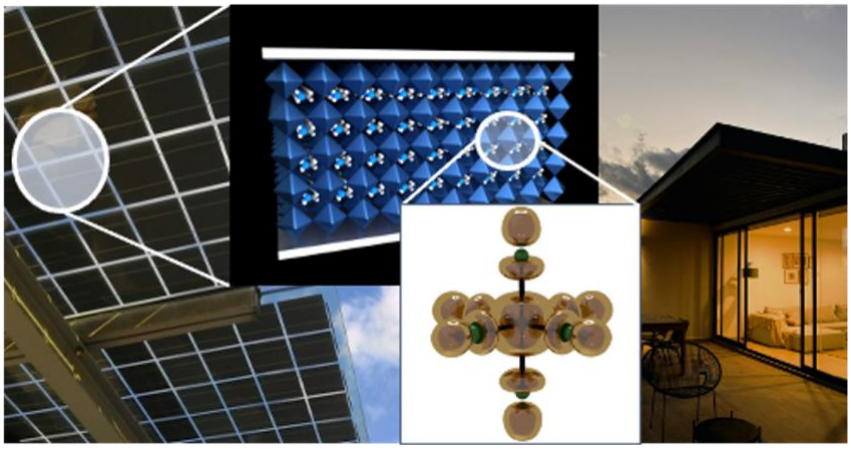
Ab initio materials design of advanced energy materials

post-doctoral position

A full-time **18-months** 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 March 2025, and will be supported by the established research team at Rennes working on the electronic structure of energy materials.



Context | The dramatic environmental impact of fossil fuels makes it essential to develop original strategies for the discovery of new materials that will enable the transition to the efficient use of renewable energies. In particular, photo-active semiconductors are key materials for the development of new high-performance technologies. For example, metal halide perovskites are materials that have revolutionized the field of emerging photovoltaics over the last decade, and today perovskite-based solar cells can outperform in terms of power conversion efficiency traditional silicon-based technologies. At the same time, quantum-based calculations are a remarkable tool for understanding the performance of such materials, but also can be used to guide the design of new, more stable, more efficient and more environmentally-friendly materials.

Project | Within this project, the candidate will explore the most advanced quantum methods (DFPT, GW, BSE) for describing the electronic structure of both prototypical semiconductors within the family of halide perovskites, but also for a selection of novel materials such as halide double salts, layered halide perovskites and their heterostructures with 3D. To this aim, the candidate will make use of the strong network of the PIs collaborators that are developing state-of-the-art ab initio codes. For the selection of new materials, the candidate will employ a rational inverse-design approach, as established by the PI, and further expand towards implementing high-throughput calculations for screening the proposed datasets. The most important materials' properties for optoelectronic applications will be explored, such as the electronic gap, the optical gap, the absorption spectrum (with and without excitonic effects) and target calculating the potential performance of the photo-active materials in particular for pho tovoltaic applications. This will include both outdoor solar cells, but we will also expand our search to look for ideal candidates with spectral sensitivity that is tuned for indoor photovoltaics, an emerging technology for ambient light energy harvesting and powering IoT 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.

Start-date | March 2025

Related publications

[1] B Cucco, et al., ACS Materials Letters 2023, 5, 52.
[2] B Cucco, et al., Solar RRL 2022, 2200718.
[3] B Cucco, et al., Applied Physics Letters 2021, 119 181903.
[4] G. Volonakis and F. Giustino, Applied Physics Letters 112 24 (2018)
[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.