Computational Studies of Spectroscopic Properties of Hydrocarbons at the Air-Ice Interface

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The interfacial non-covalent interactions between ice surface and organic molecules have been studied by different experimental techniques and computational approaches. The understanding of these physical phenomena is critical for modeling of chemical processes occurring in polar regions.

The ground state molecular dynamics simulations and DFT calculations, as well as the excited state ADC(2) calculations are used to discuss the occurrence of ground- and excited-state complexes (excimers) and other associates of benzene, naphthalene and methyl-naphthalene on the ice surface. The results of these calculations are used to interpret the excitation and emission spectra obtained in aqueous solution and at the air-ice surface.