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Photolytic production of atoms and radicals for studying chemistry of unstable species

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Electron transfer at surfaces is central to catalysis and electrochemistry. Such processes often involve nonadiabatic dynamics, which present extreme challenges for ab initio theory. Experiments have demonstrated the importance of electronically nonadiabatic dynamics in the trapping of H-atoms at metal surfaces, where the mechanism is dominated by nonadiabatic loss of translational energy to electron hole pair excitation. Experimental results are well described by phenomenological electronic friction based theories, which treat nonadiabatic interactions using a friction force that is proportional to the local electronic density. However, it is unclear if the lessons learned from H atoms are applicable to polyelectronic atoms, where friction would likely be less important due to lower velocities, but electron transfer could be an important factor. In our work, state-to-state inelastic scattering experiments will be performed at metal and semi-metal surfaces using beams of polyelectronic atoms (C, N, O) prepared by a VUV photolysis source in well-defined electronic states and with well-defined incidence translational energy and angle. The most likely mechanism for spin violation (e.g. O(1D)⟶O(3P) is the exchange of two electrons of opposite spin, since spin transitions are unlikely on the timescale of the scattering event. Effects of fine structure, surface electronic structure, incidence translational energy and atomic orbital orientation on the electronically inelastic branching ratios and final angular and speed distributions will provide the most fundamental benchmarks for theories of nonadiabatic electron transfer processes at surfaces. VUV photolysis will also be explored as a novel source of well-defined high-energy source of diatomic and polyatomic radicals to probe state-specific reactivity.

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