A Unified Framework on Molecular Mass Growth Processes to Polycyclic Aromatic Hydrocarbons - From Deep Space to Combustion Systems and Nanomaterials

Ralf I. Kaiser
University of Hawaii at Manoa

Friday, September 24th, 2021
12:30 PM

MAE Seminar Series (Virtual)

For decades, polycyclic aromatic hydrocarbons (PAHs) – organic molecules containing fused benzene rings - have been invoked in fundamental molecular mass growth processes leading eventually to carbonaceous nanostructures in the interstellar medium (grains) and in combustion processes (soot). However, the elementary steps involved in low- and high-temperature growth mechanisms of these aromatics have remained essentially elusive until recently. Extracted from gas phase molecular beam studies on the molecular level combined with isomer-selective photoionization mass spectrometry and electronic structure calculations, this talk presents a novel mechanistical framework on key elementary reaction mechanisms synthesizing aromatic molecules in extreme environments. These versatile findings are translated from the interstellar medium to combustion systems and to two- and three-dimensional carbonaceous nanostructures such as graphenes, chiral heli-cenes, nano bowls, and fullerenes. Facile low-temperature routes to complex aromatics signify a fundamental shift in the perception that PAHs can be only formed at high-temperature combustion and circumstellar conditions on electronic ground state surfaces with novel mechanisms comprising excited state dynamics, submerged barriers, and unconventional concerted reactions between aromatic radicals. An outlook is also presented on the synthesis of PAHs in low temperature, hydrocarbon-dominated solids upon interaction with (non)-ionizing radiation driven predominantly by non-adiabatic dynamics to PAHs as complex as coronene. Potential future works involving condensed phase ultrafast spectroscopies and the exploration of growth processes on surfaces of carbonaceous particles levitated in ultrasonic fields and radio-frequency multipole traps are highlighted to ultimately shed light on the aromatic universe we live in.

Ralf I. Kaiser received his Ph.D. in Chemistry from the University of Münster and Nuclear Research Center Jülich (Germany) in 1994 and conducted postdoctoral work at UC Berkeley (Department of Chemistry). During 1997–2000, he performed his Habilitation at the Department of Physics (University Chemnitz, Germany) and Institute of Atomic and Molecular Sciences (Academia Sinica, Taiwan). He joined the Department of Chemistry at the University of Hawai'i in 2002, where he is currently Professor of Physical Chemistry and Director of the W. M. Keck Research Laboratory in Astrochemistry. His research focusses on Reaction Dynamics & Materials in Extreme Environments spanning Combustion & Energy, Material Sciences & Propellants, Reaction Dynamics & Kinetics along with Astrochemistry, Astrobiology & Planetary Sciences. For his research achievements, Ralf I. Kaiser was elected Fellow of the Royal Astronomical Society (UK), the Royal Society of Chemistry (UK), the Institute of Physics (UK), the American Physical Society (APS), the American Association for the Advancement of Science (AAAS), and of the American Chemical Society (ACS).

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