ChemCatBio Webinar Series

"Artificial Intelligence for Catalysis"

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12–12:45 p.m. MT
Register: https://nrel.webex.com/weblink/register/r564abcd5cada169641f6ee1583b84144

Artificial intelligence (AI) has the potential to play a crucial role in accelerated catalyst design, discovery, and optimization of chemical processes for decarbonization. With the help of a range of AI tools—such as machine learning, deep learning, and large language models—researchers can uncover useful guidelines for designing new and improved catalysts, for both low- and high- technology readiness level research activities (i.e., innovation in catalyst research and development, advanced catalyst optimization/scale-up). To discover new and improved catalysts for efficient chemical transformation, researchers can use a combination of high-throughput computational screening (DFT-based approaches) and machine learning (supervised learning or self-supervised learning). This can reveal the influence of heterogeneous catalyst descriptors (i.e., active sites, number of hetero metal atoms, nature of grain structures) and operating conditions (i.e., temperature, pressure, concentration) on desired versus undesired reactions. Recent large language models will play a vital role in catalyst design, synthesis, and characterization, especially those based on transformer architectures that do not require knowledge of 3D structures of catalysts, as well as those based on open-source catalyst databases, such as the Materials Data Facility, Open Catalyst Project, ChemCatBio Data Hub, and Materials Project.

In this webinar, Argonne National Laboratory researcher Rajeev Assary will describe how AI and high-fidelity, first-principles simulations can help identify cost-efficient catalysts for deoxygenation chemistry. He will also describe recent efforts on using machine learning to field billions molecules to choose the best as liquid organic hydrogen carriers. Finally, he will briefly cover ongoing research directions for helping the catalysis community incorporate large language models in catalyst discovery.

For more information, please visit ChemCatBio.org or contact the consortium at https://www.chemcatbio.org/contact. ChemCatBio is funded by the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Bioenergy Technologies Office.