Investigating Ice Photodynamics Using Molecular Dynamics Simulations

Water ice found on dust grains within molecular clouds in the interstellar medium are the site of interesting photodynamics initiated by the high energy photons from nearby stars. In experiments, the dynamics involved are inferred from the observed reaction products. Molecular dynamics simulations can provide a “molecule eye view” of the dynamics as they occur.

In separate works the dynamics of the primary photoproducts due to excitation of a single water molecule in ice are followed using molecular dynamics simulations. Water excitation is described using interpolations to ab-initio potential energy surfaces for the ground and excited states of H$_2$O. Intramolecular and intermolecular interactions in all other molecules are handled by molecule specific force fields. Our initial study involves a fully classical description for the vibrational motion of all molecules leading to vibrational energies in the molecules far below zero point energy. To counter this a separate study employs a frequency dependent thermostat which provides a correct description of the vibrational energy in the matrix molecules. In my final study, reactions of the H atom with neighboring water molecules are considered through the inclusion of an ab-initio potential energy surface for H$_3$O.