Interaction of Oxygen (X,^{3}P) atom with graphenic-like surfaces for astrophysical applications

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In the interstellar medium (ISM), dust grains play a key role in mediating the formation of molecular species. In order to understand and quantitatively describe the related reactive processes, it is of a strong interest to study the interactions (and reactions) of H, C, O atoms present in the interstellar clouds with (and at) grain surfaces.

Many studies have been devoted to the adsorption of hydrogen atoms, the most abundant atomic species in interstellar clouds, and to the formation of H_2 by H recombination/abstraction processes onto the surface of carbonaceous dust grains. We have shown that the atomic adsorption characteristics (physisorption/chemisorption wells, adsorption barrier, defects) play a major role in the molecular formation [1], [2].

In the ISM, the oxygen is the third abundant element after H and He. The atomic oxygen is implied in the formation of heavier molecules such as OH [3], H_2O. In this context, we have studied the adsorption of the atomic oxygen in the fundamental state ^{3}P on a carbonaceous grain. Indeed previous works have been mainly devoted to the singlet state and only a few to the triplet state [4] [5].

Our theoretical studies have been performed by means of spin polarized DFT/GGA calculations. The grain surface is modeled either as a graphene sheet or as PAH molecules ($C_{24}H_{12}$, $C_{54}H_{18}$). We have considered several adsorption sites: on top of a C atom of the surface, bridged between 2 adjacent C atoms of the surface.

We have obtained adsorption energies and geometries in agreement with previous works [4] [5]. Our main result is the barrierless chemisorption of the atomic oxygen in the ^{3}P state onto graphenic surfaces. The chemisorption characteristics are site dependent. Regardless of the surface considered, the more stable chemisorption site is the top site.

At larger surface-oxygen distances, the physisorption of the atomic oxygen in the ^{3}P state onto graphenic surfaces is also obtained. Depending on the surface, the physisortion characteristics are weakly site dependent.

All these electronic/structural studies, including relaxation of surrounding carbon atoms, are the first step needed for the study of the OH/H_2O formation dynamics in order to obtain reaction probabilities, energy sharing between the nascent molecules and the surface.

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