

## Sorbonne Université/China Scholarship Council program 2021

### Thesis proposal

Title of the research project: **Prebiotic chemistry on the surface of cosmic dust grains: From interstellar dusts to planetary atmospheres**

Keywords: Interstellar Medium, Exobiologically-relevant species, Astronomical observations, Solid-gas interface, Radical reactivity, Interstellar ice analogs, Astrophysical models, IR spectroscopy, Mass spectrometry.

Joint supervision: no

Joint PhD (cotutelle): no

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Institution: Sorbonne University

Doctoral school (N°+name): ED 388 - Chimie physique et chimie analytique de Paris Centre

Research laboratory: MONARIS UMR CNRS-SU 8233

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## **Subject description (2 pages max):**

### **1) Study context**

More than 160 molecules have been detected in the interstellar medium (ISM). Reactions involving atoms, radical species and different astrochemical relevant organic species, and occurring on the icy interstellar grains at low temperatures have been often proposed to explain either the detection or the non-detection of many chemical species through astronomical observations. For example, aldehydes such as methanal or propanal are abundant in dense molecular clouds while there is no evidence for the detection of alcohol species larger than methanol. The knowledge of reaction pathways leading to the formation of complex molecular species in those coldest regions of the universe, represents an important step toward the understanding the chemical composition of the ISM and planetary atmospheres. Laboratory experiments at very low temperature and very low pressure are of primary importance to help understanding these reaction pathways. Among others, the formation of complex organic molecules (COM) and exobiologically-relevant species on the surface of dust grains and their processing during desorption represent an important topic of investigation. One of the hypothesis about the source of organic compounds that could serve as the basis of life on Earth is their formation in the interstellar medium (ISM) and delivery to early Earth on board of meteorites. The aim of this thesis proposal is to investigate the energetic and non-energetic processing of interstellar ice analogs in order to explain the formation of prebiotic COM and to guide the future exploratory observations looking for the astrochemical routes to prebiotic molecules in the Universe.

### **2) Details of the proposal**

The project aims to better understand the complex chemistry of the interstellar medium (ISM) in order to determine the reaction pathways leading to the formation and evolution of COM, particularly those of prebiotic interest. In this context, we propose to carry out laboratory experiments at very low temperature and very low pressure to mimic the organic synthesis of COM on the surface of interstellar dust grains and their processing during desorption. Even though, the powerful astronomical observations are now able to characterize accurately the composition of the ISM, they need to be completed with laboratory experiments mimicking the exact conditions of the ISM. Such laboratory simulations are crucial not only to validate the abundances of the species already detected but also to guide the future exploratory observations. Practically, this project is to connect for the first time in one experimental setup, organic synthesis, radical reactivity on interstellar ice analogs, mass spectrometry, infrared and terahertz spectroscopy to investigate two aspects of energetic and non-energetic processing of interstellar ice analogs:

- atom/radical addition reactions combined with UV or high energy particle bombardment.
- Physical & chemical evolution in the solid-gas interface.

Based on the state of the art instrumentation in the field of interstellar chemistry, we will investigate the evolution of COM since their formation in the solid phase till their release into the gas phase. It will be then possible to follow the transformation of species during their desorption and to characterize properly the reaction products in the gas phase, including the isomeric species. In addition to investigate how prebiotic species form in an astrophysical context, this project will improve astrophysical models and provide catalogs of rotational transitions which will allow the search of molecular species in the ISM using IRAM, ALMA and other facilities.

For the present thesis project, we intend to focus on radical reactions involving H, N or O atoms and abundant astrochemical relevant molecules (CO, H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>, CH<sub>3</sub>OH) and large unsaturated species such as H<sub>2</sub>C=C=O, HC≡CCHO, HCCNC, HC<sub>3</sub>N, H<sub>2</sub>NCONH<sub>2</sub> and H<sub>2</sub>NCHO. Those radical reactions, occurring in solid phase at very low temperature between 3 and 200 K, may lead to the formation of different prebiotic molecule such as amino acids. To this end, the experimental setup that will be used allows to reproduce the very low pressure and temperature conditions similar to those found in the ISM and in some planetary atmospheres. Our solid samples are formed, in a chamber maintained under ultrahigh vacuum 10<sup>-10</sup> mbar, by condensation of gaseous mixtures on the surface of a polished rhodiated copper mirror maintained at 3K. Atomic species H, N and O are generated in situ using a plasma discharge based on the principle of electron cyclotron resonance where low radio-frequency is coupled to the plasma gas to achieve massive dissociation of stable molecules (H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>) into atoms. Combining laboratory experiments and computational chemistry, we will investigate the evolution of COM since their formation in the solid phase till their release into the gas phase. All the studied processes occurring in solid phase are analyzed and monitored using Fourier-Transform Infrared Spectroscopy, through the transmission–reflection mode detection. The identification of reaction pathways leading to the formation of COM or exobiologically-relevant species in solid phase covers the first part of our project. The second part of the present project consists in studying the instantaneous or progressive desorption of interstellar ice analogs before and after energetic and non-energetic processing, by means of UV irradiation and thermal heating. Such induced sample desorption will allow to study the physical and chemical evolution of COM in the solid-gas interface which will be probed by coupling IR spectroscopy to mass spectrometry and Terahertz spectroscopy. While the mass spectrometry allows the identification of desorbed species, the THz spectroscopy will quantify, in the case of species with different isomeric forms, the proportion of each isomer.

### 3) References

- [1] Swings P., Rosenfeld L., 1937, ApJ, 86, 483
- [2] Potapov A., Jäger C., Henning T., Jonusas M., Krim L. 2017, ApJ, 846, L131.
- [3] Jonusas M., Guillemin J. C., Krim L. 2017, Mon. Not. Roy. Astron. Soc. 468. 4592.
- [4] Watanabe N., Kouchi A. 2002, ApJ, 571, L173.
- [5] Turner B. E. 1991, ApJ, 76, 617.
- [6] Hollis J. M., Jewell P. R., Lovas F. J. Remijan A., Møllendal H. 2004, ApJ., 610, L21.
- [7] Irvine W. M., Brown R. D., Cragg D. M., Friberg P., Godfrey P., Kaifu N., Ohishi M., Suzuki H. D., Takeo H. 1988, ApJ, 335, L89.

### 4°) Profile of the Applicant (skills/diploma...)

Applicants should be physical chemist specialized. They must have experience with atomic and molecular spectroscopy, mass spectrometry, organic chemistry with a Master's degree in chemistry of physical-chemistry.

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