Prebiotic chemistry at an oxide/water interface

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A simple prebiotic reaction ($CO+H_2O \rightarrow HCOOH$) has been investigated by computer simulations at an oxide/water interface. The MgO(001) surface was used as a model, as it promotes dissociation of protons within the two first water layers [1]. The free energy landscape for the reaction has been obtained using *ab-initio* metadynamics, a method which enables a short simulation explore reaction pathways which would otherwise occur on a longer timescale [2,3]. The energy barrier for the formation of formic acid (HCOOH) has thus been computed in the bulk liquid case, and in the near-surface case.

Results show that the product is stabilised when the temperature is increased, which is in agreement with experiments in which formic acid is obtained in hydrothermal conditions [4]. In the near-surface case, formic acid is significantly more stable than in the bulk liquid case. This shows that near-surface conditions alter free energy landscapes of chemical reactions, in a way which could be of importance for prebiotic geochemistry. Work is on-going to identify enthalpic and entropic contributions from the surface, as well as specific effects such as surface acidity and surface electric field. Perspectives involve studying the effects of a mineral surface in reactions involving formamide, which is a possible intermediate step in the formation of amino acids [5].

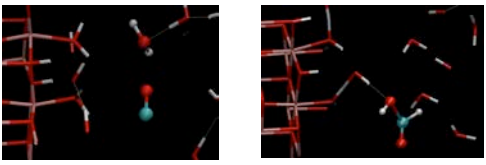

Figure 1: Snapshots of a metadynamics simulation in which the reaction $CO+H_2O$ □ HCOOH is observed.

[1] Laporte *et al.* (2015) *Phys. Chem. Chem. Phys.* **17** 20382.
[2] Pietrucci and Saitta, (2015) *Proc. Natl. Acad. Sci.* **112** 15030.
[3] Laio and Parinello (2002) *Proc. Natl. Acad. Sci.* **99** 12562.
[4] Yasaka *et al.* (2006) *J. Phys. Chem. A* **110** 11082.
[5] Saitta and Saija (2014) *Proc. Natl. Acad. Sci.* **101** 13768.