# Collision-induced dynamics of PAH-water clusters

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Polycyclic Aromatic Hydrocarbons (PAHs) are a family of molecules that have several research interests, especially in environmental science and astrochemistry. In the dense and cold regions of the interstellar medium (ISM), it is believed that PAHs could condense on the icy surface of interstellar nanograins and interact with other molecules like water[1]. Understanding PAH-water interactions motivated both experimental and theoretical studies, to which our group has contributed significantly[2,3]. With theoretical models, exhaustive studies can be conducted to cover the diversity of the PAH family in the ISM: different charge states, (de)protonation states, PAHs with side groups, PAH clusters, etc.

We present here a study on collisions involving protonated pyrene, where pyrene (Py) is a PAH ($C_{16}H_{10}$), and water clusters: (Py-H)$(H_2O)_n$. The collisions were simulated by on-the-fly Born-Oppenheimer Molecular Dynamics (BOMD), along with the Self-Consistent Charge Density Functional based Tight-Binding (SCC-DFTB) potential to compute the electronic energy[4]. This potential, which can be seen as an approximation of the Density Functional Theory (DFT) method, allows inexpensive calculations that still maintain a quantum description of the electrons. Thousands of simulations (of around 20 ps) can be run in a reasonable amount of computational time.

Low-energy (50 meV) collisions of astrophysical interest between protonated pyrene and water molecules ($n = 1 - 4$) were simulated. High-energy (7.5 eV) collision-induced dissociations by argon atoms were simulated as well ($n = 1 - 5$), to complement experimental results[5].
Properties such as sticking efficiency, influence of the protonation site, structures of the adducts, and branching ratios were derived from these calculations. Due to its symmetry, pyrene presents three non-equivalent protonation sites. Successive collisions at low energy with water molecules reveal different types of PAH-water interactions according to the protonation site (proton transfer, pyrene oxidation, etc.). As for the structural properties, they were compared to "classic" Monte Carlo simulations. On the other hand, collisions at high energy with an argon atom provide data that were gathered up as mass spectra. The question of the charge (de)localisation will also be addressed.

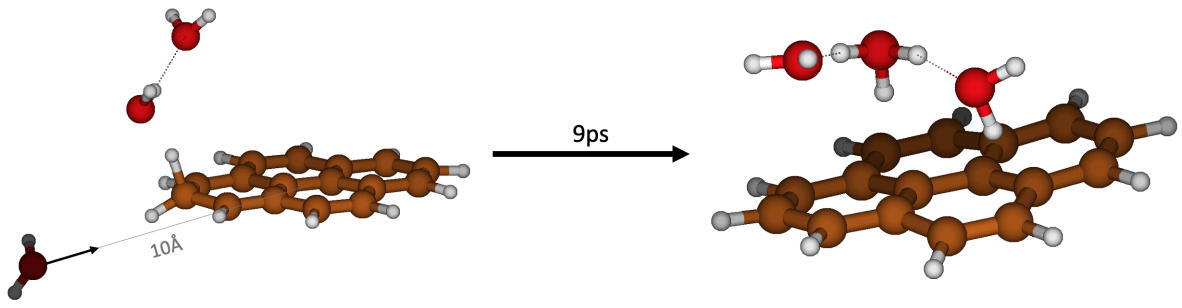


Figure 1: Illustration of a collision at 50 meV, between a water molecule and (Py-H)$(H_2O)_2$

**Keywords**: PAH, water, DFTB, molecular dynamics, collision

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