Structural and Electronic Properties of 2D Organic–inorganic Halide Perovskites.

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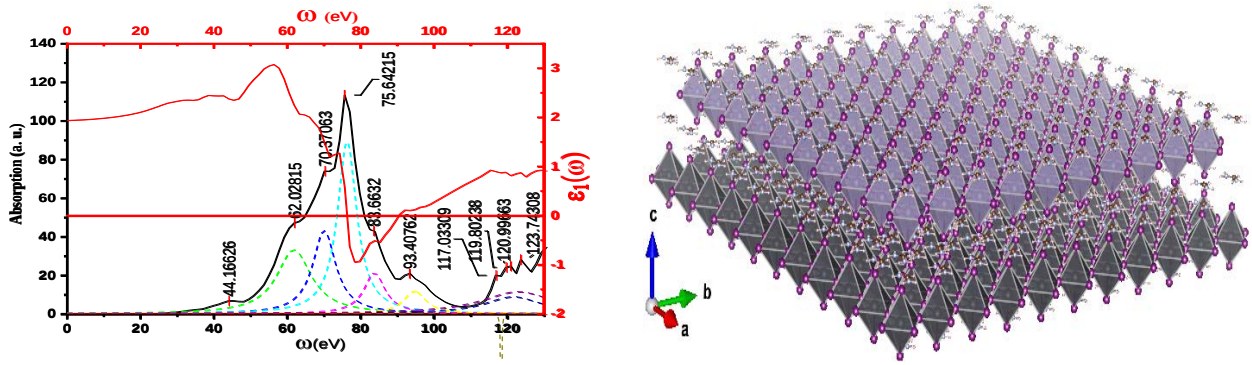

In this work, we systematically investigate the structural and electronic properties, based on density functional theory calculations. We find that a general rule to predict the bandgap of the 2D (MA,FA)PbI3 its bandgap decreases as the thickness increases and the size of metal atom decrees as well as that of the halide atom increases and the effective mass of hole increases as the thickness of 2D (MA,FA)PbI3 increases[1]. Our results confirm that the 2D (MA,FA)PbI3 may be excellent alternatives to the unstable bulk (MA,FA)PbI3 in solar energy harvesting with improved performance due to suitable bandgap, small carrier effective mass[2], and high resistance to water and oxygen molecules.

the abstract text.

[1] W. Geng, C. Tong, Z. Tang, C. Yam, and Y. Zhang, "ScienceDirect Effect of surface composition on electronic properties of methylammonium lead iodide perovskite," *J. Mater.*, vol. 1, no. 3, pp. 213–220, 2015.

[2] N. Kumari, S. R. Patel, and J. V Gohel, "Optik Superior efficiency achievement for FAPbI 3 -perovskite thin film solar cell by optimization with response surface methodology technique and partial replacement of Pb by Sn," vol. 176, no. September 2018, pp. 262–277, 2019.