O 104: Invited Talk (Alec Wodtke)

Time: Friday 13:15–14:00 Location: TRE Phy

Invited Talk O 104.1 Fri 13:15 TRE Phy

Toward a Dynamical Understanding of Surface Chemistry — •Alec Wodtke — Department of Dynamics at Surfaces, Max Planck Institute for biophysical Chemistry, Göttingen, Germany — Institute for Physical Chemistry, Georg-August University, Göttingen, Germany

Great strides in our understanding of surface chemistry have been made over the last two decades due to constantly improving computational methods that rely on the Born-Oppenheimer (electronically adiabatic) approximation and exploit the power of modern electronic structure theory, especially density functional theory. Despite this progress, describing and understanding the atomic-scale motion involved in surface reactions remains a daunting challenge. The central difficulty concerns the question: how is energy exchanged between an adsorbate and elementary excitations of the solid? To observe and understand the atomic-scale motion involved in energy conversion processes occurring in collisions between molecules and solid surfaces is a central goal of our group. Using modern molecular beams methods in state-to-state scattering experiments, we obtain a wealth of observational data. Emphasizing quantitative comparison to first principles theories, we find that energy conversion can occur by unexpected mechanisms, where the electronically adiabatic approximation separating the time scales of electronic and nuclear motion is found to be invalid. One important outcome of this work is the realization that Born-Oppenheimer breakdown can be induced by simple electron transfer events that are common in surface chemistry.