Energy dissipation and restructuring in interstellar ice

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Dust particles covered by icy mantles play a crucial role in the formation of molecules in the Interstellar Medium (ISM). These icy mantles are mainly composed of water but many other chemical species are also contained in these ices. The structure of this ice mantle plays in important role in the capacity to hold other species, promote reactions, and take up energy.
Complex organic molecules are formed through an intricated network of photodissociation and surface reactions. Both type of reactions release energy. Surface reactions are typically exothermic by a few eV, whereas photodissociation reactions are triggered by the absorption of a UV photon, resulting in the formation of highly excited products. The excited reaction products can apply this energy for desorption or diffusion, making products more mobile than predicted when considering only thermal hopping. The energy could further lead to annealing or deformation of the ice structure.

We like to quantify the relative importance of these different energy dissipation routes in two different ways: Selective pumping of specific infrared (IR) vibrational modes can aid in understanding the dissipation of vibrational energy whereas excitation of admolecules on a surface can give more information in the fate of excited reation products. The latter we have studied by performing thousands of Molecular Dynamics simulations for three different species (CO_2, H_2O and CH_4) on top of a water ice surface. We consider different types of excitation such as translational, rotational, and/or vibrational excitation. This leads to a generalize expression for non-thermal desorption which is then included in an astrochemical model and the results are compared against astronomical observations.
Selective pumping of specific infrared vibrational modes leads to restructuring of hydrogen bonding networks. Upon resonant irradiation, a modification in IR absorption band profile of ASW is observed which is analysed in terms of hydrogen bonding donors and acceptors and the experiments are complimented with Molecular Dynamics simulations to constrain the effect at the molecular level.