

# Reaction Dynamics in Extreme Environments and Astrochemistry

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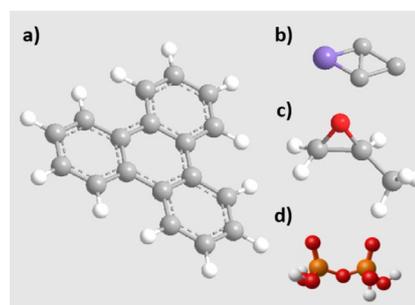


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## What is our research focus?

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

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**Figure 1.** Example of molecules of interest: a) triphenylene polycyclic aromatic hydrocarbon (PAH, a potential precursor to two-dimensional graphene sheets in the interstellar medium and in combustion systems), b) silicon tricarbonide (*c*-SiC<sub>3</sub>, an exotic bicyclic 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).

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.

## 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<sub>2</sub>) to polyatomics like the sugar-related molecule glycolaldehyde (HOCH<sub>2</sub>CHO), benzene (C<sub>6</sub>H<sub>6</sub>), and even fullerene (C<sub>60</sub>). Nevertheless, many facets of the question “How do these molecules form?” remain unanswered or contentious. Very often, observational results are

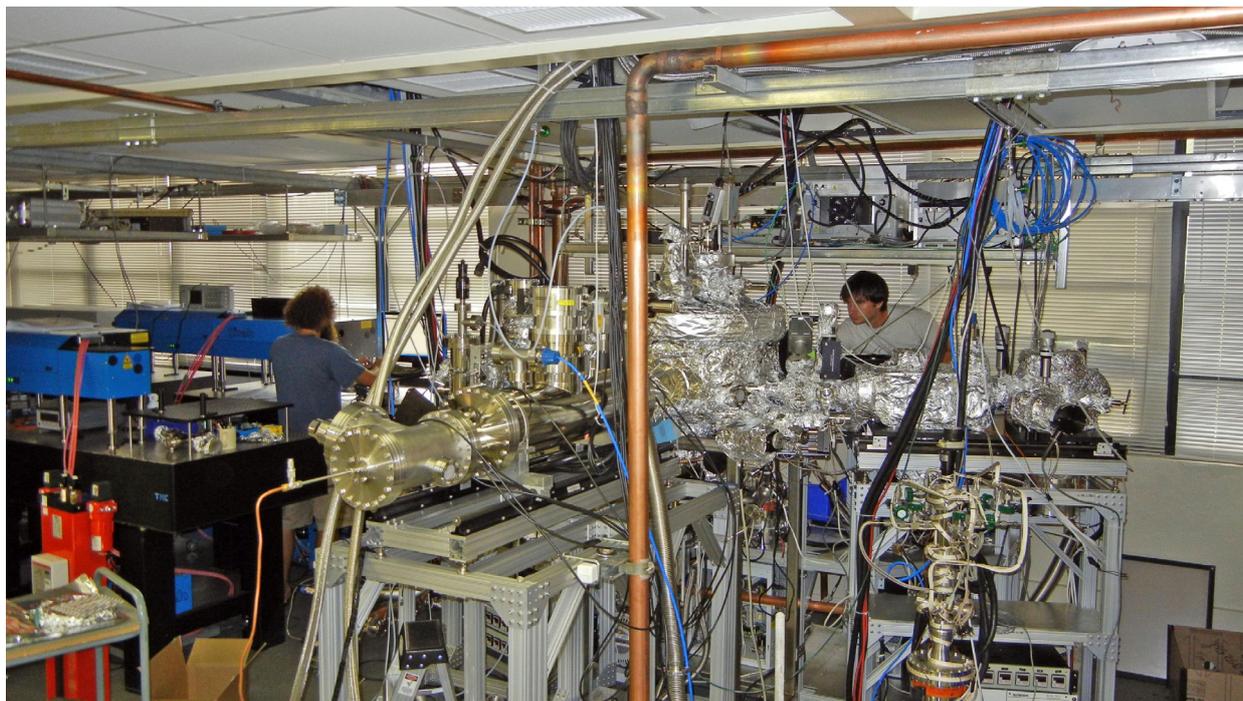


Figure 2. Photograph of the surface science setup and laser systems.

misinterpreted to suggest synthetic routes to complex molecules in deep space. However, physical chemists can now design sophisticated laboratory experiments to unravel the formation of (newly detected) molecules in extraterrestrial ices and also in the gas phase (interstellar medium, atmospheres of planets and their moons) on the molecular level. In conjunction with novel astronomical observations and cutting-edge spectroscopy, this understanding on the microscopic level exploiting reaction dynamics studies rather than guesswork is critical for astrochemistry to progress to such a level eventually predicting the formation and existence of even molecular building blocks relevant to the *Origins of Life*. The rules of chemistry, after all, are universal, even when the conditions are very different on Earth compared to deep space.

### What message shall we teach our students in astrochemistry?

The critical message to students interested in astrochemistry and in untangling the formation of molecules in extreme envi-

ronments in particular would be to focus on hardcore physical chemistry studies. Astrochemistry requires – besides a detailed knowledge in organic and inorganic chemistry – a sophisticated background in reaction dynamics: molecules in deep space are formed by chemical processes, so if a scientist lacks a fundamental understanding of basic principles in physical chemical and reaction dynamics in particular, he/she cannot make any impact in the field of astrochemistry since multiple misconceptions on postulated reaction pathways to molecules will arise. Naturally, this understanding has to be placed in the context of extraterrestrial environments, hence collaborative studies with astronomers (spectroscopists) and/or planetary scientists are highly recommended. Even though sophisticated telescope arrays such as the Atacama Large Millimeter/submillimeter Array (ALMA) have provided outstanding images and data on the molecular composition of interstellar and circumstellar environments have been collected, an understanding of the underlying physicochemical processes leading to these molecules on the molecular level is often still elusive and awaits to be solved.