Theoretical studies of collisions between gases and organic surfaces

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We will present recent approaches to simulate the collisions of a variety of gases with organic surfaces. These interfacial collisions are of interest in fields including atmospheric chemistry and material degradation in space environment. The simulations involve the calculation of classical trajectories in which gas species ranging from rare gases to chemical-warfare agents are aimed with well-controlled energy and direction at an organic surface. Critical to the accuracy of the simulations is the quality of the potential energy surface that provides the forces acting on each atom throughout the collision. The techniques utilized to develop potential energy surface for our gas-surface simulations depend on the type of system under consideration. For collisions between closed-shell gases and organic surfaces in which there is no reaction and only energy exchange takes place, most of the potential energy surface is usually well represented by harmonic force fields available in the literature. An exception to this is the non-bonding interactions between the gas and the surface, which we derive for each system based on high-accuracy ab initio calculations. When the gas species can react with the surface, an entirely different approach to represent the potential energy surface needs to be employed because common harmonic force fields do not allow for bond breakage and formation. Our approach considers a quantum-mechanics/molecular-mechanics, QM/MM, separation in which the forces acting on atoms of the region of the system in which bonds break and form are calculated on the fly using efficient QM methods. The non-reactive part of the system is treated employing standard force fields. Our simulations complement recent gas-surface molecular-beam experiments, which serve to calibrate the accuracy of the calculations.