Post-doc 1 year in
Computational Materials Discovery

A one year post-doctoral fellowship is currently available at the Theoretical Chemistry group of E4, IC2MP within the framework of the ANR PRCI France-China **PREDICT_2D_Nanomat** coordinated by Pr. Gilles Frapper.

The project relies on the use of DFT VASP and evolutionary algorithm USPEX and high throughput screening to **predict and investigate 2D/3D materials**. Our interests center around structural chemistry and the geometrical-electronic control of properties and reactivity.
This international CNRS/ANR-NSFC project involves teams of Pr. Artem R. Oganov (Skoltech and MIPT-Moscow Russia and NPU Xi'an, China), USPEX developer, and Pr. K. Su, Q. Zeng and J. Wang (NPU Xi'an, China). Applicant will have to work within this international team. Thus, excellent communication skills in English, both verbal and written, are required.

Desired qualifications: the candidate should have obtained her/his PhD in theoretical chemistry or physics in a recognized group with experience in computational material modeling at the atomic scale (periodic DFT; machine learning, high throughput screening approaches, …); a strong ability for programming in Fortran/C++/Matlab is required and an experience in using computational tools (elaboration of scripts in bash, python,...) are clearly an asset; the candidate should possess a solid track record of research accomplishments.

Funding: *The net salary should be ~2.3 k€ per month (gross salary 36 k€/y) depending on the experiences.* Partly health insurance (70% in charge of French Social Security), and a social housing support are a plus.

How to apply: Applications should be sent to gilles.frapper@univ-poitiers.fr with the subject: "**Post-doc position in Computational Materials Discovery at Poitiers U.**". The application should include:

- a Curriculum Vitae and a motivation letter,
- the name of at least two references (MSc-PhD supervisors/current employers),
- PhD diploma & copies of educational certificates,

All documents should be in PDF format and written in English. A short-list of candidates will be made, who will be contacted for an interview over videoconferencing.
The selected candidate is expected to start asap and before 1rst feb 2020.