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From computational physics to the origins of life

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Here we set the general problem of ab initio calculations in prebiotic chemistry by defining chemical networks within a new topology-based definition of reaction coordinates [1]. We thus report on the first ab initio computer simulations, based on quantum physics and a fully atomistic approach, of the celebrated Miller experiment in the condensed phase. Our study [2] shows that glycine spontaneously form from mixtures of simple molecules once an electric field is switched on. We identify formic acid and forma-mide [3] as key intermediate products of the early steps of the Miller reactions, and the cruci-ble of formation of complex biological molecules, as confirmed by our recent experimental and theoretical study on high-energy chemistry of formamide [4]. From a broader chemical per-spective, we show that formamide plays the role of hub of a complex reaction network in both the gas and the condensed phase [5]. We are now going on a larger scale, studying the atomistic mechanisms of RNA nucleotides synthesis [6], meteoritic amino acids [7] and sugars [8] in fully realistic prebiotic solution environments. All these results pave the way to novel computa-tional approaches in the research of the chemical origins of life [1].
References: [1] Physics of Life: Reviews (2019). [2] PNAS (2014). [3] PNAS (2015a). [4] PNAS (2017). [5] PNAS (2015b). [6] J. Phys. Chem. Lett. (2018). [7] ACS Earth Space Chem (2018). [8] Chem Comm (2018).

Choix de session parallèle

5.4 Physique et origines de la vie

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