Theoretical approaches for gas-phase and ice surface processes

Dahbia Talbi

LUPM, UMR5299 du CNRS, Université de Montpellier, Place Eugene Bataillon, 34095, Montpellier Cedex 5 – France

It is nowadays an evidence that both gas phase reactive collisions and heterogeneous chemistry involving interstellar grains/ices, play a fundamental role in the formation of molecules in space. For the last processes, in addition to understanding the catalytic role of the solid phase, there is also the problem of understanding the adsorption, diffusion and desorption of the reactants and/or products as well as the thermal exchanges between the products and the solid phase. Theoretical chemistry is able to address both chemistries with more or less accuracy and success but always bringing useful information for astrochemical modelling. I will through this talk, try to address in a manner accessible to an interdisciplinary audience, the approaches used by the theoretical chemists/physicists of the PCMI community to understand both this gas phase and solid state chemistry.