

Master 2: International Centre for Fundamental Physics

INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: ISMO (INstitut des Sciennces Moléculaires D'Orsay)
CNRS identification code: UMR 8214
Internship director's surname: Sabine Morisset
e-mail: sabine.morisset@universite-paris-saclay.fr Phone number: 01.69.15.78.63
Web page: <http://www.ismo.universite-paris-saclay.fr>
Internship location: ISMO, Bâtiment 520 Université Paris-Saclay 91405 Orsay Cedex

Thesis possibility after internship: YES
Funding already obtained for a PhD: NO If YES, which type of funding:

STICKING OF A H ATOM AND A GRAPHENIC SURFACE INCLUDING RELAXATION OF THE SUBSTRATE : EFFECT OF THE ANAHARMONICITY ON PHONON MODES

Molecular hydrogen H_2 , one of the most abundant molecules in InterStellar Medium (ISM), can be formed by association of H atoms on interstellar dust grains. In our study, these grains will be modelled as graphenic surfaces. Two distinct mechanisms are usually assumed for these reactive processes: (i) two H atoms, in weak interaction with the grain (physisorption), may collide to form an H_2 molecule, which is subsequently released in the gas phase; (ii) a H atom in strong interaction with the surface (chemisorption) can react with an impinging H atom from the gas phase to form H_2 . In both cases, a precise determination of the probability of the first adsorption of a H atom is crucial for subsequent simulations of the H_2 formation. This information, in turn, is essential in other more applied areas such as hydrogen storage [1] or graphene technology [2].

Both of the mechanisms of formation of H_2 involve energy transfer between the sticking particles and the surface, thus leading to energy redistribution among the phonon bath of the substrate. Consequently, in addition to describing the motion of the reacting atoms, it is very important to accurately take into account the dissipation processes (phonon modes) induced by the nuclear degrees of freedom of the surface. The H atom interaction with a graphene surface may involve either weak dispersion interactions at large distances (physisorption) or stronger interactions at shorter distances (chemisorption). More specifically, an H atom chemisorbed on a surface C atom induces a local deformation ("puckering") of the surface. This, in turn, translates into an activation barrier (of about 0.2 eV) for the chemisorption process. Conversely, the physisorption process is barrierless. In this respect, the sticking of an H atom on graphenic surfaces has been object of many dynamical studies (quantum, classical, and mixed quantum-classical), either in a chemisorbed state [3-7] or in a physisorbed state [8,9]. However, the simultaneous study of both chemisorbed and physisorbed states in a same calculation has not been tackled yet.

The objective of this internship is to treat both the chemisorption and physisorption processes in a single reaction dynamics calculation, using a novel quantum-classical trajectory method. For this, we propose the calculation of the vibrational modes and couplings between the surface and the motion of the individual H atoms. The coupling among the vibrational modes will be obtained from the eigenvectors of the dynamical matrix of the solid. In the harmonic approximation, the vibrational modes will be calculated by means of the Quantum Espresso computer code suite. Moreover, we will investigate the effect of the anharmonicity on the phonon modes. To tackle this study, notions in solid state physics would be useful. These calculations will constitute the first step in the ANR HYTRAJ project (HYbrid quantum TRAjectory approach for low temperature reactive processes in condensed phase) in which novel quantum-classical trajectory methods are being developed. This ANR project is a collaboration between three laboratories (ISMO and ICP at Orsay and LUPM at Montpellier).

[1] V. Tozzini, V. Pellegrini, Phys. Chem. Chem. Phys., 15:80-89, 2013; [2] M. Bonfanti, S. Achilli, R. Martinazzo, J. Phys.: Condens. Matter., 30:283002, 2018; [3] S. Morisset and A. Allouche, J. Chem. Phys., 129:024509, 2008, [4] M Bonfanti, B. Jackson, K.H. Hugues, I. Burghardt, and R. Martinazzo, J. Chem. Phys., 143:114705, 2015; [5] M Bonfanti, B. Jackson, K.H. Hugues, I. Burghardt, and R. Martinazzo J. Chem. Phys., 143:124704, 2015; [6] F. Karlicky, B. Lepetit, and D. Lemoine, J. Chem. Phys., 140:124702, 2014; [7] S. Morisset, Y. Ferro, A. Allouche, J. Chem. Phys., 133:044508, 2010; [8] B. Lepetit and B. Jackson. Phys. rev. Lett., 107:236102, 2011; [9] B. Lepetit, D. Lemoine, Z. Medina, and B. Jackson. J. Chem. Phys., 134:114705, 2011.

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES Soft Matter and Biological Physics: NO

Quantum Physics: YES Theoretical Physics: YES