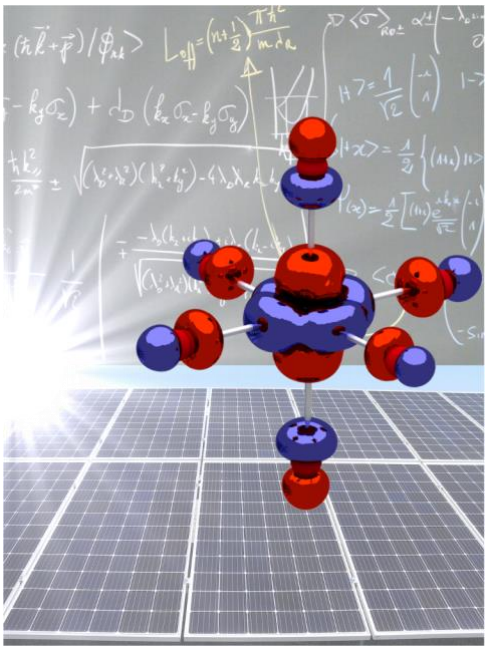
Ab initio modelling of surfaces and interfaces of novel perovskite energy materials

2-year post-Doctoral position

A full-time 24-month post-doctoral position (with the possibility of extension) 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 should start in January 2024, funded by the ANR SURFIN project (SURFaces and Interfaces of Novel perovskites and perovskitoids), and will be supported by the established research team at Rennes working on the electronic structure of energy materials.

Scientific background: SURFIN will employ an ab initio approach to systematically deal with the study of the surfaces of most prominent perovskite (and related) materials that have been recently discovered, and proposed as promising photo-active compounds for energy related applications. The candidate will investigate members of the prototypical corner-sharing 3D perovskites, new double and vacancy ordered double perovskites, and edge- or face- sharing octahedrally coordinated halide compounds like the Ag/Bi double salts. Hence, the project will build upon and support the established research activity on the computational design of novel energy materials. Within SURFIN the candidate will focus on calculating the materials' absolute energy levels, a most critical parameter for (i) identifying the potential photo-catalytic activity of the materials, (ii) designing selective contacts between device layers, and (iii) engineering optimized transport layers for opto-electronic devices.



Profile of the candidate: Applicants for this position must hold a Ph.D. in Physics, Chemistry, Materials Science, or a closely related discipline. A robust expertise in the following areas is required: solid-state physics, quantum chemistry, atomistic materials modelling approaches. The ideal candidate should demonstrate strong motivation, possess excellent communication skills, and exhibit a collaborative spirit to work closely with both theoreticians and experimentalists. Additionally, prior experience in utilizing ab initio methods for surface property calculations, and many body approaches beyond standard DFT (e.g., GW, BSE) is considered highly valuable.

How to apply: Applications are now open and candidates are encouraged to email the PI at yorgos.volonakis@univ-rennes.fr, with (i) a detailed CV, including clear description of previous research experience, and (ii) a motivation letter which should include the contact details of at least two referees.

Important dates:

July 2023: position open.
October/November 2023: notification of the candidates and interviews.
January 2024: start of the position.

Related publications:

[1] G. Volonakis and F. Giustino, Applied Physics Letters 112 24 (2018)
[2] B. Cucco et al., ACS Materials Letters 5, 52 (2023).
[3] B. Cucco et al., Solar RRL 2200718 (2022).
[4] G.Volonakis et al., J. Phys. Chem. Lett. 10, 1722 (2019).
[5] G. Volonakis et al., J. Phys. Chem. Lett., 8, 772 (2017).

Informal enquires can be addressed to yorgos.volonakis@univ-rennes.fr

The CTI team: The hired candidate 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.