Condensed Phase Adsorption and Reactivity: Extraterrestrial Ices, Isotopic Enrichment

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We present research that seeks to experimentally model surface-mediated processes occurring on icy-dust grains to develop a more complete understanding of the formation of planetary atmospheres, complex organic molecules, and origin of life in the universe. We use a state-of-the-art ultra-high vacuum (UHV) chamber that mimics the low-pressure and cold temperature conditions seen in astrophysical environments with optics for *in-situ* Reflection Absorption Infrared Spectroscopy (RAIRS). This chamber is connected to a supersonic molecular beam line that produces reactant gases with highly customizable energies for exposure onto the substrate. This talk focuses on how sticking probability, hydrogen bonding, and reactivity in condensed phase systems depends critically on the structure and morphology of the film. These mechanistic studies examine acetone on top of D_2O ices of astrophysical interest which include high-density, non-porous amorphous (np-ASW) and crystalline (CI) films as well as porous amorphous (p-ASW) films with various pore morphologies.[1] These studies also examine sticking probability differences between methane isotopologues using both experimental measurements as well as theoretical gas-surface chemical trajectory simulations.[2] For both studies, changes on the surface were monitored in real time with RAIRS and mass spectrometry techniques. Our work demonstrates that isotopically-dependent gas-surface collisional energy transfer can influence molecular sticking and condensation allowing for an enrichment of the heavier methane isotope. We also determine that more hydrogen bonds occur between acetone and the p-ASW film structure compared to between acetone and the np-ASW or CI films. In general, our results offer a clearer picture of the mechanisms that can occur when small organic hydrocarbons interact with various icy interfaces; a quantitative understanding of these interactions is essential to understand chemical processing or production of novel molecules occurring on the surface of icy dust particles.

1. Brann, M.R.; Hansknecht, S. P.; Muir, M.; Sibener, S.J. Acetone-Water Interactions in Crystalline and Amorphous Ice Environments. *J. Phys. Chem. A* **2022**, *126*, 2729-2738
2. Brann, M. R.; Hansknecht, S. P.; Ma, X.; Sibener, S. J. Differential Condensation of Methane Isotopologues Leading to Isotopic Enrichment under Non-Equilibrium Gas–Surface Collision Conditions. *J. Phys. Chem. A* **2021**, *125*, 9405–9413.