Computational design of novel 2D perovskite materials for energy applications: Electronic structure and Interfaces from first-principles.

3-year PhD position
(Oct. 2020 – Sept. 2023)

Supervisors

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A full-time PhD position is available in the department of Inorganic Theoretical Chemistry (CTI) at the Institute of Chemical Sciences of Rennes (ISCR, University of Rennes 1) for a talented and ambitious student. The position is fully funded within the framework of the 'Chaire de Recherche – Rennes Metropole'.

Owing to both the rapidly increasing global demand for energy and the dramatic environmental impact of fossil fuels, the development of efficient strategies for discovering novel materials for energy generation has become a top scientific priority. Within the proposed PhD project, we want to pursue two distinct research directions. At first the candidate will investigate the discovery and design of novel energy materials. To do so, the project targets to look at the structural, electronic and optical properties of the two-dimensional (2D) counterparts (i.e. Ruddlesden-Popper and Dion-Jacobson phases) of the lead-free halide double perovskites that have been recently discovered: $Cs_2InAgCl_6$, $Cs_2BiAgCl_6$, $Cs_2BiAgBr_6$, $Cs_2SbAgCl_6$, $Cs_2SbAgBr_6$, Ba_2IAgO_6. In particular, the candidate will assess their stability and characterize their opto-electronic properties by means of first-principles, but also will feedback with the supervisors' established experimental partners to attempt synthesis, and subsequent characterization.

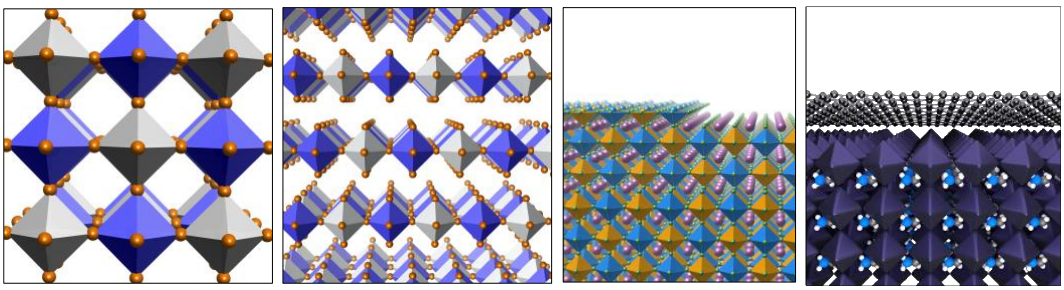

Figure: Prototype models of structures that will be investigated within the proposed PhD thesis. (From left to right) Double perovskite, layered double perovskite, surface of double perovskite, interface between 2D monolayer and prototype perovskite.

At a second stage, the candidate will move on to investigate the surface and interfacial properties of the most promising materials investigated in the first part. The interfaces that will be probed are first in combination with prototype bulk compounds like Ag, Au, TiO_2, ZnO, SnO_2, and Si, and following the same methodology, the interfaces with prototype 2D materials (e.g. graphene, MoS_2, $MoSe_2$, InSe,

Black-p, etc.) will be explored. The properties of interest are the surface stability, the absolute band energy levels, and the energy level alignment when interfaces with other compounds of interest. Moreover, we will aim to uncover possible charge-transfer and electrical dipole formations at the most important interfaces for opto-electronic application.

The CTI team

The PhD student will work in the Inorganic Theoretical Chemistry (CTI) team, in the Institute of Chemical Sciences of Rennes. The CTI team gathers several theoreticians (14 permanent staff members, 15 students) with complementary skills in theoretical chemistry but also physics, working with a broad set of quantum chemical tools, ranging from high precision *ab initio* wavefunction-based calculations to fast semi-empirical methods. The studied systems in CTI are diverse, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. This has led to fruitful joint collaborations with experimentalists from ISCR as well as major national and international groups. The team is also strongly involved in the collective effort made by the French community of theoretical chemists at the national level, in the quest of bridging the gap between state-of the art quantum tools and real life applications. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Local and national computing means are available for the purposes of the scientific projects.

Profile of the candidate

This 3-year fully funded PhD is part of the "Chaire de Recherche Rennes Metropole" project coordinated by George Volonakis. The position is fully funded for three years starting from October 2020. A Master's degree in Physics, Chemistry, Materials Science or closely related field is required. A strong background in any of the following subject is desired: solid-state physics, quantum-chemistry, materials modelling approaches, and atomistic simulations. The successful candidate should be highly motivated, with excellent communication skills and the ability to work in close collaboration with other theoreticians and experimentalists.

Application

The PhD project will start in October 2020. Applications are already open and candidates shall contact both supervisors by e-mail, with a CV and a motivation letter, including clear description of previous research experience, including any Master internship(s).

References:

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