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Reaction Dynamics in Extreme Environments and Astrochemistry

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What is our research focus?

The prime directive of our laboratory is to explore experimentally the **Reaction Dynamics and Materials in Extreme Environments** comprising the gas phase, liquids, and solids (ices, materials) in low temperature molecular clouds (10 K), atmospheres and (icy) surfaces of planets and their moons, and toward high temperature settings such as combustion systems, chemical vapor deposition processes, high energy density materials, and in circumstellar envelopes of up to a few 1,000 K. These studies are combined with electronic structure calculations embracing fundamental physical chemistry research on the molecular level together with material science and unravel basic gas phase processes and expand to the condensed phase (droplets, thin films) with implications to reaction dynamics and kinetics, astrochemistry and astrobiology, along with material sciences. Overall, our program is aimed to elucidate the decomposition/formation of (carbonaceous) nanostructures, to rationalize the origin and chemical evolution of our solar system by exploiting complex organic molecules (COMs) as molecular tracers, and to untangle the (mineral catalyzed) formation of biorelevant molecules like sugars, amino acids, phosphates, and nucleotides in deep space (Figure 1). We utilize a wide array of modern experimental techniques comprising five experimental setups such as gas phase scattering dynamics of open shell species and clusters, surface scattering experiments, singly levitated particles and droplets, and tunable vacuum ultraviolet light generated via resonant four wave mixing schemes. The surface science setup is shown in Figure 2 as an example. Experiments are also conducted at user facilities at the Advanced Light Source (Berkeley) and the National Synchrotron Radiation Laboratory (Hefei, China). These setups have the capability of untangling the formation and chemical processing of new molecular species from simple diatomic molecules (few hundredth of nanometers) via complex polyatomic species such as polycyclic aromatic hydrocarbons and biomolecules (few nanometers), to carbonaceous nanoparticles and levitated particles on the mesoscale up to macroscopic surfaces (few centimeters). Our experimental studies are often combined with electronic structure calculations (Bartlett, Chang, Head-Gordon, Mebel, Stanton) and modeling (Herbst, Millar, Shingledecker, Yung) to gain a comprehensive and predictive picture on the chemical evolution of these environments.

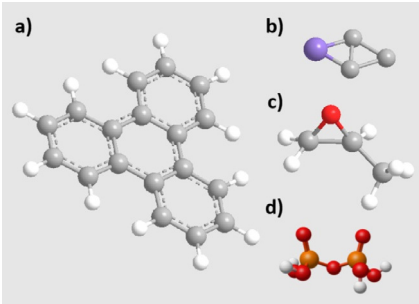

Figure 1. Example of molecules of interest: a) triphenylene polycyclic aromatic hydrocarbon (PAH, a potential precursor to two-dimensional graphene sheets in the interstellar mediu and in combustion systems), b) silicon tricarbide (c-SiC_3, an exotic bicycylic circumstellar molecule and potential building block to silicon-carbon-based nanoparticles), c) propylene oxide (a chiral molecule formed in hot molecular cores), and d) diphosphoric acid (a building block of ADP formed in interstellar ices).

Why is the future for astrochemistry and reaction dynamics so bright?

Astrochemistry and Reaction Dynamics – key areas of research of our laboratory – go hand in hand toward untangling the astrochemical evolution of the interstellar medium and of our solar system on the molecular level. Astronomical observations have revealed more than 200 gas phase molecules in interstellar and circumstellar environments ranging in complexity from diatomics such as molecular hydrogen (H_2) to polyatomics like the sugar-related molecule glycolaldehyde ($HOCH_2CHO$), benzene (C_6H_6), and even fullerene (C_{60}). Nevertheless, many facets of the question "How do these molecules form?" remain unanswered or contentious. Very often, observational results are

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