« INVESTIGATIONS OF THE IMPACT OF MINERAL IMPURITIES ON GAS TRAPPING SELECTIVITY WITHIN HYDRATES »

Description. Gas hydrates are nanoporous crystalline solids composed of hydrogen-bonded water molecules forming cages within which gaseous molecules are encapsulated. Since their initial discovery, interest in gas hydrates has grown exponentially from being of mere scientific curiosity to offering a potential new energy solution to the imminent energy crisis. Gas hydrates are considered to be pivotal terrestrial and extraterrestrial ingredients, as they make up a great part of the Earth's seafloor sediments and play a role in extraterrestrial planetary formation scenari. A very important observation common to both terrestrial and extraterrestrial gas hydrates is that they are predominantly and naturally formed in the presence of porous dusty ice media, possibly enriched in minerals, hydrated salts and/or sediments. The impact of these mineral impurities onto the physical-chemistry properties of gas hydrates (trapped-gas selectivity, thermodynamic promotion or kinetics modification) is of prime importance to track the evolution of the abundances of species taking part in the compositions of hydrate-bearing deposits on Earth and on extraterrestrial bodies. Since the hydrate morphology and distribution both depend on the medium property (chemical composition, hydrophobicity, pore space, bulk stiffness), a fundamental understanding of the hydrate selectivity, thermodynamics, formation and dissociation mechanisms onto/into mineral-like media appears to be crucial. The position falls in this research context and aims at investigating, at a fundamental level, the underlying factors governing the gas selectivity and formation/dissociation mechanisms in mixed clathrate hydrates formed in the presence of mineral defects to mimic their natural environment (e.g., planetary and cometary bodies, deep oceans, permafrost of terrestrial and extraterrestrial origin). The PhD research program will be devoted to the physico-chemical investigations by combining (ab-initio) molecular dynamics simulations, neutron scattering (inelastic and diffraction) and Raman spectroscopy. Consequently, the proposal encompasses the investigation of mixed clathrate hydrates in thermodynamics conditions relevant to geological and astrophysical environments, and will thoroughly explore the influence of mesoscopic surrogates present in these natural media during clathrate formation. The latter objective constitutes the key novelty of this project.

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