

Post-doctoral fellowship – Call for application
**Unlocking the potential of IA for the theoretical study of reactivity:
Application to the origin of Life**

Department of molecular chemistry (University Grenoble Alpes/ CNRS)

Prof. Anne Milet, DCM, SITH team

<https://dcm.univ-grenoble-alpes.fr/>

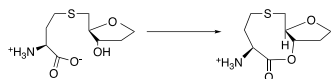
<https://dcm.univ-grenoble-alpes.fr/membre/anne-milet>

A Post-doctoral fellowship has opened up at the Department of Molecular Chemistry (DCM) at Grenoble, France. In an alpine setting and a remarkable scientific environment, the University of Grenoble Alpes welcomes more than 7000 PhD and post-doctoral students each year.

- Immediate opening
- Gross salary: from 3600 to 5000 €/month (depending on experience).
- MIAI funding : <https://miai.univ-grenoble-alpes.fr/>
- Duration: one year

Objectives:

The project focuses on the use of IA to study reactions linked to the origin of life. The project will be carried out in the SITH team in collaboration with Prof. Damien Laage (ENS, Paris) and Dr. Rolf David on the AI aspects and with Prof. Yannick Vallée and Dr. Véronique Blandin on the prebiotic chemistry aspects. We would therefore like to study a reaction in aqueous medium on the SAH molecule, derived from SAM (S-adenosylmethionine), which would be a key step in the setting up of the protein factory. This study falls within the framework of the TRP (Thiol Rich Peptide) world hypothesis, which is linked to the RNA (ARN) world hypothesis¹.



In view of the reagents used and the reaction paths proposed, simulations that explicitly include solvent effects are necessary. **We will therefore propose to use the software under construction ArcaNN coupled with**

deepMD² to determine the mechanisms involved. The candidate will interact regularly with the experimental team in Grenoble but also with our theoretical collaborator in Paris.

Applicant profile:

The successful candidate will have expertise in computational chemistry. Knowledge of neural networks potential like deepMD² or software for dynamics (cp2k or/and lammmps for example) will be appreciated. An open mind and broader chemical culture will also be a key asset for interacting with the experimental team.

Further information and application:

Contact Prof. Anne Milet by email (Anne.Milet@univ-grenoble-alpes.fr) ASAP. Please attach a letter of motivation, CV, list of publications and recommendation letter(s) (pdf format).

1 - Vallee, Y.; Shalayel, I.; Ly, K.-D.; Rao, K. V. R.; De Paëpe, G.; Märker, K.; Milet, A. At the Very Beginning of Life on Earth: The Thiol-Rich Peptide (TRP) World Hypothesis. *Int J Dev Biol* **2017**, *61* (8–9), 471–478. <https://doi.org/10.1387/ijdb.170028yv>.

2 - Wang, H.; Zhang, L.; Han, J.; E, W. DeePMD-Kit: A Deep Learning Package for Many-Body Potential Energy Representation and Molecular Dynamics. *Computer Physics Communications* **2018**, *228*, 178–184. <https://doi.org/10.1016/j.cpc.2018.03.016>.