We Are Pleased to Announce a Seminar
Presented by

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Modeling Electron Detachment from Metal Oxide & Boride Clusters
with Efficient Electronic Structure Methods

Friday, February 7, 2020
2:00 pm
SLSRC 3410/3430

Metal oxide surfaces are perhaps the most widely used catalytic materials in industrial applications utilizing reduction/oxidation chemistry. However, much remains to be learned about structural and dynamical properties leading to the desired reactivity of these systems. Indeed, such understanding will be crucial for the rational design of next-generation catalysts obeying sustainable materials targets. Due to experimental limitations and a need for atomic level understanding, computation and theory are key partners in this interdisciplinary research endeavor. Motivated by the complicated electronic structure often exhibited by these systems, our group has explored the development of spin projection methods and introduced a new scheme for describing the nature of ionization events. This talk will describe these efforts and our lab's recent investigations of metal oxide and metal boride clusters.

(Biography on back)

Refreshments will be served at 1:45 pm
Biography
Hrant P. Hratchian, a Michigan native, obtained his B.S. degree in chemistry from Eastern Michigan University (Ypsilanti, MI) and completed doctoral studies under the tutelage of Professor H. Bernhard Schlegel at Wayne State University (Detroit, MI) where he was an NSF-IGERT Graduate Fellow. From 2005-2008 he was the Ernest R. Davidson Postdoctoral Fellow at Indiana University (Bloomington, IN), where he worked with Professor Krishnan Raghavachari. From 2008-2013, he was a Research Scientist at Gaussian, Inc. (Wallingford, CT). Since 2013, he has been Assistant Professor of Chemistry and Chemical Biology at the University of California, Merced. In recent years, Prof. Hratchian has been honored with a Hellman Foundation Fellowship and an NSF CAREER award. His research group’s work has received extramural funding support from the Petroleum Research Fund, Hellman Family Foundation, National Science Foundation, and the Department of Energy. Professor Hratchian’s research interests include the development and application of efficient computational chemistry methods to explore the unique properties of transition metal systems and the chemical transformations they catalyze.