29th TcSUH STUDENT/POSTDOC SEMINAR

Tuesday, October 15, 2024 | 4:30–5:30 PM | HSC 102

Meet & Greet: Food and soft drinks will be served at **4:00 PM**!!

Steady State Machine Learning Enhancements of Kinetic Models in Heterogeneously Catalyzed Systems

Kenneth Kusima

Department of Chemical and Biomolecular Engineering

Abstract: In heterogeneous catalysis, accurate kinetic modeling remains a cornerstone for scientific advancement and industrial optimization. While kinetic Monte Carlo (KMC) simulations excel in capturing intricate surface phenomena, their computational demands often prove prohibitive. This study introduces a novel approach that harnesses the power of machine learning to enhance steady-state kinetic models in heterogeneously catalyzed systems. Our methodology synergizes an object-oriented microkinetic modeling framework with machine learning algorithms, achieving KMC-comparable accuracy at a fraction of the computational cost. By focusing on steady-state conditions, we've shown different approaches that streamline traditional mean-field approaches and significantly improve predictive capabilities for complex catalytic systems. These novel frameworks bridge molecular-scale interactions and macroscopic outcomes, offering insights into steady-state surface coverages and reaction rates across diverse conditions. By adeptly capturing subtle effects like adsorbate interactions and surface heterogeneity, our approaches open new avenues for catalyst design and process optimization. Ultimately, this fusion of microkinetic modeling and machine learning presents a transformative tool for researchers and industry professionals alike, promising to accelerate discoveries and optimizations in the field of heterogeneous catalysis.

Bio: Mr. Kenneth Kusima is a PhD candidate and current UH Graduate Energy Fellow working in the computational catalysis and interface chemistry group under the supervision of Dr. Lars Grabow in the Department of Chemical and Biomolecular Engineering at the University of Houston. He obtained his bachelor's degree in Engineering Science with a minor in Mathematics from Trinity University in 2019 and then received a master's degree in Chemical Engineering from Rice University in 2020. His current research focuses on creating novel machine-learned kinetic models and generating dynamic reactor models.

Development of Electrically Conductive Buffer for REBCO Conductors

Md. Abu Sayeed

Department of Mechanical Engineering

Abstract: An electrically conductive buffer architecture can enable defect-tolerant RE-Ba-Cu-O (REBCO) superconductor tapes by providing a current shunt path to the substrate. We are developing suitable electrically conductive buffers based on Titanium Nitride (TiN) grown on an ion beam-assisted deposition (IBAD) template on Hastelloy C276 substrate. The aim is to prevent the oxidation of TiN during REBCO's metal-organic chemical vapor deposition (MOCVD). The buffer architecture was modified to render TiN more oxidation-resistant while maintaining good electrical conductivity. A strong biaxial texture was achieved, and a low electrical resistivity of

43 μΩcm was measured with this modified buffer architecture. An oxide layer based on the $SrTiO_3$ (STO) cap layer was epitaxially grown using RF magnetron sputtering, followed by REBCO film growth by MOCVD. By avoiding oxidation of the modified buffer architecture based on TiN, we achieved a strong epitaxy of REBCO with a sharp texture without non-00L orientations. Scanning Hall Probe Microscopy (SHPM) data showed uniformly high critical current density throughout the entire REBCO tape.

Bio: Mr. Md. Abu Sayeed is a PhD candidate in the Department of Mechanical Engineering at the University of Houston, working under the supervision of Dr. Venkat Selvamanickam. He obtained bachelor's and master's degrees in Electrical and Electronics Engineering from the University of Chittagong, Bangladesh. His current research focuses on fabricating and characterizing buffer materials for high temperature superconductor tapes.

Optimization of the Thermoelectric Performance in High Entropy Zintl Alloys

Suraj Pradhan

Department of Physics

Abstract: The pursuit of waste heat recovery using advanced thermoelectric materials has led to the development of high-performance materials. Mg_3Sb_2, Sb-based Zintl compound, stands out as a promising thermoelectric material due to its non-toxic, low-cost, and earth-abundant elements. However, compared to its n-type counterpart, the p-type Mg_3Sb_2 has a lower figure of merit (zT), mainly due to weaker electronic properties. The n-type Mg_3Sb_2 achieves an impressive zT thanks to a high band degeneracy ($N_v = 6$). In contrast, the p-type ones have a significantly lower N_v of only 1, resulting from a large crystal-field splitting energy ($\Delta E = 0.3$ eV) between its two valence bands. To address this, Xin et al. proposed a strategy to minimize the crystal-field splitting energy, thereby increasing band degeneracy. They designed a series of compositions in the high-entropy material $Yb_xCa_{1-x}Mg_yZn_{2-y}Sb_2$, achieving band convergence by zeroing the weighted sum of crystal-field splitting energies from the parent compounds. These compositions demonstrated both higher power factors and lower thermal conductivities, with one composition ($Yb_{0.7}Ca_{0.3}Mg_{0.55}Zn_{1.45}Sb_2$) showing a notably higher zT of 1.2 at 773 K outperforming other p-type Zintl materials. Motivated by the good thermoelectric performance of $Yb_xCa_{1-x}Mg_yZn_{2-y}Sb_2$, we further investigated the thermoelectric properties of this Zintl compound by further incorporating Eu and Na through ball-milling and hot-pressing techniques.

Bio: Mr. Suraj Pradhan is a PhD candidate in the Department of Physics and Texas Center for Superconductivity at the University of Houston under the supervision of Dr. Zhifeng Ren. His current research focuses on enhancing the performance of Mg_3Sb_2-based thermoelectric materials.

Persons with disabilities who require accommodations to attend this seminar should call 713-498-9703