

DFT study of the optoelectronic properties of 2D multilayered perovskites

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Used alone or associated with a 3D structure in a 2D/3D heterojunction, two-dimensional (2D) halide perovskites have recently emerged as a game changer in the field of perovskites solar cells thanks to their excellent optoelectronic properties combined with an enhanced material stability^{1,2}. Therefore, we propose to explore the optoelectronic properties of various perovskites that could possibly be used in 2D-3D multidimensional solar cells or LEDs. In particular, series of 2D Ruddlesden-popper perovskites will be explored as well as the related intriguing methylhydrazinium 3D perovskite, CH₃NH₂NH₂PbBr₃³. The density functional theory (DFT) study will be supplemented by experimental results.

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