

Early Stages of Diamond Rain formation in Icy Giants

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The chemistry of icy giants such as Neptune and Uranus has attracted great attention from the scientific community in the last three decades. The interiors of such planets are believed to be mainly composed of a dense fluid which is a mixture of water, methane, and ammonia. The extreme conditions of pressure and temperature ($T > 1000$ K, and $P > 3$ GPa) in those interiors imply complex chemical transformations that dictate many of these planets' chemical and physical properties. In this regard, the formation of diamonds and super ionic water (diamonds rain) from the planetary mixture has been invoked to rationalize their luminosity and anisotropic magnetic field. The absence of direct astrochemical observation into the process, the difficulty in characterizing the transformation in situ from experiments due to the extreme conditions and chemical inhomogeneities, make atomistic simulations a valuable tool to get microscopic insights into the transformation. In this talk, I will present the results of our computational study on the reactivity of water/methane mixture under extreme conditions mimicking the icy giants' interiors.

In particular, we have combined ab initio molecular dynamics with state-of-the-art enhanced sampling techniques (metadynamics, umbrella sampling) to characterize the mechanisms and free energies of the early stages of diamond formation (hydrocarbon chain elongation, branching reactions and cyclisation).

With such approach, we have been able to identify the elementary chemical channels through which the hydrocarbon growth proceeds, providing an unprecedented mechanistic insight into the process at extreme conditions. Furthermore, the computation of the energy profiles, coupled with an accurate structural, dynamical and electronic characterization of the reaction environment, sheds light on the key role of the dissociated water in:

- i) generating carbon ions accountable for the observed reactivity
- ii) its direct implication in the hydrocarbon growth.