CO_2 Hydrogenation to Methanol within the OBIWAN Project: An Experimental and Modelling Approach

*Zhipeng Zhang, Iliyas Melnikov, Vitaly V. Ordomsky, Joris W. Thybaut, Andrei Khodakov**

E-mail: andrei.khodakov@univ-lille.fr; Joris.Thybaut@UGent.be

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OBIWAN Background

- **OBIWAN aims to develop sustainable catalytic routes for converting carbon-containing streams into valuable chemicals and fuels.**
- **Within this framework, CO_2 utilization combined with hydrogen-based conversion is a key strategy.**
- **Methanol is a particularly attractive product because it can serve as both a liquid energy carrier and a versatile chemical platform.**
- **Therefore, CO_2 hydrogenation to methanol is a central research direction in the project.**

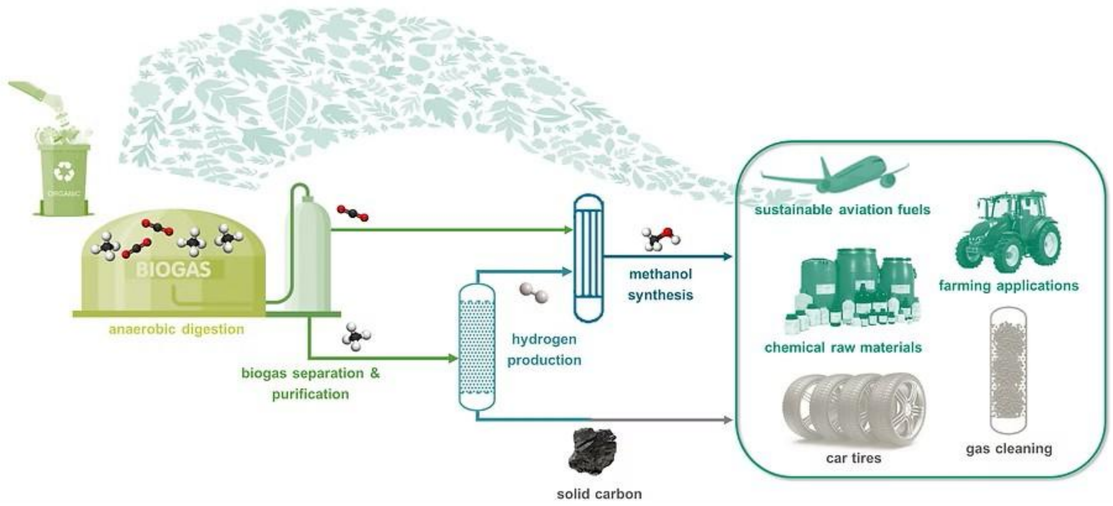


Fig. 1. OBIWAN concept: conversion of carbon-containing streams into methanol and downstream products.

My Research Focus in OBIWAN

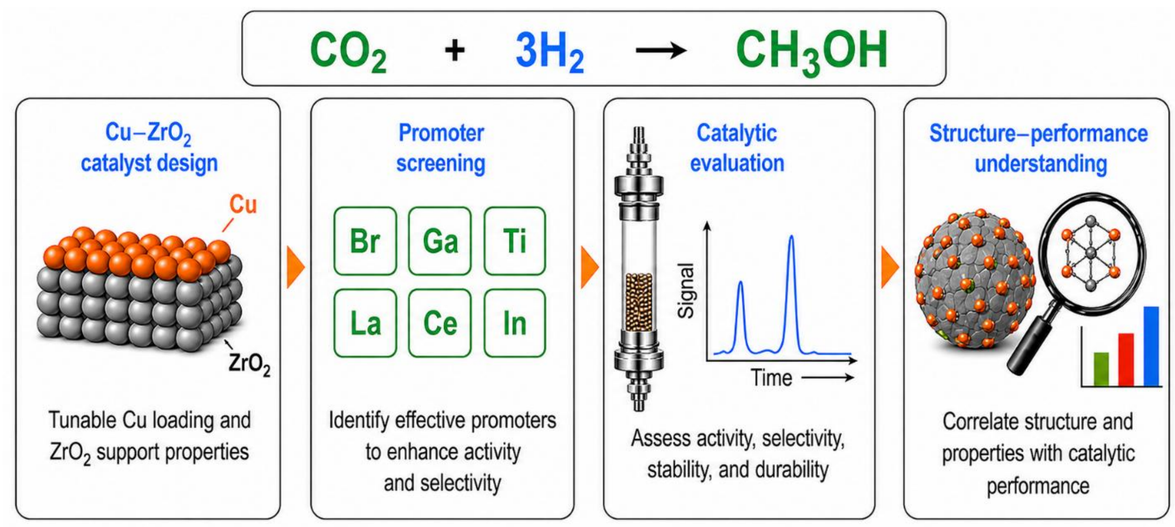


Fig. 2. Research workflow for Cu–ZrO_2 catalyst development in CO_2 hydrogenation to methanol.

Catalyst Design

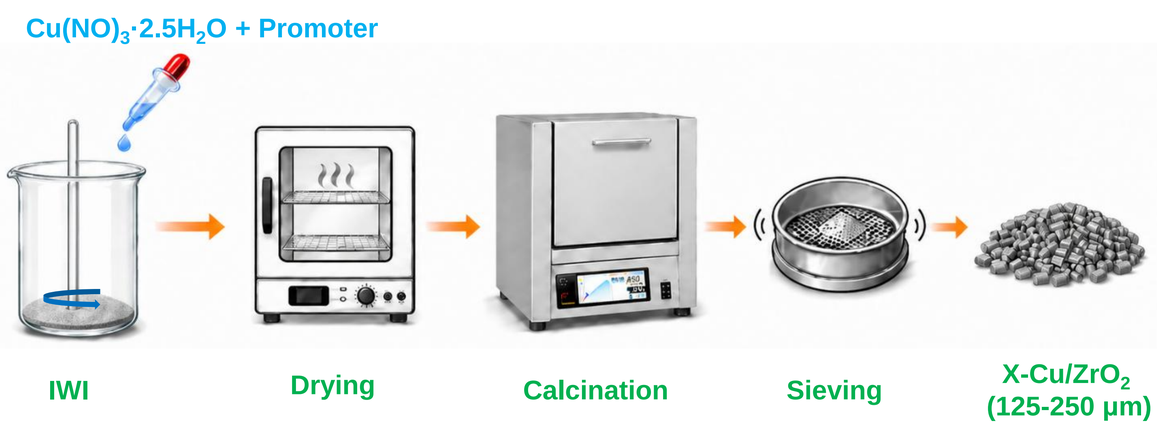
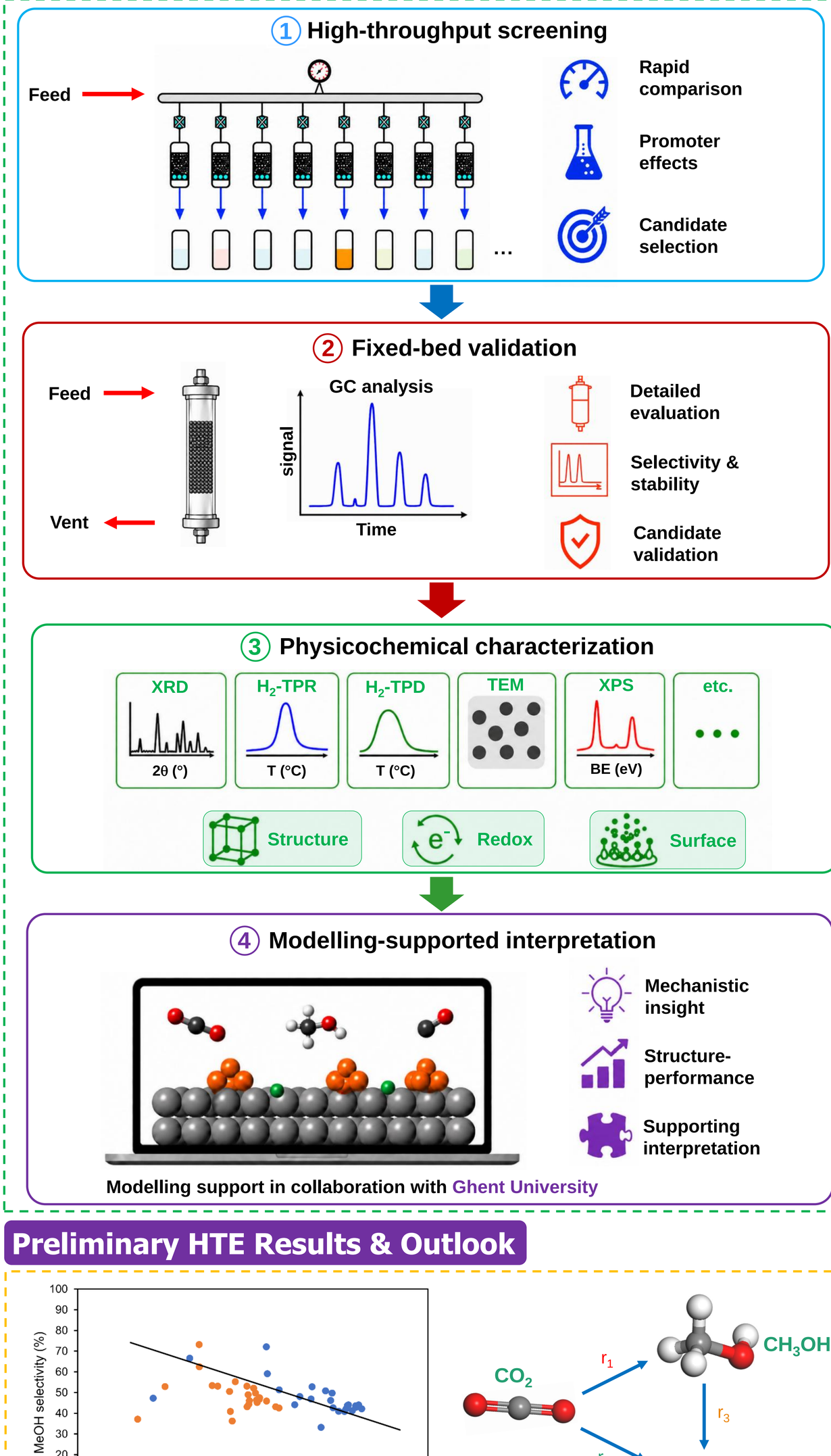


Fig. 3. Schematic preparation procedure for X–Cu/ZrO_2 catalysts.

Research Approach



Modelling support in collaboration with Ghent University

Preliminary HTE Results & Outlook

Conditions: 250 ºC; 30 bar; WHSV: 3000 and 6000 mL g_{cat}^{-1} h^{-1}

Fig. 4. Catalytic performance and main reaction pathways in CO_2 hydrogenation.

- **High-throughput screening rapidly maps the performance landscape of Cu–ZrO_2-based catalysts and identifies promising compositions for CO_2 hydrogenation to methanol.**
- **Fixed-bed validation, targeted physicochemical characterization, and atomistic modeling will be integrated to clarify structure–performance relationships and guide rational catalyst optimization.**

Reference: [1] Navarro-Jaén, S.; Virginie, M.; Bonin, J.; Robert, M.; Wojcieszak, R.; Khodakov, A. Y. Nat. Rev. Chem. 2021, 5 (8), 564–579.
[2] Corda, M.; Chernyak, S. A.; Marinova, M.; Morin, J.-C.; Trentesaux, M.; Kondratenko, V. A.; Kondratenko, E. V.; Ordomsky, V. V.; Khodakov, A. Y. ACS Catal. 2024, 14 (23), 17244–17252.

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