Implications of detailed modeling of surface chemistry in PDR codes on the processes in the Interstellar Medium

Franck Le Petit[1], E. Roueff[1], J. Le Bourlot[1,2], E. Bron[1], B. Godard[1],

[1]LERMA - Observatoire de Paris, CNRS, France, [2]Université Paris Diderot, France

It is well recognized that chemical reactions on dust grains are central processes to understand the molecular composition of interstellar gas. Several experiments in laboratory have been set up to study such processes. The first experiments have been dedicated to H2 formation. They allowed to understand the detail of mechanisms on grains surfaces, to determine reactions energy thresholds as well as excitation states of newly formed H2. New experiments focus on complex species as the ones associated to oxygen chemistry providing invaluable data for the modeling of interstellar chemistry. These works are motivated by new detections of molecules done thanks to a new generation of instruments (Herschel, ALMA, APEX, IRAM/Noema). Many recent observations of molecules in star forming regions, dark clouds and diffuse clouds, in our local environment but also in the Galactic Center and in distant galaxies are directly or indirectly related to surface chemistry. The interpretation of these new observations require that results obtained in laboratory experiments be implemented in state-of-the-art numerical models of interstellar clouds.

Among the state-of-the-art codes modeling interstellar chemistry, the Meudon PDR Code (pdr.obspm.fr) is a public 1D code that computes consistently 1) radiative transfer from far UV to sub-mm taking into account absorption and emission of photons by grains and in atomic and molecular lines, 2) individual heating and cooling mechanisms for non LTE systems, 3) chemistry of hundred chemical species related by thousands reactions. Recently, we implemented in this code the detailed mechanisms on grains surfaces based on the new laboratory experiments results. We introduced the formation of H2 in physisorption and chemisorption sites following Eley-Rideal and Langmuir-Hinshelwood mechanisms. We also introduced oxygen surface reactions network taking into account adsorption, formation of mantles, and desorption: thermal, driven by photons and cosmic rays, as well as chemi-desorption.

In this talk, we will show that, the importance to use a proper grain size distribution to reproduce well known properties of diffuse clouds as H2 excitation observed by FUSE in the far UV. We will also show that modeling precisely the chemical processes on grains surfaces in a comprehensive code as the Meudon PDR Code allow to answer to some of the key questions in the field of the interstellar medium. We will show how detailed treatment of H2 formation on grains reconcile numerical models and H2 emission observed in PDRs by ISO and Spitzer. We will show that when recent laboratory / theoretical results on H2 formation on grains are implemented in comprehensive numerical models solving both surface chemistry and radiative transfer, H2 formation on grains can become a major heating mechanism that competes with photoelectric effect and may explain the high CO excitation observed in some PDRs by Herschel. We will also show the importance to treat in detail the coupling of radiative transfer and surface chemistry to understand how molecules as methanol and formaldehyde formed on grains are released from mantles to the gas phase thanks to different mechanisms depending on the position in clouds. We will illustrate this by comparisons of our models to recent Herschel and IRAM observations in PDRs as NGC 7023 and the Orion Bar as well as the Horse Head.