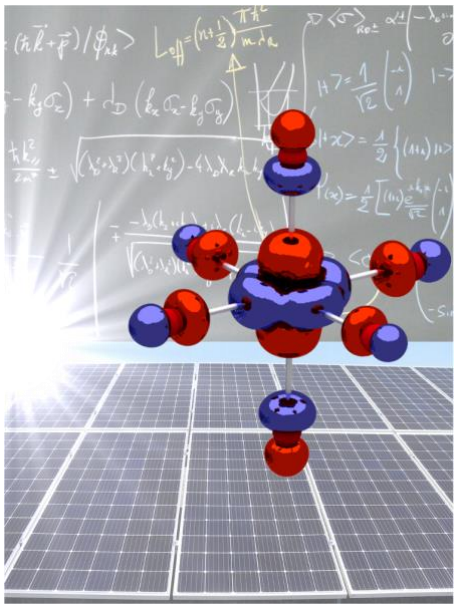
Electronic structure of novel photo-active materials for sustainable energy applications.

Fully funded 3-year PhD position

A full-time PhD position is available at the Institute of Chemical Sciences of Rennes (ISCR) of the Université de Rennes (UR). The successful candidate will be supervised by George Volonakis of the CTI group. The position is for three years starting as early as October 2023, with a funding from the PIs projects, and will be supported by the established research team at Rennes working on the computational methods for energy applications.

Scientific background: Within todays critical need for sustainable and environmental-friendly energy, this project aims to employ a computational design approach to identify and accurately model the most promising novel materials for energy applications. In particular, within this thesis the candidate will work towards a deep fundamental understanding of the most critical structural, optical and electronic properties of selected materials that pioneer the next generation opto-electronic energy devices. The candidate will employ advanced computational approaches based on first-principles to unveil the structure-property relations of prototype energy related prototype materials like halide perovskites and closely related perovskitoids and explore the materials phase-space well beyond these crystal lattices. The project supports the active research-axis of the principal investigator (PI) that has been established and developed over the past three years at the ISCR, and lead to several publications, as well as the design of novel materials like halide double perovskites, vacancy ordered double perovskites and Ag/Bi double salts. This PhD aims to identify and synthesize novel semiconducting materials and reveal known overlooked compounds with tailored properties that could advance a range of energy applications like solar-cells, photo-catalysts and light-emitters.



Profile of the candidate: A 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.

How to apply: Applications are open and candidates are encouraged to email at the soonest George Volonakis: yorgos.volonakis@univ-rennes.fr, with a CV, including clear description of previous research experience, and a motivation letter.

Important dates:

March 2023: position open.
April 2023: notification of the candidates and interviews.
October 2023: start of the thesis.

Institut des Sciences Chimiques de Rennes – Université de Rennes 1
263 avenue du Général Leclerc - CS 74205 - 35042 Rennes Cedex, France

Related publications:

[1] B. Cucco et al., ACS Materials Letters 5, 52 (2023).
[2] B. Cucco et al., Solar RRL 2200718 (2022).
[3] G.Volonakis et al., J. Phys. Chem. Lett. 10, 1722 (2019).
[4] G. Volonakis et al., J. Phys. Chem. Lett., 8, 772 (2017).

The CTI team: The PhD student will work in the Inorganic Theoretical Chemistry (CTI) team, of 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.

More positions available: *There are more opportunities to join the group coming up: 1) PhD on the 'Theory of optoelectronic properties of perovskite heterostructures' supervised by S. Thébaud at INSA, Rennes, 2) PhD 'Theoretical modelling of solid-state batteries' co-supervised by E. Furet and X. Rocquefelte, and 3) PHD 'Ab initio Modelling of excited-state absorption' co-supervised by B. Le Guennic and D. Jacquemin. Please contact the supervisors.*