

Application of Operando Spectroscopy on Industrial Catalysts

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Dynamic in-situ (Operando) spectroscopy is a technological tool used to study materials' surface structure, reaction kinetics and catalytic mechanism under real working conditions to reveal reaction mechanisms, evaluate catalytic performance and shorten the design and development cycle of new materials. According to the concept of "reasonable design and controllable preparation" of industrial catalysts, we focus on (1) Creating new strategies for the regulation of industrial catalyst structure assisted by in-situ spectroscopy (Operando) technology to study a real reaction process; (2) Explaining the relationship of structure-activity of the active sites throughout the catalyst lifecycle (preparation-structure, structure-activity-product, deactivation-regeneration). (3) Acquiring the synergistic regulation mechanisms for the process of preparation-activation-reaction-transfer in catalysts; (4) finally, greatly improving the efficiency of research and development for the industrial catalysts. We have developed a new generation of Operando spectroscopy (reaction cell up to 50 bar). The combination of kinetics, DFT, and operando spectroscopy allows us to build the relationship of structure-performance for the catalysts. The project aims to develop efficient nanocatalysts that build on the atomic-level information obtained from our mechanism studies.

Prof. Yi-Fan Han received his PhD from East China University of Science and Technology (ECUST) with honors in 1997. He worked as a postdoctoral fellow at the department of chemistry of Fudan University (Shanghai), the Catalysis and Surface Chemistry department of ULM University (Prof. R. J. Behm, Germany), and the chemistry department of Texas A&M University (Prof. W. D. Goodman & Prof. J. H. Lunsford, College Station, USA). From 2004 to 2009 he was a senior research fellow at the Institute of Chemical and Engineering Sciences (A*STAR, Singapore). He has been at East China University of Science and Technology (Shanghai, China) as a professor since 2009. He has published more than 160 papers in top professional journals like JACS, Angew. Chem.-Int. Edit., J. Catal, AIChE J., 7500 citations in SCI, 53 application for patents.

Selected Publications:

1. Weifeng Tu, Pengchao Ren, Yuanjie Li, Yongpeng Yang, Yun Tian, Zhenzhou Zhang, Minghui Zhu, Ya-Huei Cathy Chin, Jinlong Gong*, and Yi-Fan Han*. "Gas-Dependent Active Sites on Cu/ZnO Clusters for CH₃OH Synthesis" *Journal of the American Chemical Society*, 2023.
2. Minghui Zhu, Pengfei Tian, Ravi Kurtz, Thomas Lunkenbein, Jing Xu, Robert Schlögl, Israel E. Wachs, Yi-Fan Han*. "Strong Metal-Support Interactions between Copper and Iron Oxide during the High-Temperature Water-Gas Shift Reaction" *Angewandte Chemie International Edition*, 2019, 131(27), 9181-9185.
3. Minghui Zhu, Pengfei Tian, Michael E. Ford, Jiacheng Chen, Jing Xu, Yi-Fan Han*, Israel E. Wachs*. "Nature of Reactive Oxygen Intermediates on Copper-Promoted Iron-Chromium Oxide Catalysts during CO₂ Activation" *ACS Catalysis*, 2020, 10, 7857-7863.
4. Pengchao Ren, Weifeng Tu, Chanchan Wang, Sifan Cheng, Wenqi Liu, Zhenzhou Zhang, Yun Tian, Yi-Fan Han*. "Mechanism and sites requirement for CO hydrogenation to CH₃OH over Cu/CeO₂ catalysts" *Applied Catalysis B: Environmental*, 2022, 305, 121016.
5. Weifeng Tu, Chao Sun, Zhenzhou Zhang, Wenqi Liu, Haripal Singh Malhi, Wei Ma, Minghui Zhu, Yi-Fan Han*. "Chemical and structural properties of Na decorated Fe₃C₂-ZnO catalysts during hydrogenation of CO₂ to linear α -olefins" *Applied Catalysis B: Environmental*, 2021, 298, 120567.

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