A Theoretical, Neural-Network Assisted Study of Methane Formation under Astrophysical Conditions

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Dense molecular clouds are cold regions (~10-20 K) in the interstellar medium (ISM) that accommodate dust grains coated with ice, usually amorphous. The chemical components of those ices are H_2O, CO, CO_2, CH_3OH, etc. with strongly fluctuating compositions. These surfaces play a central role in the chemistry of the ISM and therefore in the evolution of molecular clouds, acting as templates of atoms, radicals and molecules, to meet on top of them [1]. Additionally these ices help to dissipate the energy of the reactions occurring on them. Hence, these surfaces enable the synthesis of a variety of chemical compounds that would not be accessible by gas phase reactions alone. In this work, we studied the formation of CH_4 by investigating the reaction of a CH_3 radical with H on the surface of amorphous solid water (ASW). Among the things we analyzed is the energy redistribution vs chemical desorption [2, 3]. A periodic model of ASW was used to mimic the reaction. As a first step, we have obtained the binding energy (BE) distribution of CH_3 on the surface with values between -500 and -4000 K. The reaction was modeled by placing CH_3 on binding sites with high, medium and low BEs for both axial and planar orientation of the CH_3 radical on the surface. Later, hydrogen atoms have been placed spherically around the CH_3 radical to sample many possible trajectories. Subsequently, molecular dynamics simulations for the reaction were carried out at a temperature of 10 K. The potential driving the dynamics is a neural network potential trained on DFT energies and forces [4, 5]. We have found that the initial orientation of the CH_3 radical hardly plays any role on the reaction. On the contrary, we found huge differences in the evolution of the reaction as a function of the CH_3 binding site and the initial orientation of the H with respect to the methyl radical.

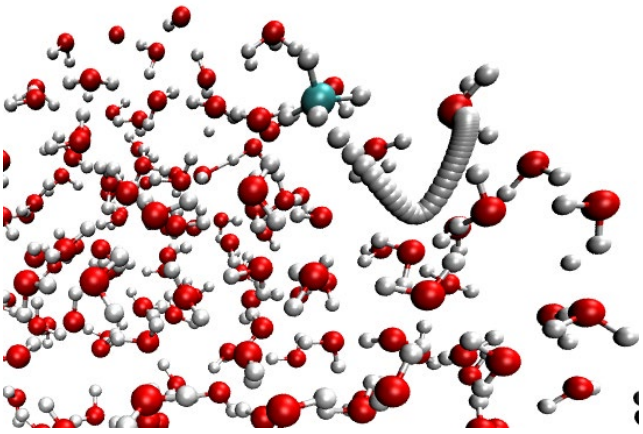

Figure 1: Trajectory of the hydrogen atom approaching the methyl radical to form methane during the MD simulation in increments of 2 fs per hydrogen frame.

References

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