

Low Temperature Reverse Water-Gas Shift Enabled by Magnetically Induced Catalysis

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Highlights

- MICat using a Cu–Al spinel-derived catalyst with carbon-coated iron nanoparticles achieves high CO₂ conversion (53%) and CO yield (48%) at mild conditions (catalyst 300 °C, reactor 123 °C)
- MICat decouples local and bulk equilibria while promoting in-situ water removal.
- These two points synergistically result in a performance that would require a reactor temperature of 650 °C in a conventionally heated gas phase reaction.^[1]

1. Introduction

The catalytic conversion of CO₂ to CO through the reverse Water–Gas Shift reaction (rWGS) is pivotal to the establishment of a sustainable chemistry–energy nexus. However, this reaction is endothermic and equilibrium-limited, and thus plagued by the need for high operation temperatures (>500°C).^[2]

2. Methods

Cu–Al spinel catalyst^[3] functionalized with carbon-coated Fe NPs was tested for CO₂ hydrogenation under magnetic induction^[4,5]. Local heating was induced by an alternating magnetic field, and product analysis was performed by online GC.

3. Results and discussion

the Fe@C-Cu/Al₂O₃ multifunctional catalytic system proved robust and delivered a maximum CO yield of 62% (90% selectivity; H₂:CO₂ = 3:1) at a reactor temperature (point of contact with the catalyst bed) of 123 °C and a catalyst temperature estimated to 300 °C, which is one of the best rWGS performance at low temperature reported to date (Fig. 1b). Strikingly, reaching the same CO yield in a conventionally heated gas phase rWGS would require a reactor temperature of ca. 650 °C (Fig. 1b).

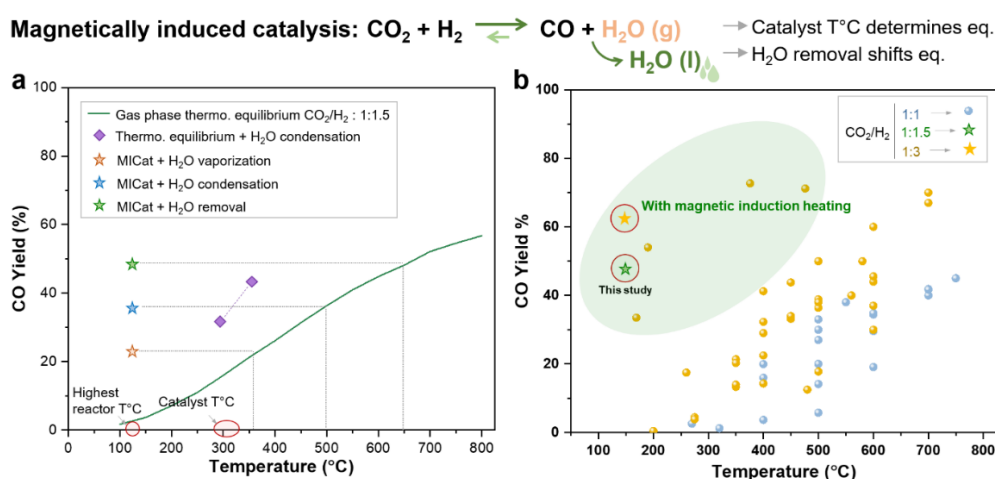


Fig. 1. CO yield as a function of temperature and comparison with literature data. a) Plot of CO yield as a function of temperature. The stars represent the data obtained in this study. The green line shows the gas-phase thermodynamic equilibrium, while the violet points indicate the thermodynamic equilibrium while accounting for water condensation (see SI for details). b) Comparison of the best result of this study (circled green star and yellow star, MICat + in-situ water removal) with literature data (individual colored disks).

4. Conclusions

Our results show that the striking enhancement as compared to the gas phase equilibria predicted by Gibbs free energy minimization at the same temperatures (CO yield of 3% at 125 °C, 16% at 300 °C) originates from two main interlinked factors: 1) in MICat, the gas phase equilibrium composition is determined by the local catalyst temperature and not by the reactor temperature, and 2) MICat helps overcoming gas phase thermodynamic equilibria by promoting the in-situ water removal from the reactive environment.

These findings substantiate the potential of MICat to decouple local and bulk equilibria and enable effective rWGS under particularly mild conditions, and may pave the way toward a broader application of MICat in challenging equilibrium-limited endothermic reactions.

References

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Keywords

Reverse water gas shift; Magnetically induced catalysis (MICat); Fe@C nanoparticles; Cu/Al₂O₃; thermodynamic equilibrium.