

## MASTER2 INTERNSHIP

Institut des Sciences Chimiques de Rennes - Theoretical Inorganic Chemistry group (Fr) and  
Laboratoire de Chimie des Matériaux Nouveaux, Université de Mons (Be)

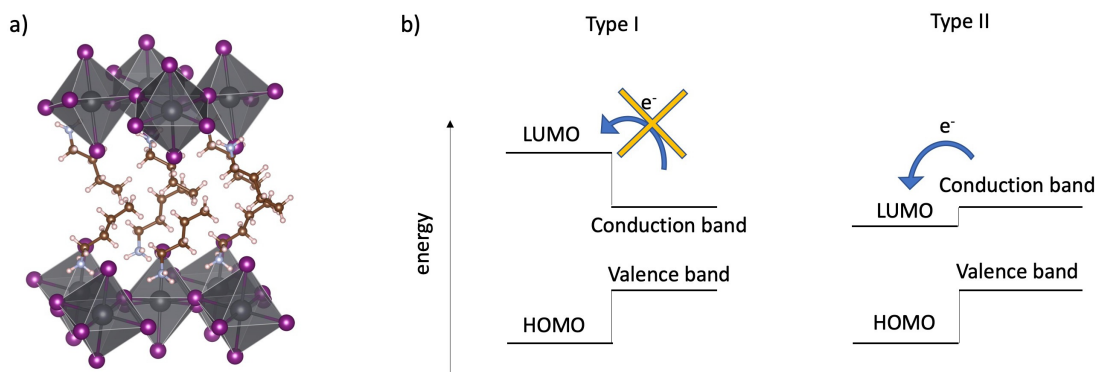
Supervisors: Mikael KEPENEKIAN, Claudio QUARTI

Contacts: [mikael.kepenekian@univ-rennes1.fr](mailto:mikael.kepenekian@univ-rennes1.fr), [claudio.quarti@umons.ac.be](mailto:claudio.quarti@umons.ac.be)

### Layered perovskites meet organic chromophores: electronic processes at the inorganic/organic interface

Theoretical Chemistry/Physics, Materials Science, Solid State Chemistry, Semiconductor Physics, Photovoltaics  
November 2020 – June 2021

With almost 20% of world's energy consumption related to illumination,<sup>1</sup> improvement in the performances related to both light-emitting materials and devices are pivotal, in order to reduce carbon footprint associated to human activities. In this frame, layered halide perovskites are emerging as potential candidates for effective light-emission applications.<sup>2</sup> The crystalline structure of these systems consists in atomically thin semiconducting layers of corner-shared MX<sub>6</sub> octahedra (M=metal and X=halide), spaced by bulky organic, insulating cations (Figure 1a), and provides unique optical properties as efficient and narrow excitonic emission.<sup>3</sup> However, additional functionalities can be envisaged by substituting the electronic inert organic cation with optically active chromophores. This case in fact results in the transition from most common type I electronic interface between the organic/inorganic components, to a type II interface (Figure 1b), which opens the path for a plethora of charge and energy transfer phenomena.<sup>4</sup> Still, the basic understanding of these electronic phenomena in presence of optically active organic chromophores is currently poor.<sup>5</sup> In this internship, we propose computational investigations of the electronic structure of layered halide perovskites containing optically active organic cations.



**Figure 1.** (a) crystalline structure of layered 2D perovskite; (b) type I and type II electronic interfaces associated to the mixed organic/inorganic system. Electronic levels of interest are indicated, as well.

The candidate will first carry out a systematic review of the literature works related to the optical response of layered perovskites containing electroactive organic cations.<sup>3-5</sup> Subsequently, she/he will perform state-of-the-art Density Functional Theory simulations within periodic boundary formalism, considering case studies for the most relevant model systems from the literature. The target will be *i)* to determine the energy alignment between the delocalized band-like states of the inorganic frame and the localized states of the molecular moieties; *ii)* to estimate the degree of electronic communication between electronic states residing on the organic and inorganic components; *iii)* to develop a procedure for the quantification of an electronic coupling. This will likely take advantage of a Wannierization scheme for the crystalline wavefunction, as proposed in the Wannier90 package.<sup>6</sup> The stage enters in the frame of the collaboration between two institutes, the Theoretical Inorganic Chemistry group at ISCR of the University of Rennes (M. Kepenekian), and the laboratory for Chemistry of Novel Materials of the University of Mons (C. Quarti), which are at the forefront of the research on hybrid perovskites<sup>7</sup>. A short stay (3 to 6 weeks) at the University of Mons is envisaged. The student will benefit from a dual expertise in solid state and molecular chemistry provided by the two institutions and will gain, together with a sound knowledge of optoelectronics processes at the atomistic scale, practical skills in the use of state-of-the-art computational methods for the simulation of the electronic structure of materials.

#### References

- (1) G. Zissis, *Energy Consumption and Environmental and Economic Impact of Lighting: The Current Situation from Handbook of Advanced Lighting Technology*, Springer International Publishing Switzerland 2016.
- (2) D. N. Congreve et al., *ACS Photonics*, **2017**, *4*, 476-481.
- (3) C. Katan et al., *Chem. Rev.*, **2018**, *119*, 3140-3192.
- (4) K. Ema et al., *Phys. Rev. B*, **2008**, *100*, 257401/1-4.
- (5) F. Lédée, C. Quarti et al. *Manuscript in preparation*.
- (6) G. Pizzi et al., *J. Phys. Cond. Matt.* **2020**, *32*, 165902/1-25.