



The Department of Chemistry Presents:

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"On-Surface Chemical Dynamics Elucidated with with Molecular Beam Scattering, Scanning Tunneling Microscopy, and Molecular Dynamics Simulations"

We have developed the capability to elucidate interfacial reaction dynamics using an arguably unique combination of supersonic molecular beams combined with in situ STM visualization and FTIR spectroscopy. These capabilities have been implemented in order to reveal the complex spatio-temporal correlations that govern heterogeneous reactions spanning atomic, nano, and meso length-scales. For example, time-lapse visualization of reacting interfaces is allowing us to probe the reactivity of specific sites at interfaces and how the presence of a reacted site or local region influences the subsequent reaction probability at proximal sites. Such correlations are important in chemisorption, catalysis, materials oxidation and erosion, and growth. This approach also opens up a new view for interfacial reaction dynamics where incident beam kinetic energy and angle of incidence can be used for reaction control parameters with outcomes such as site-specific reactivity, changes for overall time-evolving mechanisms, and where the on-surface fate of chemisorbed species can be ascertained. In this work the time-evolving interface can be probed either in real-time or, for reactions occurring under extreme thermal conditions, using time-lapse sequential imagery. This presentation will examine H reactivity with SAMs, oxidative reactivity of HOPG graphite, O interactions with single and multilayer moiré graphene superlattices, and N₂ chemisorption on Ru to elucidate non-adiabatic effects. In situ studies of molecular embedding, reactivity, and sticking under non-equilibrium gas-surface collision conditions will also be discussed, including isotopic dependencies in condensation. Taken together, these results provide a direct and information-rich complement to traditional gas-surface scattering which monitor only volatile products, especially with respect to uncovering the important on-surface chemical and physical events that inform energy transfer dynamics and interfacial reactivity. If time permits, this talk will conclude with a brief overview of our work on the optimization of superconducting materials based upon Nb and Nb₃Sn important for superconducting radio frequency (SRF) based accelerators and x-ray free electron lasers.

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1260 Chemistry Building