Abstract for IAS International Conference on Energy Materials (January 19-23, 2026)

Interpretable Artificial Intelligence for Heterogeneous Catalysis

Wei-Xue Li

Department of Chemical Physics, University of Science and Technology of China, P. R. China

Email: wxli70@ustc.edu.cn

Achieving high stability in metal catalysts is critical for their practical application in industry, yet remains a long-standing challenge due to sintering and chemical degradation under working conditions. Traditional approaches often fall short in systematically understanding and tuning the complex interplay between catalyst structure, composition, and environment.

Our team has developed an AI-driven theoretical framework to address this challenge. By integrating big data with interpretable artificial intelligence, we unified the theory of catalyst growth kinetics and established a Sabatier-like principle for tuning metal–support interactions (MSI) to enhance sintering resistance. This framework allows for rational support selection based on MSI strength and catalyst performance. To go further, we constructed a massive space of over 30 billion mathematical expressions and, using experimental data, identified a physically transparent MSI control equation. This equation successfully describes a wide range of catalytic interfaces, including oxide-supported nanoparticles, single-atom catalysts, and metal-on-oxide systems. We also introduced a criterion for strong metal–metal interactions, resolving long-standing experimental puzzles such as the encapsulation of metal catalysts by oxide supports.

This AI-guided approach not only accelerates the discovery of fundamental catalytic principles but also provides powerful design rules for building next-generation catalysts with both high activity and long-term stability under industrial conditions.

References:

[1] S. Hu, W. X. Li, Sabatier principle of metal-support interaction for design of ultrastable metal nanocatalysts, *Science*, **374**, 1360 (2021).

[2] T. R. Wang, J. Y. Hu, R. H. Ouyang, Y. T. Wang, Y. Huang, S. Hu, W. X. Li, Nature of metal-support interaction for metal catalysts on oxide supports, *Science*, **386**, 915 (2024).

[3] S. Hu, W. X. Li, A Data-driven Leap Towards Stable Catalysts, *Nature Catalysis*, **8**, 981, (2025).