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Gas trapping at the ice surface and in clathrate hydrates under astrophysical conditions, as studied by GCMC simulations

MR. JULIEN JOLIAT[1], ANTOINE PATT[2] AND SYLVAIN PICAUD[3]

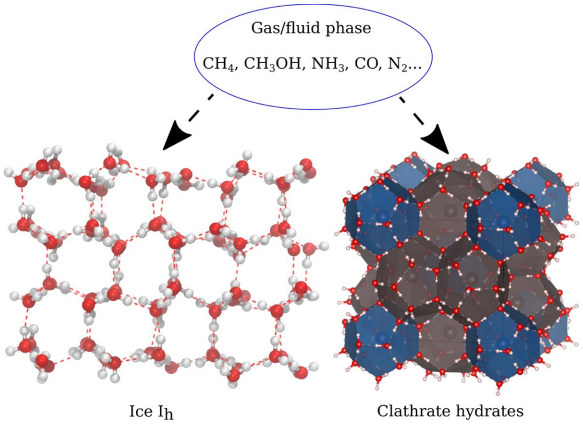
[1]Institut UTINAM
[2]Centro de Fisica de Materiales, CSIC – UPV/EHU
[3]Institut UTINAM - UMR 6213 CNRS/UBFC

Presenting Author: julien.joliat@edu.univ-fcomte.fr

The prevalence of water ice in the Solar System and interstellar medium has been evidenced, with examples found on icy moons such as Enceladus, Europa, Titan, and Triton, as well as on interstellar grains. These ices may be able to trap organic molecules, as it has been theoretically inferred on Enceladus [1].

Natural clathrate hydrates may also be present in these environments where they are suspected to play a role in the evolution of planetary atmospheres and/or oceanic compositions. Moreover, due to the unique environmental conditions present in extraterrestrial environments, clathrate hydrates not observed on Earth may be stabilized there.

Because of the difficulty of reproducing these conditions in laboratory experiments, Monte Carlo molecular simulations in the grand canonical ensemble (GCMC) have been used to study, at the molecular scale, the surface adsorption of organic compounds on ice [2,3] and to characterize the trapping of gas mixture in clathrate hydrates [4,5]. These simulations have been used primarily in astrophysical contexts, where experimental data are limited, to provide useful information to the planetary and astrophysical communities.



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