MAR14-2013-008809

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Collisions of Sodium Atoms with Liquid Glycerol: Insights into Na Atom Solvation and Ionization and the Reactions of Near-Interfacial Electrons

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Over the last 70 years, thousands of reactions between solvated electrons and dissolved species have been investigated in water and other protic solvents. Electrons born at the surface of the solvent, however, may react differently than those created within it. We have explored this interfacial reactivity by directing sodium atoms at the surface of liquid glycerol in vacuum. Gas-liquid scattering experiments show that electrons generated from the Na atoms produce hydrogen atoms and hydrogen molecules, hydroxide ions and water, and glycerol fragments. Remarkably, nearly half the hydrogen atoms created near the surface escape into vacuum before reacting with the solvent. Complementary ab initio molecular dynamics simulations of Na striking a 17-molecule glycerol cluster indicate that the glycerol hydroxyl groups reorient around the Na atom as it makes contact with the cluster and begins to ionize on the picosecond timescale. The experiments and simulations together indicate that Na-atom deposition provides a low-energy pathway for generating solvated electrons in the near-interfacial region of protic liquids.