

Department of Chemistry and Molecular Biology Seminar  
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## **Reaction Dynamics Relevant to Spacecraft in Low-Earth Orbit: Atomic-Oxygen Reactions with Gases and Surfaces**

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Hyperthermal reactions of  $O(^3P)$  occur at the surfaces and in the exhaust gases of spacecraft that travel through the residual atmosphere of the Earth at high altitudes (100-800 km). These reactions may degrade materials through oxidation and erosion, and they may yield internally excited reaction products which emit radiation and contribute to the “signature” of a rocket plume. Underlying the practical problems associated with space vehicle operations in the upper atmosphere are fundamental chemical and physical processes that have remained elusive in laboratory studies. Technical challenges have inhibited detailed investigations of  $O(^3P)$  reactions even with simple hydrogen and hydrocarbon model systems. The challenges stem from the difficulty of producing a high velocity beam of atomic oxygen in the ground  $O(^3P)$  state and the opening up of new, high-barrier, reaction pathways at hyperthermal collision energies that may involve multiple potential energy surfaces. New experimental studies of hyperthermal  $O(^3P)$  reactions are facilitated by a high-velocity O-atom source, known as a laser-detonation source, that has been developed for the simulation of space environmental effects. Crossed-beams experiments were used to study model reactions that can form the foundation upon which to build an understanding of atomic-oxygen chemistry in an unknown regime of hyperthermal collision energies. Specifically, the reactions of  $O(^3P)$  with CO, CH<sub>3</sub>CH<sub>3</sub>, HCl, and H<sub>2</sub>O have been studied at center-of-mass collision energies in the range of 2.5 – 4.0 eV, depending on the O-atom collision partner. Additional beam-surface scattering experiments on the initial reactions of 3.0 and 5.3 eV  $O(^3P)$  atoms with a continuously refreshed hydrocarbon surface have shown that gas-phase-like reactions at the gas-surface interface play a major role in the degradation of polymers under O-atom attack. The interpretation of the experimental results has been deeply strengthened by related theoretical calculations carried out by collaborators.