Formation of molecules at the gas-surface interface: experimental and theoretical advances

S.Morisset[1]

[1] *Institut des Sciences Moléculaires d'Orsay, CNRS/ Université Paris-Sud, UMR 8214, Orsay, France*

In the interstellar medium, dust grains catalyze the formation of molecules. In order to understand and quantitatively describe such processes, it is necessary to study the interactions (and reactions) of H, C, O atoms from interstellar clouds with (and at) grain surfaces, and the dynamics of molecular formation of H_2, OH, H_2O, etc.

Molecules can be formed from two atoms which are adsorbed on a dust grain (Langmuir-Hinshelwood mechanism), from one adsorbed atom and an atom from the gas phase (Eley-Rideal mechanism), or by a mixture of these two mechanisms.

In this talk, I will present theoretical and experimental studies of the formation of H_2 and OH molecules on dust grains. Theoretically, the structure of dust grains can be modelled using electronic structure calculations or analytical potentials, and is then used for simulating the dynamics of the reactions. This leads to the calculation of physical quantities such as cross section of reactions, ro-vibrational excitations, and energy repartitions between molecules and dust grains.