Atomic-scale insights of the chemistry occurring in the interstellar medium. Clues from quantum chemical methods

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The existence of cosmic molecules is of great relevance due to due their connection with the chemical evolution steps occurring in the universe [1,2]. A key role of this chemical evolution is played by gas-grain processes, which involve in part the interaction of gaseous molecules with dust particles and the subsequent chemical reactivity. The current knowledge of these gas-grain processes is mostly based on spectroscopic observations, helped by laboratory experiments and astrochemical models. This combination has been fruitful to determine some important phsyico-chemical properties, such as the chemical activity of the gas-grain interactions [3,4]. However, this approach cannot provide atomic-scale information such as the precise mechanistic steps of the reactions or the exact role played by the grains, a serious limitation to fully understand the basic physical and chemical steps that lead to the chemical complexity in space. This information gap can be filled in by using theoretical calculations based on quantum mechanical approaches [5]. In this talk, examples on how these theoretical calculations can contribute to interstellar-related chemical studies from providing an atomistic interpretation of the gas-grain processes will be presented. In particular, results obtained from simulations devoted to the formation of H_2 through H recombination on bare olivine surfaces (Figure 1a) [6] and to the formation of interstellar H_2CO and CH_3OH through H additions to CO on water ice particles (Figure 1b) [7] will be shown. Results will provide both structural details of the systems involved and energetic data of the reactions, which in turn can be used as input parameters in astrochemical modelling studies. Estimates of tunneling contributions by calculating both tunneling crossover temperatures and transmission coefficients will also be presented.

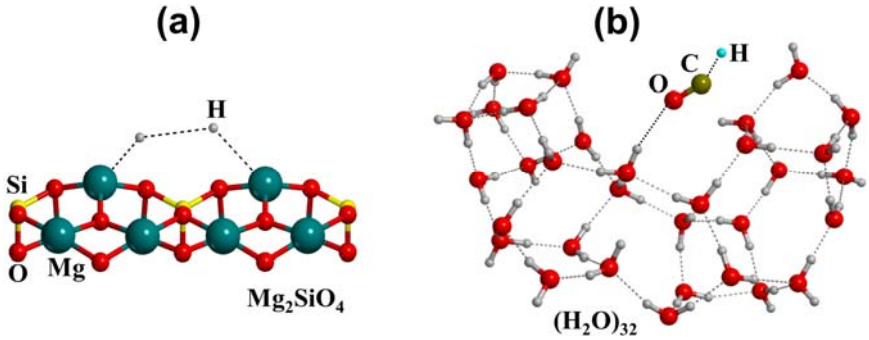

Figure 1: Transition state of (a) H_2 formation from H recombination on a Mg-rich olivine surface model and (b) HCO formation from H addition to CO on a water ice particle model.

References

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