July 22, 17:00-18:00
Online

Seminar

Designing Quantum-Size Supported Nanocluster Catalysts

Wissam A. Saidi, PhD

Department of Mechanical Engineering and Materials Science University of Pittsburgh

Speaker introduction

Dr. Saidi is an Associate Professor in the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh. He received his Ph.D. degree in Physics from the Ohio State University. Dr. Saidi's research is focused on material design using quantum mechanical and machine learning multiscale simulations. His research is multidisciplinary with collaborations spanning several areas in engineering and science. Current research thrusts are centered on advanced nanomaterials for energy applications (solar cells, electrochemistry and photocatalysis), corrosion under extreme conditions, and nanoparticle growth. Dr. Saidi has published over 150 publications in top peer-reviewed journals and is in the top 2% of world scientists based on a recent report by Princeton University.

Invited by Dr. Christian Tantardini, Research Scientist at CEST.

Seminar abstract

Developing sustainable and environmentally clean energy technologies requires addressing not only the production of the energy but also its storage and transformation. Electrocatalysts promise to play a central role in this goal, due to the efficiency with which they can convert transient-but-green energy sources, such as wind and solar, into storable, high-value products like hydrogen. However, the high cost of platinum (Pt), which is the current best-performing catalyst for the hydrogen evolution reaction (HER), prohibits its widespread commercial application. Thus, the grand challenge in HER is to develop catalysts that can match or outperform Pt while reducing or replacing the precious metal content.
In this talk, I will show that quantum-sized Pt nanoclusters (NCs) supported on two-dimensional MoS2 offer a practical solution to solve this grand challenge. In the NC limit, each atom counts, and the specific atomic arrangement is a key feature that affects the NC functionality. Hence, as a first step, I apply an integrated theoretical-experimental approach to determine the atomic structure of the NCs atom-by-atom – a problem that cannot be solved by either experiment or theory alone. Electrochemical modeling is then employed to determine the HER mechanism of the atomically resolved NCs in conjunction with machine learning and ab initio thermodynamics. Further, using a Butler–Volmer kinetic model of the linear sweep voltammogram, I show that the exchange current density of the NC is higher than that of bulk Pt despite the orders of magnitude reduction in metal content. These findings demonstrate that the synergy between atomistic modeling, advanced characterization, and machine learning deepen our understanding of catalysis, and offer a roadmap to optimize the catalysts at the nanoscale.

Skoltech