25th TcSUH STUDENT/POSTDOC SEMINAR

Tuesday, February 13, 2024 - 5:00 pm, HSC 102

Meet & Greet: Food and soft drinks will be served at **4:30** p.m!!

Structure Design and Performance Modulation of Water Electrolysis Catalysts

Dr. Luo Yu

Department of Physics

Abstract: Hydrogen (H_2) is an ideal alternative to fossil fuels. We need to embrace hydrogen as a global energy solution now more than ever. Water electrolysis is an efficient technology for green-hydrogen production with zero-carbon emission, which is of great significance to the worldwide decarbonization. However, due to the lack of efficient and low-cost electrode materials, hydrogen production from water electrolysis faces the bottleneck of high cost, which seriously impedes the commercialization of green-hydrogen technology. Focusing on low-cost non-precious metal-based materials, we have performed systematic studies on the structure design and performance modulation of water splitting electrocatalysts. To address the issues of unsatisfactory intrinsic activity, poor durability, and low selectivity, we have proposed heteroatom doping and construction of three-dimensional core-shell structure strategies to modulate the electronic and geometric structures of electrocatalysts. We have uncovered the mechanism of how electronic structure modulates the electrocatalytic water splitting performance and realized selective adsorption and activation of reactants, thus fabricating good water splitting electrocatalysts that can work efficiently under large current densities. Guided by the strategies of heteroatom doping and core-shell structure design, we have further developed a variety of economical and efficient methods for scalable and controllable synthesis of high-performance low-cost electrode materials.

Bio: Dr. Luo Yu is currently a researcher in Dr. Zhifeng Ren's group. His research has been focusing on developing non-precious metal-based materials and fabricating high-performance devices for hydrogen production from water/seawater electrolysis. He received his B.S. and Ph.D. degrees from Central China Normal University (China) in 2013 and 2018, respectively. From 2016-2018, he was a visiting Ph.D. in Dr. Ren's group, and continued to work as a post-doctoral fellow from 2019-2021.

Effect of Charge on Scaling Property of Adsorbates on Catalyst Surfaces

Dr. Shengguang Wang

Department of Chemistry

Abstract: Linear scaling relationships between binding energies of molecules adsorbed on catalytic surfaces have greatly contributed to understanding and prediction of catalytic activity in chemical reactions. These linear scaling relationships are intimately tied to the Sabatier principle stating that moderate strength adsorption of reaction intermediates is ideal for achieving the highest catalytic rate. We investigated the effect of surface charge on scaling relationships with a focus on binding energies of oxygen-containing molecules on transition metal surfaces. Our results indicate that these linear relationships do not hold on charged surfaces. However, the binding energies of oxygenates can be linearly correlated to OH* on charged transition metal surfaces. The unique scaling property on charged transition metal surfaces is rationalized by combinational analysis of density of states and charge density difference before and after adsorption. Our study identifies the opportunity for breaking traditional linear scaling relationships by charging catalysts practically using catalytic condensers.

Bio: Dr. Shengguang Wang is post-doctoral fellow and lab manager of the Computational Catalysis and Interface Chemistry Group at the University of Houston. Shengguang received his PhD from the Institute of Coal Chemistry, Chinese Academy of Sciences. He completed postdoc appointments at the University of Delaware (Vlachos group) and DTU (Nørskov group) and worked as a research scientist at Synfuels China. His current research focuses on transient kinetics and programmable catalysis using experimental and computational techniques.

Boltzmann Machines and Irreducible Representations of Hamming Space

Dr. Yang He

Department of Chemical and Biomolecular Engineering

Abstract: Machine learning involves constructing a statistical model and applying constraints learned from the training data to the parameter space of this model. In this brief presentation, we'll examine the dataset in Hamming space and contend that a higher-order Boltzmann machine is a collection of irreducible representations of the group covering Hamming space. A complete dataset yields a unique parameter space configuration of a Boltzmann machine. The discussion will extend to elucidate the geometric structures within this statistical manifold. A dually flat structure can be obtained when this manifold is equipped with Fisher information metric. In such a way, we can build the information geometry with dual affine connections as a generalization of Riemannian geometry. Towards the end of the talk, we'll highlight that an inadequate parameter space results in multiple optimal configurations to represent the training data, one must employ multiple statistical models to reproduce the training data. At the same time, datasets often contain a minuscule portion of all possible states. The missing states can be thought of as comprising a separate, high-entropy phase separated by an extensive energy gap from the states sampled during training.

Bio: Dr. Yang He is currently a postdoctoral fellow working in Prof. Vassiliy Lubchenko's group. He obtained his Ph.D. in Physics from the University of Houston in 2022. His primary research field is theoretical physics with emphasis on basics of artificial intelligence, and his current efforts focus on interpretability of free-energy-based generative models.

Persons with disabilities who require accommodations to attend this seminar should call 713-743-8212