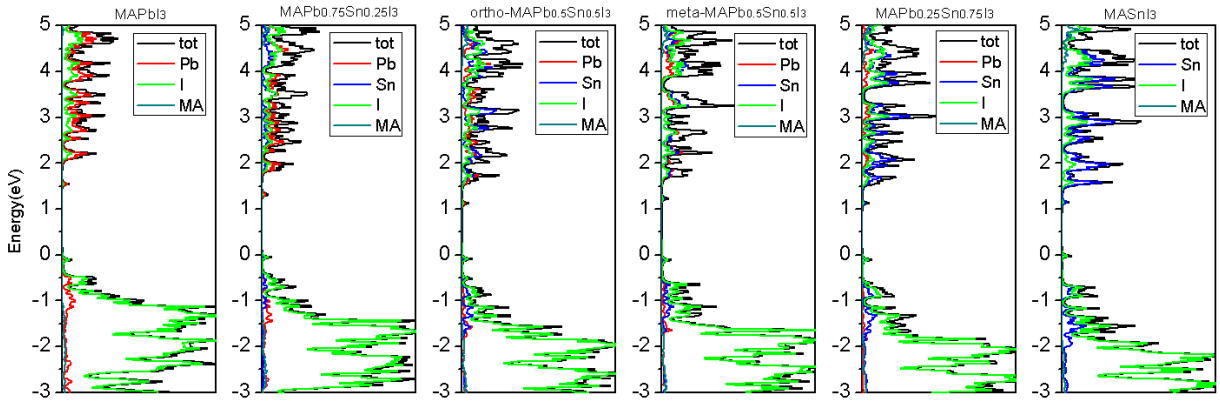

Fig. 4: Density of states of the compounds $MAPb_xSn_{1-x}I_3$ with symmetry *I4cm* computed by PBE0 functional with SO coupling. The valence band top is set to zero.

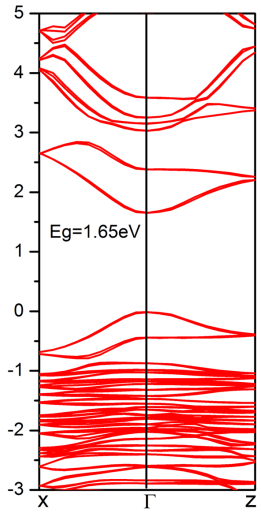

Fig. 5: Band diagram of the compounds $MAPbI_3$ with symmetry *I4cm* computed by PBE0 functional with SO coupling with hard PAW potentials for carbon and nitrogen, which have a maximum cutoff of 400 eV. The valence band top is set to zero.