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## Reaction Dynamics and Charge Transfer in the Scattering of State-Selected Ions on Surfaces

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REACTION DYNAMICS AND CHARGE TRANSFER IN THE SCATTERING  
OF STATE-SELECTED IONS ON SURFACES

A Dissertation

Submitted to the Graduate School  
of the University of Notre Dame  
in Partial Fulfillment of the Requirements  
for the Degree of

Doctor of Philosophy

by

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# REACTION DYNAMICS AND CHARGE TRANSFER IN THE SCATTERING OF STATE-SELECTED IONS ON SURFACES

Abstract

by

Patricia Lynn Maazouz

Investigating the detailed dynamics that govern gas-surface reactions is critical to understanding and predicting chemical behavior at the gas-solid interface. As energetic atomic and molecular ions scatter from surfaces, many fundamental chemical processes can be observed, including electron transfer, dissociation, and atom abstraction. The interactions of  $\text{Br}^+(^3P_2)$  with Pt(111),  $\text{Br}_2^+(^2\Sigma_{g3/2}, \nu=0 \text{ and } \nu=2)$  with Pt(111), and  $\text{NO}^+(\text{X}^1\Sigma^+)$  with oxygen-covered Al(111) provide three unique systems to investigate various reaction processes activated within the 5 – 105 eV energy regime. In contrast to conventional charge transfer theory, the scattering of  $\text{Br}^+(^3P_2)$  and  $\text{Br}_2^+(^2\Sigma_{g3/2})$  on Pt(111) show a dramatic enhancement in the formation of negative ions at an impact velocity near 8 km/s. Coincident with this resonance, the anions scatter with additional translational energy. For the  $\text{Br}^+$  projectiles a three-site model is developed to fit the product velocity-, energy-, and angular-distributions. The observed scattering behaviors are consistent with a surface site-specific collision-

induced deformation of the lattice that rebounds in phase with the departing projectile. The sensitivity of the emergence of  $\text{Br}^-$  to the  $\text{Br}_2^+$  incident energy suggests a collision-induced dissociation mechanism at higher collision energies and dissociative resonant neutralization at lower collision energies. The latter mechanism is further supported by the reduction of the  $\text{Br}^-$  yield when the initial vibrational state changes from  $v=0$  to  $v=2$  at low collision energies. The strong electronic coupling between the motion of the platinum lattice and the surface electronic states responsible for charge transfer is further evidenced by the unique relationship between the surface temperature and the formation of negative ions. Energetic collisions of  $\text{NO}^+(\text{X}^1\Sigma^+)$  with  $\text{O}/\text{Al}(111)$  results in a highly improbable abstraction reaction. The relative ion yields and mean translational energies of scattered  $\text{NO}_2^-$  are presented as a function of oxygen exposure and  $\text{NO}^+$  collision energy. The formation of  $\text{NO}_2^-$  is assigned to the direct, Eley-Rideal abstraction of an adsorbed  $\text{O}^-$  atom by an incident  $\text{NO}$  molecule. These results suggest further experimental and theoretical investigations are necessary to fully understand the transient couplings that operate when reactive projectiles scatter on clean and adsorbate-covered metal surfaces.