Bridging new Collaborations: A Dialogue with the Center for Low-Carbon Conversion Science and Engineering (SARI-CAS)

We are pleased to welcome **Prof. Gao Peng, Prof. Li Shenggang, Prof. Zhang Jun, Prof. Wang Hui**, Center for Low-Carbon Conversion Science and Engineering, Shanghai Advanced Research Institute, Chinese Academy of Sciences (SARI-CAS) to the Chemistry Department at the **Sapienza University of Rome**, to improve our research activities and international partnership related to our bilateral research agreement and scientific collaboration.

Our estimated guests will present their scientific activities:

30.06.2025 h 15.00

Prof. Hui Wang: "CCUS application in carbon neutrality"

Abstract: The excessive emission of CO_2 has caused severe climate changes and the waste of carbon resources. If CO_2 is regarded as a new carbon source and combined with green hydrogen, it can be converted into a variety of high-value chemicals. Methanol Economy is an important means to achieve carbon neutrality, as methanol can be served as a green fuel and carrier of hydrogen. In this talk, we will discuss the progress and engineering aspects of CO_2 hydrogenation to produce green methanol. Besides, the progress of CO_2 hydrogenation to other oxidized chemicals will also be introduced, thereby promoting the application in carbon neutrality.

http://old.sari.ac.cn/gradedu/gdzssz/gdszdw2024/dtzh/stxkx202401/202407/t20240704_7210314.html

30.06.2025 h 15.30

Prof. Peng Gao: "CO_2 Hydrogenation to Chemicals and Liquid Fuels"

Abstract: The hydrogenation of carbon dioxide (CO_2) to produce chemicals and transportation liquid fuels in huge demand *via* heterogeneous thermochemical catalysis achieved using renewable energy has received increasing attention, and substantial advances have been made in this research field in recent years. In this presentation, we summarize our progress in the rational design and construction of highly efficient catalysts for CO_2 hydrogenation to methanol, higher alcohols, olefins, aromatics, and gasoline- and jet fuel-range hydrocarbons. The structure–performance relationship, the nature of the active sites, and mechanism of the reactions occurring over these catalysts are extensively explored by combining computational and experimental evidence. We hope that this presentation will promote further fundamental studies and industrial applications of heterogeneous catalysts for CO_2 hydrogenation to produce bulk chemicals and liquid fuels.

30.06.2025 h 16.00

Prof. Shenggang Li: "Computational Study of Heterogeneous Catalysts for CO_2 Hydrogenation: Towards Rational Design of Efficient Catalysts"

Abstract: CO_2 hydrogenation using renewable hydrogen is an eco-friendly and viable approach for the sustainable synthesis of chemicals and fuels. Despite the extensive mechanistic studies on the relevant catalyst materials, such as the In_2O_3-based catalysts for the rather simple CO_2 hydrogenation to methanol reaction, there remain debates on the catalyst structure under the reaction condition and the quantitative structure-activity relationship, which hinders the rational design of these catalysts. Through density function theory calculations and microkinetic simulations, we examined the reaction pathways and kinetics of different model surfaces of In_2O_3-based catalysts and showed that both the surface structure and the coordination environment of the active site significantly affected the catalytic activity and product selectivity. These computational simulations further lead to the rational design of both hexagonal In_2O_3 and Ni or Pt atomically dispersed In_2O_3 catalysts. Recently, we further extend our computational studies to the CO_2 hydrogenation reactions for synthesizing multi-carbon products, such as alcohols, olefins, and aromatics. This presentation will also cover how interfacial sites were designed to promote the C-C coupling reactions to produce these value-added products.

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