

Theory of molecular scattering from and photochemistry at ice surfaces

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Abstract. The classical trajectory methodology for studying scattering of ions, atoms, or molecules from ice surfaces, and photodissociation of water at or in the surface of ice, will be presented. In the methodology used, the forces between the collider and the water molecules, or between the fragments of a dissociating molecule and the surrounding water molecules, are based on pair potentials often taken from ab initio calculations. Dynamical observables like sticking probabilities and kinetic energy distributions of desorbing fragments are computed by solving Newton's equations of motion starting from representative initial discussions. Three example studies will be presented. In the first example, we will show that the sticking probability of CO and its dependence on the collision energy are the same for the amorphous ice prevalent in interstellar space and crystalline ice (Al-Halabi et al. 2004). In the second example, we will show that protons can be reflected from ice at low incidence energies (≤ 0.2 eV), and that proton absorption can be accompanied by ejection of water molecules (Cabrera Sanfelix et al. 2005). Finally, we will present results for the photodissociation dynamics of a water molecule in both crystalline and amorphous ice surfaces at temperatures relevant to diffuse and dense clouds. As we will show, photodissociation in the first bilayer leads mainly to H atoms desorbing, while deeper in the ice trapping of H and OH dominates (Andersson et al., in press). Good agreement between the theoretical and experimental absorption spectrum can be obtained by adjusting the charges of the molecule excited to its first electronic state (Andersson et al., in preparation). Differences between crystalline and amorphous ice will be discussed.

References

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