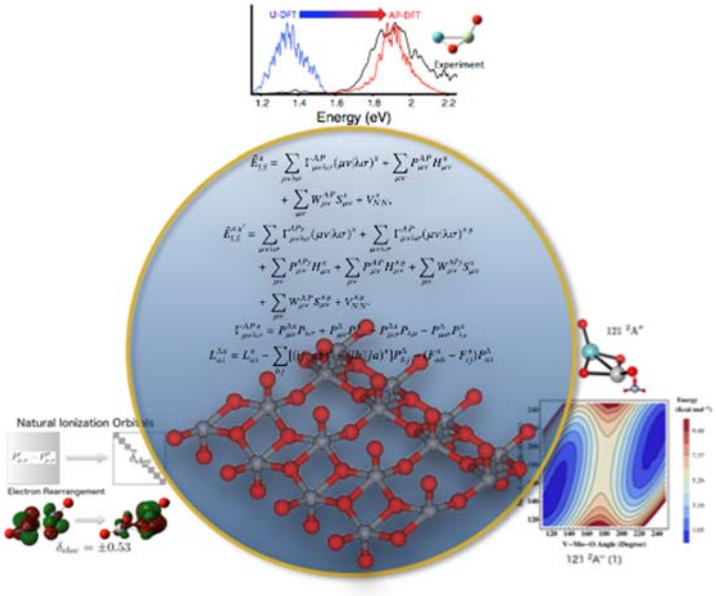
EMU Chemistry Seminar

Expanding the Computational Chemistry Toolbox to Explore the Structure and Dynamics of Metal Oxide Clusters



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. Inspired by the complicated electronic structure often exhibited by these systems, our lab has explored the development of approximate projection methods to efficiently treat unpaired and/or strongly correlated electrons. This talk will describe our lab's recent exploration of the structure and dynamics of metal oxide cluster models and will highlight our recent method developments facilitating these studies.

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Dr. Hratchian is a Michigan native and an alumnus of the EMU chemistry department

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4:00 PM, Monday, October 24th
Room 154 Science Complex