



ÉCOLE DOCTORALE

SCIENCES DE LA TERRE ET DE L'ENVIRONNEMENT ET PHYSIQUE DE L'UNIVERS, PARIS

ed560.stepup@u-paris.fr

Advisor: **CARACAS Razvan, (DR), caracas@ipgp.fr**
Host lab/ Team : **IPGP- Equipe CAGE – UMR7154**
Financing: **Doctoral contract with or without teaching assignment**

Subject title: HOW IMPACTS SHAPED THE EARLY EARTH'S SURFACE AND ATMOSPHERE

We are proposing one PhD position to work on the large impacts that shaped the geological history of our planet during the Hadean, its first half a billion years. During this period, ongoing chemical reactions, volatile degassing, and interactions with the molten silicates played a crucial role in shaping the Earth's secondary atmosphere. The constant incoming of extraterrestrial material further shaped both this atmosphere and the warm surface. They contributed to the Earth's budget of volatile and moderately volatile elements, and helped preserve the active state of the surface, by fracturing the young thin crust and resurfacing fresh lava. Here we propose to study the chemistry promoted by shock at Hadean atmospheric conditions and the fate of various volatile elements during these highly energetic impact processes.

To address this, we will employ a combination of advanced ab initio molecular dynamics simulations and thermodynamic integration to obtain the free energy and the entropy generated by the impacts. Then we base on the results from the ab initio simulations to construct machine learning interatomic potentials. They will help scaling up our simulations in terms of both time scales and size scale. They will allow us to study the chemical reactions in detail.

Simulations will be conducted on national and European supercomputing facilities. The successful candidate needs to have a strong background in condensed matter sciences, molecular dynamics, and Python programming. Fluency in English is required. The PhD student will be hosted at the Institute de Physique du Globe de Paris (IPGP). IPGP is a world-renowned geosciences research institute founded in 1921, associated with the CNRS, a component of the Université Paris Cité and employing more than 500 people. The group of Razvan Caracas is highly active in computational mineralogy, study of matter at extreme conditions, and planetary mineralogy. We offer a competitive salary and benefits package and the opportunity to work in a stimulating and supportive research environment. The internship is supported by the ERC Advanced Grant DAWN.