Adsorption of PAHs on interstellar ice viewed from molecular dynamics

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Polycyclic Aromatic Hydrocarbons (PAHs) have had an astrophysical interest since they were proposed, in the mid-eighties, to be the carriers the Aromatic Interstellar Bands (AIBs), a set of infrared (IR) emission bands observed in the [3 - 15 µm] range in many regions of the interstellar medium (ISM). PAHs would also be potential candidates to carry the Diffuse Interstellar Bands (DIBs), which are weak absorption bands measured between 0.38 and 1.3 µm on the extinction curve of our galaxy. Besides, PAHs are likely to play a role in the chemistry of the ISM as, for instance, they would form stable complexes with iron, thus contributing to the iron depletion from the gas phase of the ISM. In molecular clouds, some gases are condensed on dust particles and form ice mantles essentially made of water. PAHs may also condense on/in these ices and contribute to the complex grain chemistry [1]. This heterogeneous chemistry plays a fundamental role in presence of the adsorbed water, which catalyzes photochemical processes.

Although ice has been extensively investigated by IR spectroscopy [2], few studies of ices containing PAHs have been reported. To shed light on the unexpected role played by PAHs in cosmic ice chemistry, IR spectroscopy experiments on the cryogenic codeposition [3] of PAH and water are achieved at the Institut des Sciences Moléculaires (ISM, Bordeaux).

In connection with these experiments, we model PAHs interacting with various icy environments using a multi-method approach. The aim is to identify configurations that could best describe the experiments and provide quantitative indications on the effect of the environment on the IR spectra. Our strategy consists in (i) determining the most relevant PAH-ice configurations with a MD/FF (Molecular Dynamics/Force Field) approach [4] and (ii) extracting from such structures starting point finite-size configurations for further Density Functional based Tight Binding (DFTB) calculations, the latter approach describing the electrons explicitly. Results on the effects of the icy environment on the ionization potentials of PAHs and on PAHs' IR spectra - and reciprocally on the effect of PAH adsorption on the IR spectrum of ice- obtained with such a DFTB-based approach will be presented.

References

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Funding : Program ANR-08-BLAN-0225-03.