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Influence of structural distortions on the optoelectronic properties of 2D multilayered perovskites : a DFT study

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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}. Hence, we propose to explore the optoelectronic properties of various perovskites that could be used in 2D-3D multidimensional solar cells or LEDs. In particular, series of 2D Ruddlesden-popper perovskites will be explored as well as its intriguing methylhydrazinium 3D perovskite counterpart, CH₃NH₂NH₂PbBr₃³. Here, experimental and density functional theory (DFT) results, suggesting a substantial influence of polar distortions and long range incommensurate lattice instability on the electronic properties of this class of material⁴⁻⁶, will be described.

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