

Advancing Scientific Discovery in Catalysis with Artificial Intelligence



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Friday, 3 October 2025 3pm 66-110

Hongliang Xin's research focuses on developing an explainable artificial intelligence (AI) platform for a catalysis science. In this seminar, he will discuss how AI and machine learning can accelerate the discovery of catalytic nanostructures and enable new opportunities for sustainable chemistry. Xin received his Ph.D. in Chemical Engineering from the University of Michigan and completed postdoctoral research at Stanford/SLAC. He is a recipient of the 2019 NSF CAREER Award and has been recognized as an Emerging Investigator by Journal of Materials Chemistry A and as an Influential Researcher by ACS Industrial & Engineering Chemistry Research. He serves on the Editorial Board of Chem Catalysis and has contributed to the field through editorial leadership, including guest-editing special issues for the Journal of Catalysis and the Journal of Chemical Physics on data science for catalysis. He is Communications Director of the North American Catalysis Society (NACS). He initiated and co-chaired the 2024 AI for Multidisciplinary Exploration and Discovery (AIMED) Workshop on Heterogeneous Catalysis. He also served as Scientific Co-Chair of the 2025 North American Catalysis Society Meeting (NAM29) in Atlanta and is o-Chair of the inaugural 2026 Gordon Research Conference on AI for Materials, Energy, and Chemical Sciences (AIMECS).