PhD position | Energy levels and band offsets at semiconducting interfaces from first-principles.

Contract	Fully funded 3-year PhD position starting October 2024
Institution	Institut des Sciences Chimiques de Rennes (ISCR) Theoretical Spectroscopy Group (LSI)
Contact	Prof. George Volonakis, Email: yorgos.volonakis@univ-rennes.fr Dr. Matteo Gatti, Email: matteo.gatti@polytechnique.fr

A full-time 3-year PhD position is available in a **joint project** between the Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR) and the Theoretical Spectroscopy Group (LSI) of the École Polytechnique de Paris under the supervision of Dr. Matteo Gatti, Prof. George Volonakis, and Dr. Vitaly Gorelov. The position is for three years starting October 2024. The project is dedicated to the energy levels and their alignment, using ab initio computational approaches, for advanced photo-active materials for photovoltaic applications.

Context | The MINOTAURE project addresses questions raised within the call "reliability of advanced technologies of photovoltaic (PV) cells". Its aim is to accelerate the energy transition and to strengthen photovoltaic power generation, the reliability of novel and future PV technologies has become a critical research focus. Within MINOTAURE the atomistic interface and heterostructure properties of photo-active semiconductors will be characterized using state-of-the-art computational methods from first-principles. These will be adapted and used to determine properties of heterostructures and interfaces including dielectric profiles, work functions, interface and surface dipoles, passivation layers, and band alignments, which are critical for solar cell performance. Ab initio approaches to calculate band offsets for interfaces of devices will be adapted and accelerated, in order to determine photoemission spectra of realistic interfaces based on feedback from experimental partners of the project, and exchanging results of photoemission spectroscopies.

Project | Within this thesis, our aim is to unveil the energy level alignment across the different interfaces of the perovskite-based PV device, which remains one of the most critical parameters for the performance of both single junction and tandem solar cells. With this joint thesis (LSI/ISCR) we propose to develop a computational approach from first-principles that would enable the accurate and efficient calculation of band offsets for a selection of interfaces of the perovskite photovoltaic devices. Different flavors of ab initio calculations have been proposed for the determination of band offsets, and we will establish the most appropriate one by benchmarking our results. We will use recently established methods to accelerate the calculations, and we will apply them to realistic interfaces.

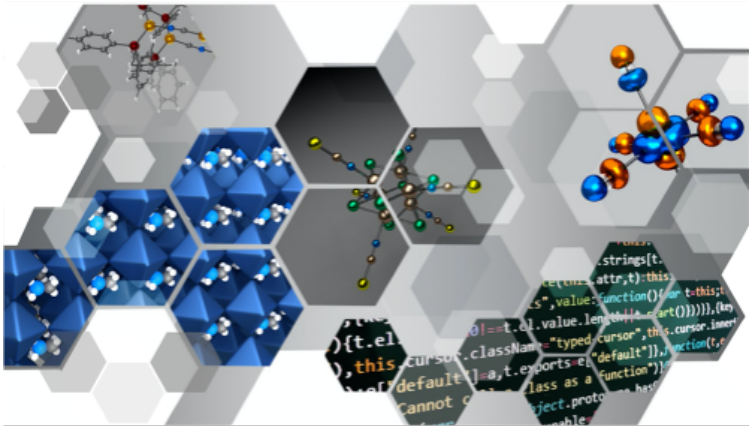
Related references

[1] B Cucco, C Katan, J Even, M Kepenekian, G Volonakis *ACS Materials Letters* **2023**, *5*, 52-59

[2] G. Volonakis and F. Giustino *Applied Physics Letters* **2018**, *112*, 243901

Profile of the candidate | A master's degree (or equivalent) in Materials Science, Physics, Chemistry or

related disciplines is required. A strong background in any of the following subject is desired: quantum chemistry, solid-state physics, 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.



The successful candidate will work in close collaboration with the: **1. CTI** | Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR). The CTI team gathers computational chemists and physicists (15 permanent staff members, 15 students) with complementary skills, working with a broad set of quantum chemical tools, ranging from high precision ab initio wave function-based calculations to fast semi-empirical methods. CTI team members are interested in diverse type of systems, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Considerable local, national and European computing resources are available for the purposes of the scientific projects. **2. LSI** | Theoretical Spectroscopy Group (*Laboratoire des Solides Irradiés*, LSI) team at the École Polytechnique de Paris.

How to apply | Applications are open and candidates are encouraged to email the supervisors: yorgos.volonakis@univ-rennes.fr, matteo.gatti@polytechnique.fr, and vitaly.gorelov@polytechnique.edu with a CV, including clear description of previous research experience, and a motivation letter.