

Application of Reactive Molecular Dynamics on Astrochemical interest systems.

M. Pezzella¹

¹University of Basel

The combination of quantum and classical methodologies is a winning strategy for studying astrochemical phenomena, making possible to explain telescopic observations. In this work two reactive events are studied in this way, using Reactive dynamics performed using MS-ARMD (Multi-Surface Reactive Dynamics) [1] module present in CHARMM[2].

The first study regards the formation of O₂ in the Interstellar Media (ISM): this species is considered the first reservoir of atomic Oxygen, but there are only few observations that support this hypothesis. Mass-spectrometric observations of comet colas suggest that O₂ is highly correlated with water ice grains[3]. After characterizing the ice structure at ISM temperature regime, 50 K, reactive simulations are performed inside the ice bulk and on top of its surface, using a MRCI Potential Energy Curve to describe O₂. The majority of the reactions are observed within the first 5 ps of simulation, showing the ability of the ice morphology to catalyze the reaction. The scarce interaction between O₂-H₂O has as consequence a slow relaxation of the new formed molecule that is estimated on the 100 ns time scale., in the meanwhile it acts as a heat source for the bulky ice increasing the temperature of 15 K during a 5 ns time scale.

The second example investigates the interaction of fullerene cations with hydrogen (C₆₀H⁺ and C₆₀H₂⁺). It results of particular interest in both astrochemical (as can be used to trace the fullerene contributions to the Carbon abundance in the Universe) and technological (due high capacity of these species of storing Hydrogen) fields. The energetic profiles are characterized via B3LYP/6-31g(d) calculations. The chemisorption of one hydrogen atom on fullerene results in 85.87 kcal/mol stabilization, and consequent possibility of diffusion on top of the adsorbate specie (barrier of 29.45 kcal/mol). Nanosecond MD simulations shows the equivalence between the different adsorption sites. In agreement with previous studies on Carbon Nanotubes [4], H₂ bond is broken during the chemisorption.

In both example the use of MS-ARMD techniques shows up to be important: Ab-Initio levels results can be easily reproduced at cost of a classical simulations. The inclusion of possibles diabatic crosses between PES is planned as further improvement of this module, opening the possibility to study more complicated photochemical processes.

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