

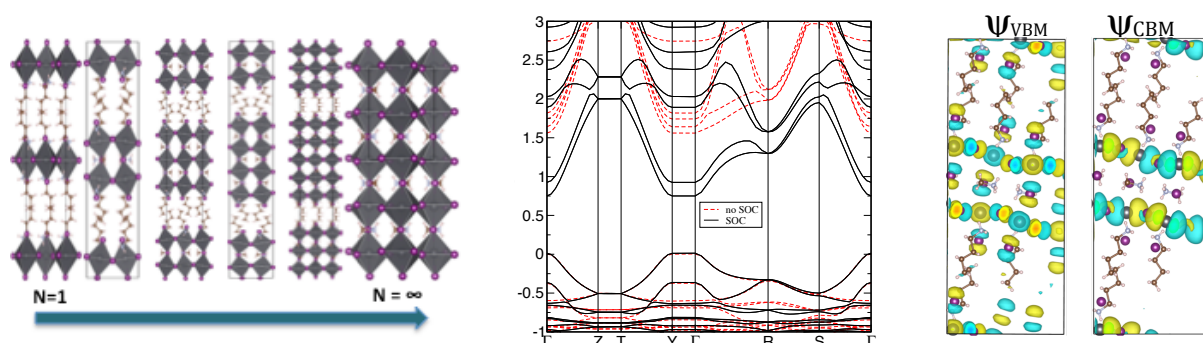
## Theoretical study of 2D-layered Ruddlesden-Popper hybrid organic-inorganic perovskites

B. Traore<sup>1</sup>, L. Pedesseau<sup>2</sup>, M. Kepenekian<sup>1</sup>, J. Even<sup>2</sup>, C. Katan<sup>1</sup>

<sup>1</sup>Institut des Sciences Chimiques de Rennes, UMR 6226, CNRS, Université de Rennes 1, 35042 Rennes, France

<sup>2</sup>FOTON, CNRS, INSA– Rennes, 35708 Rennes, France

3D organic-inorganic (hybrid) perovskites have raised great technological interest over the past few years owing to their high potential in photovoltaics and optoelectronics. This is in great part due to their high light power conversion efficiencies, currently exceeding 22%<sup>1</sup>. Recently, their 2D layered counterparts have gained renewed interest as, among others, they demonstrate excellent photostability under operating conditions and resistance to humidity and heat stress<sup>2</sup>. However, these interesting properties need to be theoretically understood in order to get physical insights that shall help the engineering of improved devices. In this regard, various theoretical tools, including tight-binding models<sup>3</sup>, are of particular value. Here, we present DFT based results on perovskites adopting the crystal structure of the Ruddlesden–Popper type (Fig.1), to understand the mechanisms that are prominent in their exciting photo-physical properties. For instance, both their electronic (Fig.1) and dielectric properties will be discussed with particular attention on quantum and dielectric confinement effects. Thanks to the information gained, excitonic effects will be subsequently tackled<sup>4,5</sup>.



**Fig.1.** (left) Structures of 2D RP and 3D  $\text{CH}_3\text{NH}_3\text{PbI}_3$  perovskites. (right) Band structure of  $N=2$  member of 2D-RP perovskites and corresponding maximum valence and minimum conduction bands' wave functions at  $\Gamma$ . SOC stands for spin-orbit coupling.

### References :

1. M. Saliba et al., "A molecularly engineered hole-transporting material for efficient perovskite solar cells", *Nature Energ.*, vol. 1, 2016.
2. Tsai et al. "High-efficiency two-dimensional Ruddlesden–Popper perovskite solar cells", *Nature*, vol. 536, 2016
3. S. Boyer-Richard et al., "Symmetry-Based Tight Binding Modeling of Halide Perovskite Semiconductors", *J. Phys. Chem. Lett.*, vol. 7, 2016.
4. C. C. Stoumpos et al., "High Members of the 2D Ruddlesden-Popper Halide Perovskites: Optical Properties and Solar Cells Based on  $(\text{CH}_3(\text{CH}_2)_3\text{NH}_3)_2(\text{CH}_3\text{NH}_3)_4\text{Pb}_5\text{I}_{16}$ ", *Chem.*, vol. 2, pp. 427–440, 2017,
5. L. Pedesseau et al., "Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors", *ACS Nano*, vol. 10, pp 9776–9786, 2016.

The project leading to this work has received funding from the European Union's Horizon 2020 programme, through a FET Open research and innovation action under grant agreement No 687008.