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► To cite this version:

Ashanti Bergonzoni, Xiaotong Li, Sébastien Pillet, Kamel Boukheddaben, Aymen Yangui, et al.. Influence of structural distortions on the optoelectronic properties of 2D multilayered perovskites: a DFT study. Journée de l'École doctorale, Jun 2022, Rennes, France. . hal-04434508

HAL Id: hal-04434508

<https://hal.science/hal-04434508>

Submitted on 2 Feb 2024

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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.

This work was supported within the framework of the Israeli-French scientific cooperation (Joint Research Projects 2019-2021 entitled: ALLPOA (From Atomic Level to layered Perovskite for Optoelectronic Applications)) by the Ministry of Science & Technology of the State of Israel (MOST) and France's Centre National de la Recherche Scientifique (CNRS).

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