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Fundamental Investigations of Electrocatalyzed Transformations of Organic Compounds

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Sustainable energy generation calls for a paradigm shift away from centralized, high-temperature catalysis to decentralized, low-temperature conversions that can be powered using replenishable, renewable energy sources. Electrocatalytic conversion of biomass derived feedstocks offers a promising avenue to effectively allow carbon recycling of distributed, energypoor resources using underutilized energy resources. To retain economic viability of this target technology, rational design of electrocatalysts with high activity and selectivity towards producing value-added chemicals and fuels is necessary. Despite extensive research done in electrocatalysis, there exists a lack of mechanistic exploration and molecular-scale understanding of electrocatalytic conversion of organic compounds specifically pertaining to biomass feedstocks. Moreover, these reactions occur at the solvated electrode-electrolyte interface where complex interactions between the electrode and solvent molecules have a critical influence on the reaction chemistry. In this talk, we address the confluent influence of the solvent distribution and the charged metal electrode on the reaction intermediates and their capacity to undergo reduction/hydrogenation. Results obtained using density functional theory (DFT) calculations and molecular dynamics (MD) simulations will be presented to demonstrate our efforts in securing molecular-scale representations of the structural/electronic properties of the electrochemical interface and the reaction energetics of target organic compounds. The inferences drawn will be used to postulate design criteria for electrocatalytic conversion of organic compounds from an experimental and theoretical perspective.

Recent Publications

1. Liang, T., Antony, A. C., Akhade, S. A., Janik, M. J., & Sinnott, S. B. (2017). Applied Potentials in Variable Charge Reactive Force Fields for Electrochemical Systems. The Journal of Physical Chemistry A Article ASAP
2. Akhade, S. A., Bernstein, N. J., Esopi, M. R., Regula, M. J., & Janik, M. J. (2017). A simple method to approximate electrode potential-dependent activation energies using density functional theory. Catalysis Today, 288, 63-73.
3. Akhade, S. A., McCrum, I. T., & Janik, M. J. (2016). The impact of specifically adsorbed ions on the copper-Catalyzed electroreduction of CO2. Journal of the Electrochemical Society, 163(6), F477-F484.
4. Akhade, S. A., Luo, W., Nie, X., Asthagiri, A., & Janik, M. J. (2016). Theoretical insight on reactivity trends in CO_2 electroreduction across transition metals. Catalysis Science & Technology, 6(4), 1042-1053.
5. Akhade, S. A., Luo, W., Nie, X., Bernstein, N. J., Asthagiri, A., & Janik, M. J. (2014). Poisoning effect of adsorbed CO during CO_2 electroreduction on late transition metals. Physical Chemistry Chemical Physics, 16(38), 20429-20435.1

Biography

Dr. Sneha Akhade completed her Ph.D. in Chemical Engineering from Penn State University in 2016 and obtained a M.S. from Carnegie Mellon University. She is currently a postdoctoral research associate at the Pacific Northwest National Laboratory and works across theory and experiment to investigate electrocatalysis at a fundamental and applied scale. Her research interests broadly include catalysis, fuel cells and batteries, high-throughput computational screening and rational design of materials for alternative energy storage and conversion technologies.

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