DEPARTMENTS OF CHEMISTRY
Seminar Series

FRIDAY, October 23, 2026 - 12:00 Noon
MC H313

Learning How to Computationally Design Better Catalysts

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This talk will describe my group's use of density functional theory calculations combined with automation tools, ligand libraries, and machine learning to design new and more selective homogeneous catalysts. The first act of the talk will first emphasize transition metal catalysts that were either designed or identified for generating alpha olefins. The second act of the talk will emphasize new tools and workflows that enable faster catalyst designs. Overall, this talk will also highlight the success, frontiers, and challenges associated with interfacing computational chemistry with experiments.

Bio: Daniel H. Ess is a professor in the Department of Chemistry and Biochemistry at BYU (https://esslab.byu.edu/). He received his B.S. from BYU and Ph.D. from UCLA followed by postdoctoral work at Scripps-Florida, Caltech, and UNC Chapel Hill. His group uses and develops computational chemistry tools to discover reaction mechanisms, reactivity and selectivity principles, and design catalysts. His research ranges from applied catalyst prediction and realization with collaborators to fundamental insights from molecular dynamics studies. He is the creator of the BYU Chem Camp program (https://chemcamp.byu.edu/), which has provided chemistry experiences for over a 1000 children and youth. For education, he creates interactive learning tools, such as the "iORA" application that displays reactive organic trajectories and is available on the iPhone App Store.