

July 16-21, 2017 at UC San Diego, CA, USA

From quantum computational physics to the origins of life

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Computational approaches are nowadays a full, self-standing branch of chemistry, both for their quantum-based (“*ab initio*”) accuracy, and for its multiscale extent. In prebiotic chemistry, however, due to the intrinsic complexity of the chemical problems, *ab initio* atomistic simulations have so far had a limited impact, with the exception of a few relevant studies, including the elucidation of the chemical interactions between biomolecules with surfaces, such as ice and minerals, or the simulation of the effect of the pressure/temperature shock waves induced by meteorite impacts in the early Earth. Surprisingly, even the celebrated Miller experiments, which historically reported on the spontaneous formation of amino-acids from a mixture of simple molecules reacting under an electric discharge, have never been studied at the quantum atomistic level.

Here we set the general problem of chemical networks within new topology-based concepts, using search algorithms and social network data analysis. This allows a very efficient definition of reaction coordinates even in the complex chemical environments which are typical of likely prebiotic scenarios. We thus report on the first *ab initio* computer simulations, based on quantum physics and a fully atomistic approach, of Miller-like experiments in the condensed phase. Our study [1] shows that glycine spontaneously form from mixtures of simple molecules once an electric field is switched on. We identify formic acid and formamide [2] as key intermediate products of the early steps of the Miller reactions, and the crucible of formation of complex biological molecules, as confirmed by our recent experimental and theoretical study on high-energy chemistry of formamide [3]. From a broader chemical perspective, we show that formamide plays the role of hub of a complex reaction network in both the gas and the condensed phase [4]. We are now going on a larger scale, studying the atomistic mechanisms of RNA nucleotides synthesis in fully realistic prebiotic solution environments [5]. All these results pave the way to novel computational approaches in the research of the chemical origins of life.

References: [1] Saitta AM and Saija F (2014) *Proceedings of the National Academy of Sciences USA* 111:13768-13773. [2] Saitta AM, Saija F, Pietrucci F, and Guyot F (2015) *Proceedings of the National Academy of Sciences USA* 112, E343-E343. [3] Ferus M et al. (2017) *Proceedings of the National Academy of Sciences USA*, to appear. [4] Pietrucci F and Saitta AM (2015) *Proceedings of the National Academy of Sciences USA* 112, 15030-15035. [5] Perez-Villa A et al. (2017) *in preparation*.

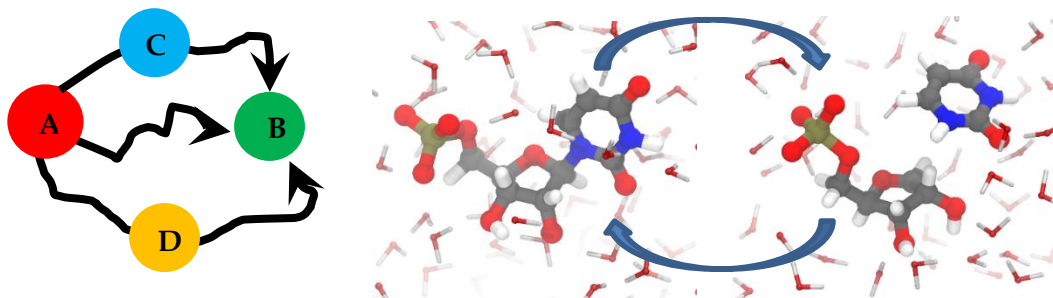


Figure 1 – Left, pictorial representation of the reaction paths connecting A and B, with possible C or D intermediates. Right, example of a fully quantum atomistic simulation of the A-to-B degradation/synthesis reaction between one uridine mono-phosphate nucleotide and one uracil plus a phosphoribose, in explicit water solution.