

# Expanding the Boundary of Biocatalysis: From Directed Evolution to Autonomous Experimentation

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**Abstract:** Biocatalysis has been increasingly used for practical synthesis of chemicals, fuels, and materials thanks to recent advances in enzyme engineering, synthetic biology, artificial intelligence (AI)/machine learning (ML), and laboratory automation. In this talk, I will discuss our recent effort in designing novel synthetic routes and repurposed enzymes for synthesis of fine chemicals by exploring the synergy between enzymatic catalysis and non-enzymatic catalysis. Particularly, I will highlight our new strategies of combining photocatalysis with biocatalysis for abiological transformations. In addition, I will highlight the development of AI/ML and laboratory automation tools for enzyme discovery and engineering. Finally, I will introduce our new AI/ML tools for synthesis planning that integrates chemical catalysis and biocatalysis. All these strategies and tools should greatly accelerate the development of biocatalysts for applications related to human health, energy, and sustainability.

## References

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**Bio:** Dr. Huimin Zhao is the Steven L. Miller Chair of chemical and biomolecular engineering at the University of Illinois Urbana-Champaign (UIUC), director of NSF AI Institute for Molecule Synthesis ([moleculemaker.org](http://moleculemaker.org)), NSF iBioFoundry ([ibiofoundry.illinois.edu](http://ibiofoundry.illinois.edu)), and NSF Global Center for Biofoundry Applications ([gcba.illinois.edu](http://gcba.illinois.edu)), and Editor in Chief of *ACS Synthetic Biology*. He received his B.S. degree in Biology from the University of Science and Technology of China in 1992 and his Ph.D. degree in Chemistry from the California Institute of Technology in 1998. Prior to joining UIUC in 2000, he was a project leader at the Dow Chemical Company. Dr. Zhao has authored and co-authored over 480 research articles and over 30 issued and pending patent applications. In addition, he has given over 570 plenary, keynote, or invited lectures. Forty (40) of his former graduate students and postdocs became professors or principal investigators around the world. Dr. Zhao received numerous research and teaching awards and honors such as ECI Enzyme Engineering Award and NSF CAREER Award. His primary research interests are in the development and

applications of synthetic biology, artificial intelligence, and laboratory automation tools to address society's most daunting challenges in health, energy, and sustainability.