SME

School of Microelectronics, SUSTech

Academic Frontier Lecture
NO: 023

Title: Machine-learning for Designing Catalysts

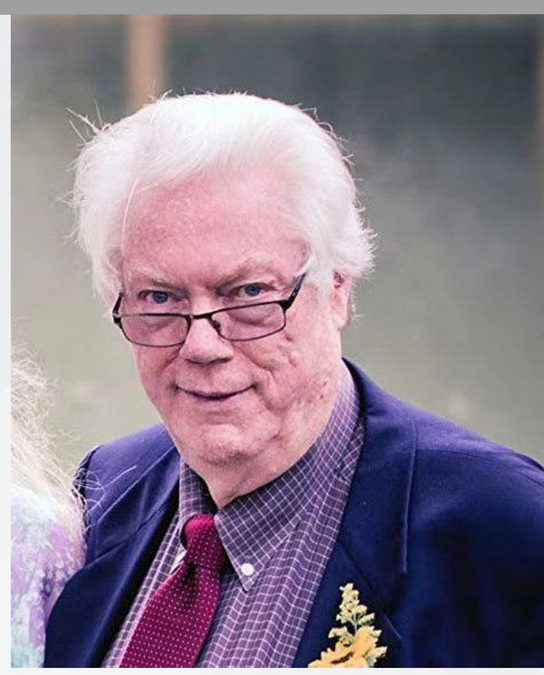
TIME: Monday 3:00pm-4:00pm, July 22, 2019

VENUE: Room114 Taizhou Hall(台州楼)

SPEAKER: James P. Lewis, Professor, Department of Physics and Astronomy West Virginia University

HOST: Prof. Quan Chen

INTRODUCTION



Professor Lewis graduated in 1996 with a Ph.D. from Arizona State University under the supervision of Otto F. Sankey, a pioneer in density functional theory local-orbital formalism for molecular-dynamics simulations. After graduating, he spent two years as a postdoctoral associate with Yang Weitao at Duke University. From there, he was affiliated with the University of Utah and Brigham Young University. In 2006, he moved to West Virginia University as an Associate Professor and has been promoted to Full Professor since 2013. James P. Lewis is the primary developer and distributor of the FIREBALL ab initio density-functional theory (DFT) package which is based on local-orbitals and pseudo-potentials. FIREBALL is a computation and simulation tool, utilizing parallel programming, for studying large and complex materials systems; it is widely used by several dozen research groups.

Professor Lewis' research group works on properties of materials for a broad variety of systems including in biology, chemistry, physics, and geology. His research efforts include investigating, for example, 1) interfaces between biomolecules and gold nanoparticles; 2) the electronic structure and optical properties of semi-conducting materials; and 3) catalysts. More recently, he has become a leader in applying machine-learning algorithms to physical chemistry research and materials by design, culminating in two recent machine-learning publications in J. Am. Chem. Soc. during 2018. This research has also led to a recently awarded Department of Energy grant to develop machine-learning software for petascale computing applications. In March 2018, he was appointed as a Thousand Talent Professor at the Institute of Coal Chemistry, State Key Laboratory of Coal Conversion. In May 2018, he was appointed as a founding member of the Editorial Board of the new journal Machine Learning: Science & Technology published by the Institute of Physics.

ABSTRACT

Machine learning, a computational dream for decades, has now been realized. With speed-ups in computational speed, the age of big data has enabled society to apply machine-learning algorithms to all aspects of life. In this lecture, we will discuss two prominent examples of our success with machine learning (both published in J. Am. Chem. Soc. in 2018): 1) The first example is a machine-learning approach to evaluate global reaction coordinates. Our approach was applied to azobenzene, but can be readily applied to any system where interest in the reaction coordinates are desired. Azobezene is a very important system that is often studied for better understanding light-activated mechanical transformations via photoisomerization. We report on a global reaction coordinate (containing all internal coordinates) to thoroughly describe the reaction mechanism for azobenzene photoisomerization, a detailed mapping is obtained in our approach; 2) The second example is a machine-learning approach to predict adsorbate interactions of Ag-alloyed Au catalysts. Here, we utilize a machine-learning model, based on the random-forest method, to predict CO adsorption in thiolate protected nanoclusters. One advantage to a machine-learning approach is that correlations in defined features disentangle relationships among the various structural parameters. For example, in Au25, we find that features based on the distribution of Ag atoms relative to the CO adsorption site are the most important in predicting adsorption energies. Our machine-learning model is easily extended to other Au-based nanoclusters, as well as other catalysts, and we demonstrate predictions about CO adsorption on Ag-alloyed Au36 and Au133 nanoclusters.

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