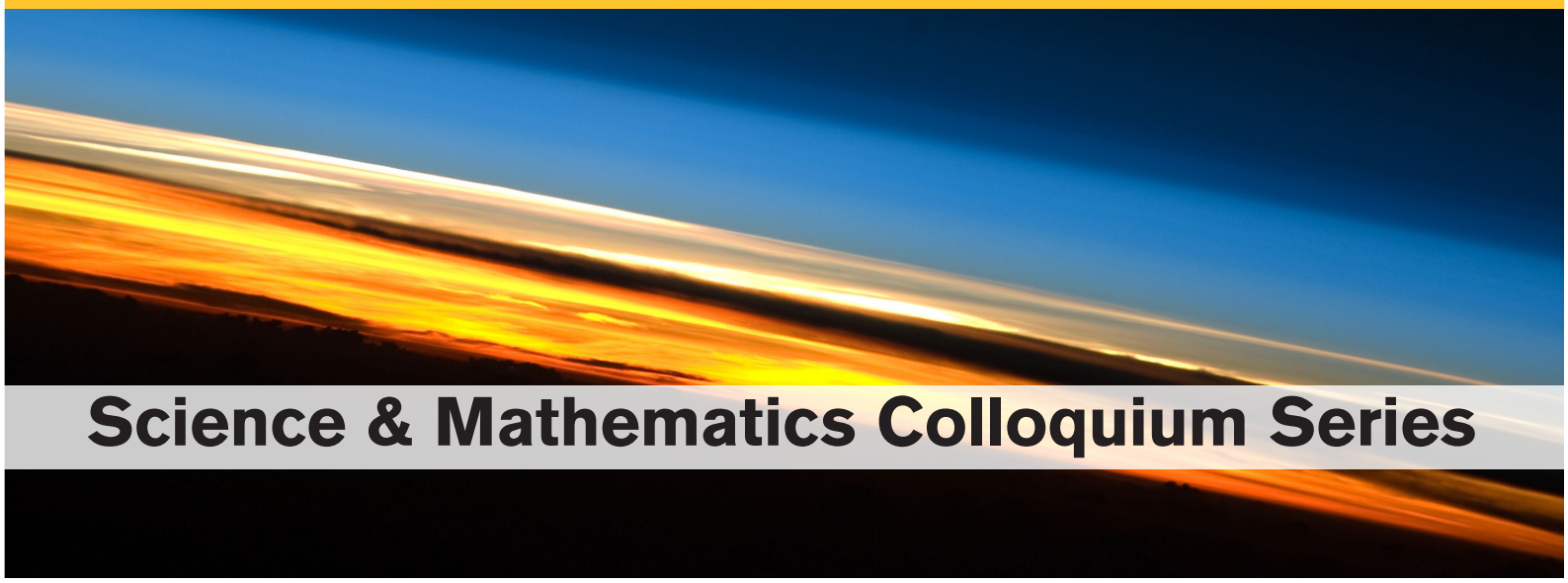
Molecular Modeling of Atmospheric Chemistry



Science & Mathematics Colloquium Series

Presentation by Manoj Kumar

Postdoctoral Researcher, University of Nebraska-Lincoln

Wed., March 22, 2017, 3 pm

Cooley Ballroom C, Student Union
ASU Polytechnic campus

Over the last five years, Criegee chemistry has become one of the most intensely studied topics in atmospheric research. Despite being extensively explored, a complete fundamental understanding of the Criegee reactivity is still lacking.

The *ab initio* molecular dynamics simulations suggest that, in contrast to the well-established view of a concerted reaction in gas-phase, a significant fraction of the Criegee-water reaction at air-water interface follows a stepwise path. The calculations further suggest that the nature of heteroatom in H2X also plays a crucial role in governing the reactivity of Criegee-H2X interaction.

An important implication of these results is that thiolaldehydes, which are important in planetary atmosphere and solution chemistry and difficult to detect because of their tendency to oligomerize, could be synthesized barrierlessly.

Manoj Kumar grew up in the northern state of Himachal in India. He did a master's in chemistry at Panjab University, Chandigarh, India, and then moved to the U.S. to pursue the PhD in computational chemistry from the University of Louisville. As a doctoral student, he worked with Prof. P. M. Kozlowski to better understand the Cobalamin-Dependent Enzymatic Reactions.

In his first postdoc, at the University of Kansas under Professor W. H. Thompson, he used electronic structure methods to model Industrially Important Processes (olefin ozonolysis and Rh-catalyzed hydroformylation). In 2015, he joined Dr. Joseph Francisco's group at the University of Nebraska-Lincoln, where he is currently studying various atmospheric processes.

cisa.asu.edu

Faculty and practitioners discuss their current research and field projects in the college's Science and Mathematics Colloquium Series, held throughout the academic year at the ASU Polytechnic campus. All seminars are free and open to the public.

ASU College of Integrative Sciences and Arts
Arizona State University