MASTER DE PHYSIQUE ET APPLICATIONS - 2ème année

Spécialité Sciences des Matériaux et Nano-objets

UPMC Paris 6, ENS Ulm, Chimie ParisTech, ESPCI et l'École Polytechnique

Proposition de stage 2015-2016

Laboratoire : Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC)

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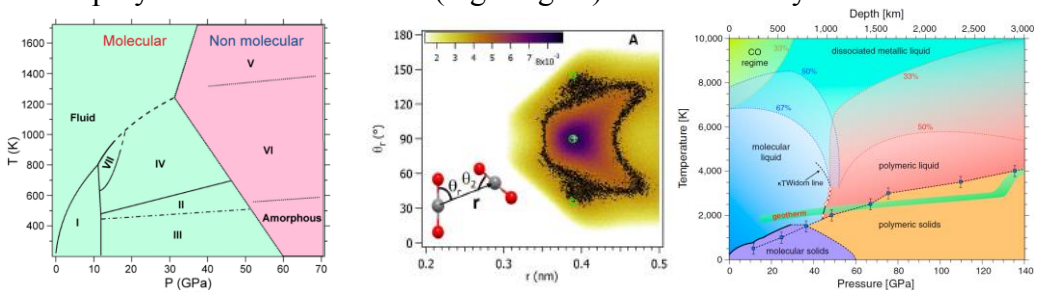
Ab initio metadynamics study of CO_2 polymerization at extreme conditions

Projet scientifique: Carbon dioxide is a predominant actor of greenhouse effect and global warming, and also a major component of geological fluids in the depth of Earth. However, the study of its structural properties and transformations at such high-pressure/high-temperature conditions is an experimentally challenging task, and the corresponding data often extremely difficult to treat. In this context, atomistic calculations represent an indispensable complement both in interpreting experimental data and in predicting novel behaviour and thus guiding experiments. In particular, our experimental/theoretical team has been particularly active in recent years in determining the phase diagram of solid CO_2 (Left figure, PRLs from our group in 2009 and 2012), as well as the structural transformation occurring in the liquid at moderate conditions (Middle figure, article submitted to PRL). However, the behaviour of fluid CO_2 at extreme conditions is unsolved yet, and its molecular-to-polymeric transformation (Right figure) unconfirmed yet.



In the present project, we aim at investigating in full depth the high-pressure/high temperature diagram by using state-of-the-art free-energy methods such as metadynamics, combined with topological, social-network-inspired approaches for the CO_2 phase space exploration (F. Pietrucci and A.M. Saitta, PNAS, under review). We look for a student willing to learn these innovative methods and determined to carry out the project in collaboration with the experimentalists of our group. Besides the above-mentioned articles, our theoretical team has a consolidated expertise and a strong publication record in the study of molecular systems under extreme conditions, including 4 PNAS in 2015, 1 PNAS and 1 SciRep in 2014, 2 PRL in 2013, 2 PRL in 2012. The ANR project "MOFLEX" supports since mid-2014 the experimental and theoretical activity on this project.

Techniques utilisées : Density-Functional Theory, Ab initio molecular dynamics, Metadynamics
Qualités du candidat requises : Basic computer and programming skills, strong motivation, basic knowledge and interest in physical chemistry.

Rémunération éventuelle du stage : oui, ~430 €/mois
Possibilité de poursuivre en thèse ? oui (en fonction des appels à projet en cours)
Quel est le mode de financement envisagé : Ministère, LabEx MATISSE, ANR, Sorbonne