



# ÉCOLE DOCTORALE

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

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**Subject title:** TOPOLOGY OF SILICATE LIQUIDS

**Advisor:** **CARACAS, Razvan (DR), [caracas@ipgp.fr](mailto:caracas@ipgp.fr)**

**Host lab/ Team :** **IPGP- Team CAGE – UMR7154**

**Financing:** PR[AI]RIE-PSAI Institute

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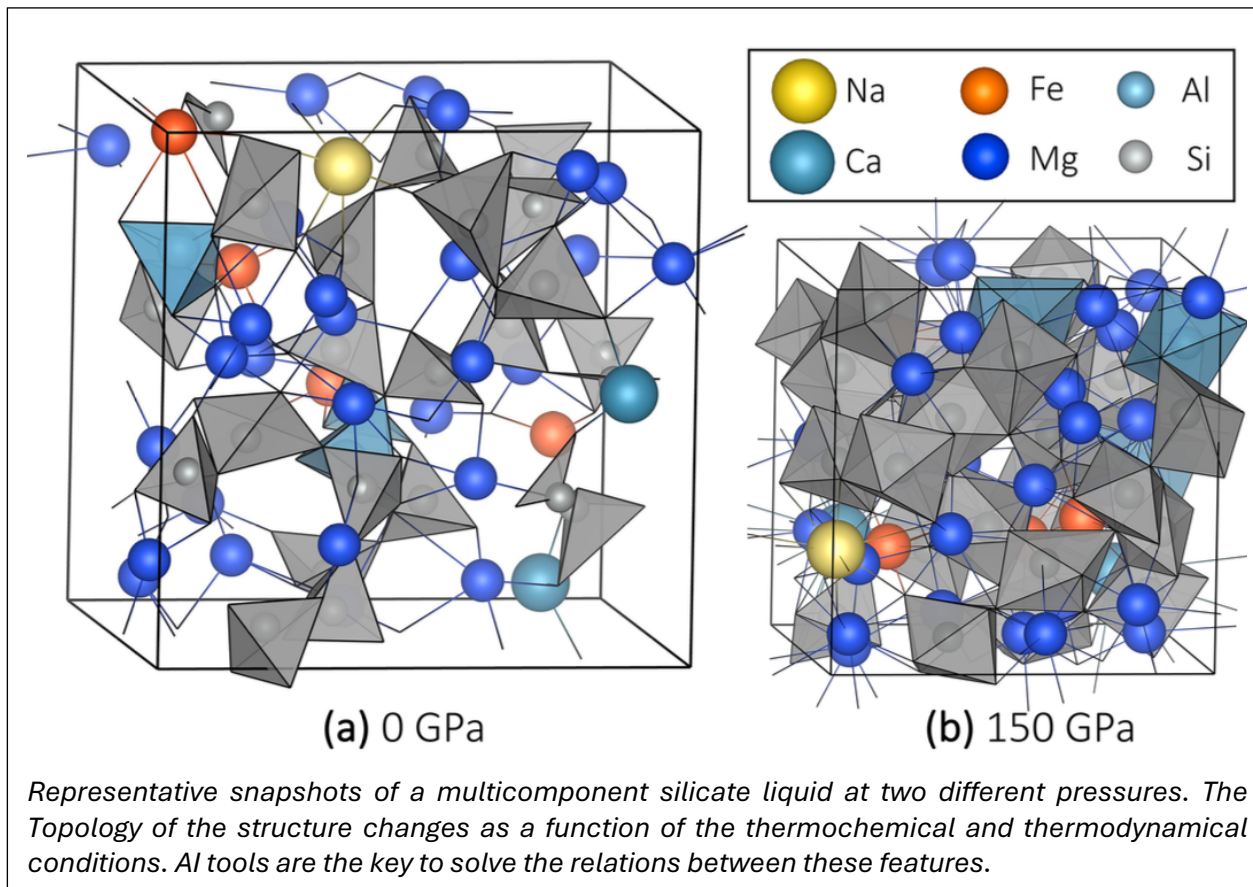
Silicates constitute the largest part of our planet. They constitute almost all the rocks we are walking on, down to almost 3000 kms depth. Their physical and chemical behavior contributed to make everything possible on our planet, including our own existence. At high temperatures, silicate lavas and magmas shaped the entire evolution of our planet, also producing some of the most catastrophic events in our history. In lavas and magmas, behind a large chemical variability atomic-scale structural units and their polymerizations determine all their physical properties and behavior at all scales.

Here, we focus on the analysis of silicate liquids. Starting with results of ab initio molecular dynamics simulations, we aim at using artificial intelligence to decipher the fundamental topological relations present in silicate lavas and magmas. We want not only to identify them, but also to relate them to variations in chemistry, pressure and temperature. Then we make connections over different scales and identify their relations with the macroscopic behavior of lavas and magmas. On this basis, we use the results of the AI analysis to propose new interatomic potentials that include both the topological analysis and the results of the molecular dynamics calculations.

The successful candidate needs to have a strong background in condensed matter sciences, molecular dynamics, and Python. She/he needs to have a strong interest in artificial intelligence techniques. 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 thesis will be led by Razvan Caracas (<https://razvancaracas.info/> [caracas@ipgp.fr](mailto:caracas@ipgp.fr)). The group of Razvan Caracas is highly active in computational mineralogy, study of matter at extreme conditions, and planetary mineralogy.

The successful candidate will be funded and thus be part of the PR[AI]RIE-PSAI Institute, an Institute for Interdisciplinary Research and Education in AI, founded by academic and industrial members. The PhD candidate will be part of a larger group of up to 16 PhD students with activities in AI, with whom active interactions are expected.



We offer a competitive salary and benefits package and the opportunity to work in a stimulating and supportive research environment.

Non-discrimination, openness, and transparency. All partners of PR[AI]RIE-PSAI are committed to supporting and promoting equality, diversity, and inclusion within their communities. We encourage applications from diverse backgrounds, and we will ensure that they are selected through an open and transparent recruitment process.