Dynamics of Surface Reactions: Reactant Mode Specificity and Product Energy Disposal

Hua Guo

Department of Chemistry and Chemical Biology, University of New Mexico

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 dissociative chemisorption, Eley-Rideal reactions, and desorption, are explored theoretically on metal surfaces. Classical trajectories either on analytical potential energy surfaces or with forces calculated on the fly are used to explore reaction dynamics in the presence of surface phonons and electron-hole pairs. Signatures of dynamics, such as reactant mode specificity and product energy disposal, are examined and compared with available experimental data to shed light on unique features of surface reaction dynamics.