SEMINAIRE ISMO (LCAM - LIXAM – LPPM)

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Theoretical study of simple molecules formation in interstellar media : the H_2 case

How can simple molecules, in particular the most abundant H_2 molecule, form in the interstellar space considering that even in the densest interstellar clouds atoms are too spread out? It has been proposed that molecular hydrogen may be formed on carbonaceous surfaces of dust particles. Due to the low temperatures of interstellar media, to be viable the discussed process should have no, or very little, barrier. In this presentation I will discuss the results of DFT simulations of atomic H chemisorption onto different graphitic like surfaces. First, I will analyze the hydrogen interaction with perfect graphene. Beyond several earlier works on this topic, I will focus on some new key points which have not been discussed so far. Then, I will propose a new point of view on which topological defects play a key role for molecular catalysis at dust grains. In that case DFT-NEB calculations will be used to find out the reaction path and the associated reaction barriers.

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Mardi 19 janvier 2010 à 11 h 00
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