PhD in Computational Materials Discovery at Poitiers U. (France)

A PhD position is currently available under the supervision of Dr. Gilles Frapper, *Applied Quantum Chemistry* group at IC2MP (Poitiers University – CNRS, France).

The project relies on the use of Crystal Structure Prediction (CSP) algorithms to predict and investigate low Tc superconducting ternary hydrides under pressure within the framework of the ANR *Tc_Predictor* coordinated by Dr. Julia Contreras-Garcia (CNRS, LCT Sorbonne U.). At IC2MP, our interests center around structural chemistry and the geometrical-electronic control of properties, prediction of new materials, and development of CSP methodologies.

The doctorate candidate will have (1) to apply machine learning interatomic potentials to accelerate the potential energy surface scan, (2) to develop a double-objective optimization method to find the optimal set of solutions using evolutionary algorithms, here Tc descriptor and enthalpy, and (3) to perform MLIP-based CSP searches, periodic DFT calculations (e.g. VASP code), and bonding analysis.

Desired qualifications: solid background in physics and chemistry and understanding of quantum mechanics with experience in computational material modeling at the atomic scale; ability for programming is required (Python; Fortran/C++ expertise is a plus); Applicant will have to work within an international team (Spain, US, France). Thus, excellent communication skills in English, both verbal and written, are required.

Funding: *The net salary should be ~1 750 € per month (3-year CNRS contract funded by ANR).* Partly health insurance (70% in charge of French Social Security), and a social housing support are a plus.

Starting date: from October 15th to December 1rst 2022. The candidate will be enrolled at Rosalind Franklin Doctorale School of Poitiers U.

How to apply: Applications should be sent to gilles.frapper@univ-poitiers.fr before september 1, 2022. The application should include:

- a motivation letter,
- a detailed Curriculum Vitae,
- transcripts of M.Sc. courses and copy of M.Sc. diploma
- a copy of your research training report (M2 or equivalent).
- a list of three professors who have supervised you in M.Sc. research projects or current employers and who are willing to provide a letter of recommendation.

Applications submitted before the deadline (1rst September) will be evaluated and applicants selected for a remote interview will be contacted before september 7th.

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