

EPFL Valais/Wallis SEMINAR

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Steady-state Study on Hydrogenation of the Intermediate of CO₂ methanation

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Carbon dioxide (CO₂) hydrogenation over transition metal catalysts is a method to produce synthetic fuels from renewable energy in a CO₂ neutral cycle. The methanation reaction, which is the primarily fully hydrogenated carbon reaction, proceeds in multiple reaction paths on a solid catalyst. It is crucial to understand the active sites and the related reaction mechanisms of CO₂ hydrogenation in order to improve the efficiency and selectivity of the reaction. Recently, we have unraveled the relationship between activity and metal/metal oxide composition, and the pathway of CO₂ methanation reaction on transition metal based catalysts. The results showed the metal oxide play important roles in CO₂ adsorption and activation. The pathway after CO₂ activation is to form adsorbed CO* species on the metal site. This CO* is the main intermediate of CH₄ formation. However, the observation of the intermediates between CO* and CH₄ has been missing over decades. Here, we present the newest discovery of intermediates on the pathway of CO* to CH₄ through a steady-state study in operando using diffuse reflectance infrared Fourier transform spectroscopy-mass spectroscopy.

References:

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2. Zhao, K. *et al.* Identifying Reaction Species by Evolutionary Fitting and Kinetic Analysis: An Example of CO₂ Hydrogenation in DRIFTS. *J. Phys. Chem. C* **2019**, *123*, 8785.
3. Zhao, K. *et al.* Unraveling and optimizing the metal-metal oxide synergistic effect in a highly active Co_x(CoO)_{1-x} catalyst for CO₂ hydrogenation. *J. Energy Chem.* **2021**, *53*,241.
4. Zhao, K.; *et al.* A Combined Diffuse Reflectance Infrared Fourier Transform Spectroscopy-Mass Spectroscopy-Gas Chromatography for the *Operando* Study of the Heterogeneously Catalyzed CO₂ Hydrogenation over Transition Metal-Based Catalysts. *Rev. Sci. Instrum.* **2020**, *91*, 074102.
5. Zhao, K. *et al.* Hydrogen storage by reduction of CO₂ to synthetic hydrocarbons. *Chinima* **2021**, under prep.



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2012 BS Chemistry and Physics, Central China Normal University, Wuhan, China.
2015 MS Physical Chemistry, Central China Normal University, Wuhan, China. Maser thesis on photocatalysis of molecular oxygen activation.
2020 PhD Physical Chemistry, École Polytechnique Fédérale de Lausanne, Sion, Switzerland. Doctoral thesis on catalyzed CO₂ hydrogenation reaction.
2020.07-08 Working on DFT calculations of the transition states of electrochemical CO₂ reduction on Cu single crystalline surface in Prof. Hannes Jonsson's group at Iceland University.
2020.07-11 Postdoc at EPFL working on microkinetics of heterogeneously catalyzed CO₂ hydrogenation