Study of the Adsorption of Volatiles and Surface Processes on Astrophysical Ices and Clathrates using Molecular Simulations

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Solid water in the universe can be found as crystalline or amorphous ices, according to the local thermodynamic conditions. Besides, solid water can also exist in the form of clathrate hydrates when water molecules are mixed with other gases. Indeed, these compounds, while ubiquitous on Earth, have also been suspected to be widely present in various astrophysical environments.

The relevance of solid water in astrophysics research is associated with the role that ice may play in interstellar chemistry, the latter now being recognized as a significant pathway for the synthesis of molecules in space. Namely, an important question linked to astrophysical ices is the origin of prebiotic materials. However, most often, only exothermic and barrierless reactions can proceed in the gas phase, and some species, especially organic molecules, cannot be efficiently produced without invoking surface reactions. Henceforth, a thorough characterization of the surface processes on astrophysical ices appears to be of fundamental interest for enhancing our understanding of the celestial formation of prebiotic molecules.

In this astrophysical context, interactions of gaseous compounds with solid water surfaces have been widely studied in the laboratory during the past decades. To gain more insights regarding the details of the adsorption and surface processes, numerical simulations can well complement experimental investigations. Here, we discuss the results of molecular simulations of the adsorption of several volatiles, including ones of prebiotic interest, performed at astrophysical temperatures and pressures, on four different solid water surfaces: crystalline hexagonal ice, low density amorphous ice, and structures I and II clathrate hydrates. As far as clathrates are concerned, we also characterize the competition between trapping at the surface and incorporation in the bulk of the system. The thermodynamic interpretations of those results and their implications on several astrophysical scenarios are presented.