MASTER2 INTERNSHIP

Institut des Sciences Chimiques de Rennes - Theoretical Inorganic Chemistry group and
Institut FOTON – INSA Rennes
Supervisors: Claudio QUARTI, Laurent PEDESSEAU
Contacts: claudio.quarti@univ-rennes1.fr, laurent.pedesseau@insa-rennes.fr

Computational screening of lead-free metal halide perovskites: a step towards green and performant photovoltaic materials

Theoretical Chemistry/Physics, Materials Science, Solid State Chemistry, Semiconductor Physics, Photovoltaics
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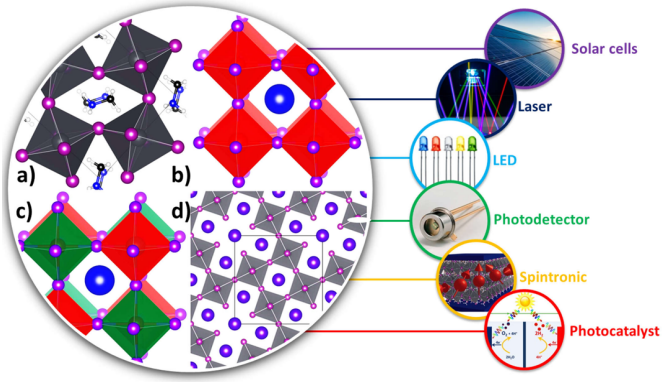
The **climate change** and its impacts are nowadays well established and cannot be ignored[1]. The international community agrees to have a fast energy transition, which translates in developing more efficient photovoltaic cells, light emitting and photocatalytic devices. Since 2009, hybrid metal halide organic perovskites came in the limelight because of the impressive photovoltaic performances, which have currently overcome the 25%[2], and because of their great potential for other optoelectronic applications such as Laser, Light Emitting Devices (LED), Photodetection, Photocatalysis. Nevertheless, the full exploitation of this novel class of semiconductors is nowadays limited by the presence of lead in their composition, which raises a serious toxicity issue. Within this frame, great effort is currently devoted in finding alternative compositions for perovskite-like structures, compared to the reference $A(I)Pb(II)X_3$ (A=monovalent element/molecule like methylammonium CH_3NH_3, X=halide). Several strategies have been proposed for lead removal, which are illustrated below: *a*) substitution of lead with other divalent metal atoms $A(I)B(II)X_3$ (B=Sn, Ge)[3]; *b*) investigation of non-perovskite structures, as rudorfittes, characterized by $A(I)_3B(III)_2X_9$ composition and by a peculiar BX_6 octahedral connection[4]; *c*) double perovskites with composition $A(I)_2B(IV)X_6$ and $A(I)_2B(I)B'(III)X_6$ [5]; *d*) deficient perovskite, $d\text{-}A(I)Pb(II)X_3$, characterized by a reduced content of lead[6].



During this internship, the candidate will perform computational screening of the main properties of lead-free compounds, using first principle methods, i.e. methods free from any external parametrization. The workhorse will be Density Functional Theory within periodic boundary conditions, with focus on predicting thermodynamic properties (stability), electronic and optical properties, aiming to find suitable lead-free candidates for photovoltaic and light emitting applications. The stage enters in the frame of the collaboration between two institutes, the Theoretical Inorganic Chemistry group at ISCR (C. Quarti), and FOTON Institute – INSA Rennes (L. Pedesseau), which are at the forefront of the research on hybrid perovskites[7], and fits in the context of freshly founded European (DROP-IT) and national (MORELESS) projects, with connections with experimental research groups. The student will benefit from a dual expertise in materials chemistry and physics provided by the institutions and will gain, together with a sounded knowledge of photovoltaics and optoelectronics applications, practical skills in the use of state-of-the-art computational methods for the simulation of the electronic structure of materials.

(1) Obama, B. The Irreversible Momentum of Clean Energy. *Science* **2017**, *355* (6321), 126–129.
(2) https://www.nrel.gov/pv/cell-efficiency.html
(3) Noel, et al. *Energy Environ. Sci.* **2014**, *7* (9), 3061–3068.
(4) Turkevych, I. et al. *ChemSusChem* **2017**, *10* (19), 3754–3759.
(5) Volonakis, G. et al. *J. Phys. Chem. Lett.* **2017**, *8* (4), 772–778.
(6) Leblanc, A. et al. *Angew. Chem Int. Ed.* **2017**, *56* (50) 16067-16072.
(7) Katan, C. et al. *Chem. Rev.* **2019**, *119* (5), 3140-3192.