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Rotational excitation of carbon dioxide due to collision with a liquid surface

Michael Valliere & John Adams

To improve our understanding of collisional energy transfer at a gas-liquid interface, we have investigated collisions of carbon dioxide molecules with a simple atomic liquid surface. Our particular focus here is on the transfer of the impinging molecules' initial kinetic energy to its rotational degrees of freedom. In these simulations, CO₂ molecules are treated as rigid rotors, thus permitting unambiguous isolation of the fraction of the initial (purely translational) kinetic energy flowing into rotations. The first phase of this work involved modifying the molecular dynamics code to incorporate molecular species rather than atoms as impinging particles and the evaluation of the rotational state of the molecules after leaving the surface.