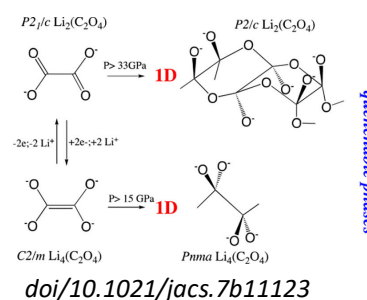


## PhD position in Computational Materials Discovery at Poitiers U. (France)

A PhD student position is available in Professor Gilles Frapper's theoretical chemistry research group at IC2MP, Poitiers university (France). The project will utilize mainly DFT VASP and evolutionary algorithm USPEX to predict and investigate **CO<sub>2</sub>-based materials** in the context of capture and storage of CO<sub>2</sub> and renewable organic-based materials batteries. Our interests center around structural chemistry and the geometrical-electronic control of properties and reactivity.

The project also requires regular visits to our partners from USPEX community for work discussions and theoretical development, *ie* USPEX leader Pr. AR Oganov groups at NPU (Xi'an, China) and MIPT/Skoltech (Moscow, Russia). This project follows our recent *JACS* article in CSP, *crystal structure prediction*, on Li-CO<sub>2</sub> phases under pressure.



**Desired qualifications:** 1) Master degree in theoretical chemistry, condensed physics or materials science, 2) solid understanding of quantum mechanics and experiences in computational material modeling at the atomic scale, 3) comprehensive experience on bonding analysis, and 4) scientific programming skills.

Excellent communication skills (English and/or French), both verbal and written, are required.

**Funding:** the net salary will be ~1 400 € /month during 3 years, starting October 1st (Ecole doctorale Gay Lussac at Poitiers U., national fellowship). 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](mailto:gilles.frapper@univ-poitiers.fr) before **April 15, 2018**, with the subject: " **PhD position in Computational Materials Discovery at Poitiers U.**".

The application should include:

- a detailed Curriculum Vitae,
- a cover letter describing why you should be considered for this position, answering the following questions: What materials modeling technique(s) do you have expertise in? What materials do you look at? What is your experience with software development (if any)? When might you start?
- transcripts of B.Sc. and M.Sc. courses and grades,
- copies of educational certificates, and
- a list of two professors who have supervised you in your B.Sc. and/or M.Sc. research project and who are willing to provide a letter of recommendation.

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 Skype (In CV, Skype address must be included).