Towards Practical and Accurate Simulations of Electron Detachment from Transition Metal Oxide Clusters

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**Abstract**

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 lab 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 applications of such models in investigations of metal oxide clusters.

**About the Speaker**

Hrant P. Hratchian, a Michigan native, obtained his B.S. degree in chemistry from Eastern Michigan University and completed doctoral studies under the tutelage of Professor H. Bernhard Schlegel at Wayne State University where he was an NSF-IGERT Graduate Fellow. From 2005-2008 he was the Ernest R. Davidson Postdoctoral Fellow at Indiana University, where he worked with Professor Krishnan Raghavachari. From 2008-2013, he was a Research Scientist at Gaussian, Inc. Since 2013, he has been Assistant Professor of Chemistry and Chemical Biology at the University of California, Merced. Professor Hratchian is a recipient of the Hellman Faculty Fellowship and the NSF CAREER award. His current research interests include the development and application of computational quantum chemistry methods to explore the structure, properties, and reactivity of transition metals.