An 18-months postdoctoral position is offered at the Université Pierre et Marie Curie – Sorbonne of Paris, under the supervision of Profs. A. Marco Saitta and Fabio Pietrucci.

The project, focused on advanced ab initio free-energy methods (metadynamics and beyond) to model the synthesis of fundamental biochemical bricks under realistic prebiotic conditions, will develop within a larger research consortium. This includes the experimental groups of Profs. M.-C. Maurel (Muséum National d'Histoire Naturelle), J.-F. Lambert and T. Georgelin (Chemistry Department of UPMC), and F. Guyot (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie), all in Paris. The fellowship, funded by the Sorbonne Excellence Cluster "MATISSE" (MATerials, InterfaceS, Surfaces, Environment), should start in 2016, at the earliest convenience.

The candidate should have a PhD in computational physics or chemistry, a solid background in reaction chemistry in solution and/or interface, a good experience in ab initio molecular dynamics and, ideally, in free energy methods. She/he will carry out ab initio, metadynamics-based, explorations of the synthesis channels of biochemically-relevant molecules, reconstruct free-energy landscapes and identify new reaction mechanisms. The candidate will also play a central role in interacting with the experimental partners, to suggest the most relevant experiments, and interpret experimental data and observations.

Interested candidates can apply electronically (CV including full publication list and references) by sending an email to: marco.saitta@upmc.fr

Our theory group is a young, dynamical and attractive one, including, besides Profs. Saitta and Pietrucci, 2 postdocs, 5 PhD students and 2 undergraduate interns. Our recent implication in prebiotic chemistry/origins of life is highlighted by recent invitations at the prestigious Goldschmidt and Gordon conferences; we will also organise in Paris in June 2016 the first CECAM workshop on prebiotic chemistry.

Publications related to the subject:

Saitta A.M., Saija F. (2014) *Miller experiments in atomistic computer simulations*. Proceedings of the National Academy of Science (PNAS) **111**, 13768.

Pietrucci F., Saitta A.M. (2015) *Formamide reaction network in gas phase and solution via a unified theoretical approach: towards a reconciliation of different prebiotic scenarios*. Proceedings of the National Academy of Science (PNAS) **112**, published online on Nov 23rd.

Tel: 33-(0)1 44 27 22 44 --**Fax**: 33-(0)1 44 27 37 85 - **Email**: marco.saitta@upmc.fr

Laporte S., Finocchi F., Paulatto L., Blanchard M., Balan E., Guyot F., Saitta A.M. (2015) *Strong electric fields at a prototypical oxide/water interface probed by ab initio molecular dynamics: MgO (001)* Phys. Chem. Chem. Phys. **17**, 20382-20390

Pietrucci F., Andreoni W. (2011) *Graph Theory Meets Ab Initio Molecular Dynamics: Atomic Structures and Transformations at the Nanoscale* Phys. Rev. Lett. **107**, 085504.

https://www.researchgate.net/profile/Antonino_Saitta2
https://www.researchgate.net/profile/Fabio_Pietrucci