

**When:** 16 December, 16:00-17:00**Where:** Blue Bld. (TPOC-3), room 408**COMPUTATIONAL MATERIALS SCIENCE SEMINAR:****FORMATION OF CARBONACEOUS MATERIALS IN COMBUSTION  
ON EARTH AND IN DEEP SPACE****Speaker:****Alexander  
M. Mebel****Department  
of Chemistry  
and Biochemistry,  
Florida International  
University, Miami,  
Florida 33199, USA****ABSTRACT**

The presentation will overview results of quantum chemical calculations of potential energy surfaces combined with RRKM-Master Equation calculations of reaction rate constants, carried out in order to unravel reaction mechanisms of the growth of polycyclic aromatic hydrocarbons (PAHs) at temperatures and pressures relevant to combustion as well as to carbon-rich circumstellar environments and the interstellar medium. We will describe our recent efforts directed toward the development of a comprehensive mechanism of PAH growth and consider possible formation routes to three- and four-ring PAHs, as well as the Hydrogen Abstraction aCetylene Addition (HACA) and Hydrogen Abstraction Vinylacetylene Addition (HAVA) growth mechanisms of larger PAHs. The computational results will be compared with the experimental findings by R. Kaiser's (University of Hawaii at Manoa) and M. Ahmed's (Lawrence Berkeley National Lab) groups utilizing a pyrolytic chemical reactor and product identification by means of photoionization spectroscopy using the quasi-continuous tunable vacuum ultraviolet light from the Advanced Light Source at LBNL. The complementary nature of the HACA and HAVA mechanisms and their role in the build-up of two-dimensional graphene-type nanostructures and three-dimensional carbonaceous nanostructures holding corannulene units through the incorporation of five-membered rings will be discussed. Additionally, we will consider and debate possible mechanisms of carbon particulate (soot) inception via chemical dimerization of PAH molecules.

**BIOGRAPHY**

Alexander M. Mebel received his bachelor's degree in physical chemistry in 1984 at the Moscow Institute of Steel and Alloys and his Ph.D. degree in physical chemistry in 1990 at Kurnakov's Institute of General and Inorganic Chemistry of Russian Academy of Sciences in Moscow, Russia. After postdoctoral appointments in Germany, Japan, and USA, his first faculty position was at the Institute of Atomic and Molecular Sciences (Academia Sinica, Taiwan), and in 2003 he joined the Department of Chemistry and Biochemistry of Florida International University in Miami, Florida, USA, where he is currently Professor of Chemistry. Since 2017, he also leads a megagrant "Development of physically proved models of combustion" from the Ministry of Science and Higher Education at Samara National Research University. His current research interests include theoretical quantum chemical studies of mechanisms, kinetics, and dynamics of elementary chemical reactions related to combustion, atmospheric, and interstellar chemistry.

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