

## Post-doc in Computational Materials Discovery at Poitiers U. (France)

A **post-doc position** is currently available in the group of Dr. Gilles Frapper at IC2MP (Poitiers University – CNRS, France). Our interests center around geometrical-electronic control of properties, prediction of new materials, and development of Crystal Structure Prediction (CSP) methodologies.

The project relies on the use of CSP algorithms to predict and investigate high T<sub>c</sub> superconducting ternary hydrides, as well as novel hydrogen storage materials through an experimental collaboration (2 projects funded by ANR).

Dr. Frapper is looking for a postdoctoral associate interested in Computational Materials Discovery. The project can entail one (or a combination) of the following: (i) application of machine learning interatomic potentials to accelerate the potential energy surface scan, (ii) set up of an accurate and efficient CSP methodology to scan a ternary phase diagram at (P,T) conditions, and (iii) development of a double-objective optimization method to find the optimal set of solutions using evolutionary algorithms, here T<sub>c</sub> descriptor and DFT enthalpy.

**Desired qualifications:** a PhD (< 3 years) in computational chemistry, solid state physics or a closely related area is required. The candidate should have some skills in programming languages (Fortran, C/C++, Python) and Linux; managing codes under High Performance Computing center (GENCI) is required; an experience in CSP methodology is a plus (e.g., random/evolutionary algorithms). A good knowledge of written and spoken English is essential to communicate with our external collaborators and to write reports/articles.

**Funding:** The net salary should be ~2 300 € per month (CNRS contract funded by ANR, PhD defense < 3 years). The initial contract will be for one year, with a possible 1-year extension upon mutual agreement.

**Starting date:** from December 1<sup>st</sup> 2022 until the position is filled (~winter 2023).

**How to apply:** your application should be sent to [gilles.frapper@univ-poitiers.fr](mailto:gilles.frapper@univ-poitiers.fr), detail your motivations, starting date, and relevant experience (complete CV +PhD diploma). If interested by your profile, we will ask you to arrange for two letters of recommendation from current and former research supervisors.

Poitiers is a peaceful and lively city close to Paris (1h20 by TGV), Atlantic Ocean (1h30 drive), tasting places of wonderful wines and delicious French cuisine are close by! Poitiers is ranked among the first student cities in France: 28 000 students over a population of about 100 000, in a medieval university founded in 1431; cheap rental, lively medieval city, many local attractions, and events... Our *Applied Quantum Chemistry* group is composed of two faculty members, and up to ~8 non-permanent researchers (Master&PhD students and associated researchers). We develop mainly two research fields: reactivity in green chemistry, conceptual DFT (leader F. Guégan <https://orcid.org/0000-0002-4932-8643>); computational materials discovery and structural/electronic relationships using bonding analysis tools (leader G. Frapper <https://orcid.org/0000-0001-5177-6691>), an appropriate environment for fruitful cooperation!