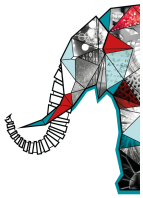
25e Congrès Général de la Société Française de Physique



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Hydrothermal prebiotic reactions of biological building blocks: A study from ab initio molecular dynamics simulations

jeudi 11 juillet 2019 09:45 (15 minutes)

Synthesis and degradation of biological building blocks in the primitive Earth is one of the most challenging issues in the origins of life field. In this context, many works have been dedicated to address their reactivity under different plausible prebiotic conditions, including the catalytic function of mineral surfaces, the role of salts or lipid compounds, the exposure to drying/wetting cycles, and so forth. Nowadays, one of the main goals is to achieve the formation of nucleotides and amino acids, under plausible primitive environments and starting from prebiotically relevant substrates.

In this work, we explore the reactivity of nucleotides and amino acids under mild hydrothermal prebiotic conditions, performing ab initio molecular dynamics simulations in explicit water molecules. Moreover, we exploit free-energy methods in combination with a topological approach developed in our team that accurately tracks the chemical bond network along a reaction path. From this methodology, we are able to unveil the thermodynamical properties and the mechanistic features of the plausible prebiotic chemical reaction at atomistic level.

Choix de session parallèle

5.4 Physique et origines de la vie

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Classification de Session: Séance Parallèle