

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

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 Gilles Frapper.

The project relies on the use of DFT VASP and evolutionary algorithm USPEX to predict and investigate **2D materials** (structure, bonding and chemical reactivity). It involves teams of Pr. Artem R. Oganov (Skoltech and MIPT-Moscow, Stony Brook – NY USA, and NPU Xi'an, China), USPEX developer, and Pr. K. Su and Q. Zeng (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. Moreover, a one-year contract extension is envisaged to work at NPU (Xi'an, China) under the supervision of Pr. A.R. Oganov and G. Frapper.

Desired qualifications: solid background in physics and chemistry and understanding of quantum mechanics with experience in computational material modeling at the atomic scale; comprehensive experience on bonding analysis; experience in using computational tools (elaboration of scripts in bash, python,...) is required and ability for programming is a plus; possess a solid track record of research accomplishments.

Funding: *The net salary should be about 2.4 k€ per month.* 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 by email to Dr. Gilles Frapper (gilles.frapper@univ-poitiers.fr). They should include:

- 1- An up-to-date CV with publication list
- 2- Two letters of reference from academic supervisors or current employers (to be sent via email directly to gilles.frapper@univ-poitiers.fr)

The application deadline is 25 december 2017. The selected candidate is expected to start during the first semester 2018 (ideally 1st feb).

IC2MP – CNRS & Poitiers University: <http://ic2mp.labo.univ-poitiers.fr>

Theoretical Chemistry group: <http://yargla.labo.univ-poitiers.fr/>