Laboratoire d'Étude du Rayonnement et de la Matière en Astrophysique

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## Projet de recherche sous-jacent à l'invitation de Albert RIMOLA au LERMA en 2016

### Contexte scientifique

In regions where stars are forming, about one percent of the mass is in the form of sub-micrometer sized ***dust particles.*** However small and insignificant these dust grains may seem, they are now recognized as powerful i***nterstellar catalysts*** and are responsible for most of the production of the simplest ($H_2$) to the most complex (pre-biotic) molecules observed in our Universe. In addition, since dust particles are interacting with the gas, the chemical composition and thermodynamics of a gas cloud forming stars depends on gas-dust interactions.
Theoretical models have begun to consider the interplay between gas and dust to reproduce observations from different astrophysical environments. To constrain the different chemical processes involved in the gas-dust interplay, the need for **laboratory experiments** under astrophysically relevant conditions has increased considerably in the last decades. However, the step to go from laboratory results to astrochemical models is far from being trivial (different time scales, simplified conditions, assumptions made to derive the parameters needed for models...), and **need specific efforts to be integrated into current astrophysical models**. One of the major point to validate the pertinence laboratory data is to understand the chemical mechanisms at play thanks to the **solid state quantum chemistry**.

### Complémentarité et synergies des expertises.

The focus of the research of Dr. A. Rimola has always been on modeling chemical processes by accurate quantum chemical calculations using both molecular and periodic ab−initio approaches. Authors of about 50 publications in his domain, A. Rimola has turned is interest on the modeling of processes of astrochemical and prebiotic interest in which solid state systems (namely, cosmic dust, dirty ices and natural minerals) play an important role. On the other hand LERMA Cergy group is a well established expert of the solid-state chemistry devoted to astrophysics. Very recently, A. Rimola and F. Dulieu have worked on the formation of methanol on very cold surfaces[1], one from the chemical chemist's point of view and the other using the methods of surface science. Comparing this two complementary approaches of this key astrophysical problem should lead to very rapid an precious results.

### Enjeu pour le laboratoire

Avec la création récente (2014) d'un département d'astrochimie, le Max-Planck-Institut fur extraterrestrische Physik (MPE) de Garching s'est positionné comme l'un des acteurs majeur de notre discipline https://www.mpe.mpg.de/2169/en. Paola Caselli en a pris la direction. Une collaboration avec ce nouveau groupe a été définie comme l'une des priorités du LERMA, assignée par la direction du conseil scientifique de l'Observatoire de Paris. A la fois A. Rimola et F. Dulieu sont déjà associés à un programme clé d'Observation (**SOLIS, 40 partenaires, PI : P. Caselli et C. Ceccarelli**). L'une des 5 molécules cibles de l'observation est le méthanol. L'invitation de A. Rimola s'inscrit donc dans la même logique que celle d'Anton Vasyunin en 2015, qui fait également partie du groupe de Garching et du programme SOLIS. L'invitation de l'an passée a été fructueuse puisqu'un article est sur le point d'être soumis et que F. Dulieu a été sollicité pour une conférence invitée à Berlin en octobre 2015[5].

Gennevilliers le 10/09/2015

## *ANNEXES :*

**Work Plan**

1. *H addition to CO vs. H abstraction of $H_2CO$. Clues from quantum mechanical calculations.*

It is well known that successive H additions to CO leads to the formation of $H_2CO$ first and then $CH_3OH$. However, recent results of Cergy's group[2] indicated that H abstraction of $H_2CO$ via the H + $H_2CO$ reaction yielding formation of $H_2$ and CO can also take place. With the aim to rationalize these puzzling results, we plan to investigate by means of quantum chemical calculations these two competitive processes both in the gas phase and on icy grains. These calculations will allow us to understand the electronic structure nature of the reactions and to characterize the respective energy profiles, where several energy-related data (e.g., activation energies) will be obtained helping us elucidate the most favorable paths.

2. *Ab initio molecular dynamics simulations of O diffusion on water ices.*

Recent results of Cergy's group revealed that O atoms on water ices diffuse relatively faster than one would expect considering the very low temperatures of the experiments [34]. Moreover, it was found that such an O diffusion was dependent on the water ice structural state. In order to understand the O surface diffusion, we plan to develop a theoretical study based on ab initio molecular dynamics simulations (AIMD) where the O diffusion will be simulated on different water ice phases; i.e., hexagonal ice, cubic ice, and amorphous ice. AIMD will allow us to study how the systems evolve with time at a given temperature, and diffusion coefficients will be derived, which will be compared with the experimental ones.

## *References*


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4. Congiu, E. *et al.* Efficient diffusive mechanisms of O atoms at very low temperatures on surfaces of astrophysical interest. *Faraday Discuss.* **168,** 151 (2014).
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