Dynamics of Surface Scattering and Reactions

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Chemical reactions at gas-solid interfaces are of great importance in many heterogeneous processes such as catalysis, corrosion, and material fabrication. In this talk, dynamics of several prototypical surface processes, including scattering and recombinative desorption, are explored theoretically on metal surfaces. Ab initio molecular dynamics (AIMD) is used to explore the dynamics of bond breaking/formation and energy transfer. High-dimensional potential energy surfaces including the surface degrees of freedom are constructed from on-the-fly AIMD trajectories and static DFT calculations. These potential energy surfaces allow a ~10^6 acceleration for dynamical calculations, which is vital for studying rare events such as trapping. Energy dissipation due to electron-hole pairs is also considered, using the local density friction approximation. I will focus on our recent work on CO scattering from Au(111)[1,2] and CO oxidation on Pt surfaces.[3,4]

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