A Novel Dual-Function Material: Amine-Modified Ru-Based Heterogeneous Catalyst for Simultaneous CO_2 Capture and Conversion

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Significance and Relevance

To address CO_2 reduction and utilization, we developed a dual-functional material (DFM) capable of simultaneous CO_2 capture and conversion under ambient pressure. The DFM integrates a Ru-based organometallic component functionalized with amine groups, enabling effective 15% CO_2 capture and conversion into methanol at 160 °C in the presence of H_2 gas. This study demonstrates the potential of this material as an innovative solution for addressing CO_2 challenges by combining efficient capture with chemical conversion, paving the way for sustainable applications in carbon management.

- *Preferred and 2nd choice for the topic: CO_2 utilization and recycling / Air cleaning and combustion*
- *Preferred presentation*: Short Oral

Introduction and Motivations

Global warming has been accelerated by the increasing concentration of CO_2. To address this issue, research on CO_2 capture and utilization has been actively conducted.[1,2] In this context, various sorbents and catalysts have been developed, demonstrating excellent CO_2 capture capabilities and efficient conversion into useful chemicals. However, using two separate materials for CO_2 capture and conversion is energetically inefficient, and aligning the operational conditions for each material is equally impractical. To address this, dual-functional materials (DFMs) have been developed, primarily based on metal oxides, which enable simultaneous CO_2 capture and conversion.[3] However, metal oxide-based DFMs typically require high adsorption and conversion temperatures, making them energy-intensive.

In this study, we synthesized a novel organometallic-based DFM capable of adsorption and conversion at relatively low temperatures. The Ru-based organometallic catalyst functions as a homogeneous catalyst, capable of converting CO_2 into methanol with the aid of amine at low temperatures (150 °C. By heterogenizing this catalyst, we synthesized a porous polymer and further incorporated amines through postsynthetic modification. The resulting material, containing amines in the solid phase, demonstrated efficient CO_2 adsorption and catalytic activity for converting CO_2 into methanol. This showcases its potential as an innovative and energy-efficient solution for CO_2 management.

Results and Discussion

We successfully polymerized a Ru-based organometallic catalyst by employing a crosslinker (Figure 1a). N_2 adsorption experiment revealed that while the Ru-based organometallic catalyst itself did not exhibit N_2 adsorption, the synthesized polymer demonstrated N_2 adsorption, confirming the formation of pores in the material (Figure 1b). Furthermore, we introduced amine functionalities into the polymer structure through additional modification, which was confirmed using Infrared (IR) spectroscopy (Figure 1a). The characteristic amine-related peak at 3300 cm^{-1} in the IR spectrum indicated the successful incorporation of amines into the polymer framework (Figure 1c).

Subsequently, each sample was subjected to 15% CO_2 adsorption, followed by exposure to 99% H_2 atmosphere to observe the conversion of CO_2 into methanol using mass spectrometry (Figure 1d-e). The polymer without amine functionalization demonstrated CO_2 adsorption but did not facilitate methanol formation during desorption in the presence of H_2. In contrast, the amine-functionalized polymer successfully converted adsorbed CO_2 into methanol under H_2 atmosphere during desorption.

These findings validate that the amine-functionalized Ru-based polymer is not only capable of capturing CO_2 but also effectively converting it to methanol at low temperatures, demonstrating its potential as a dual-function material for CO_2 capture and utilization.

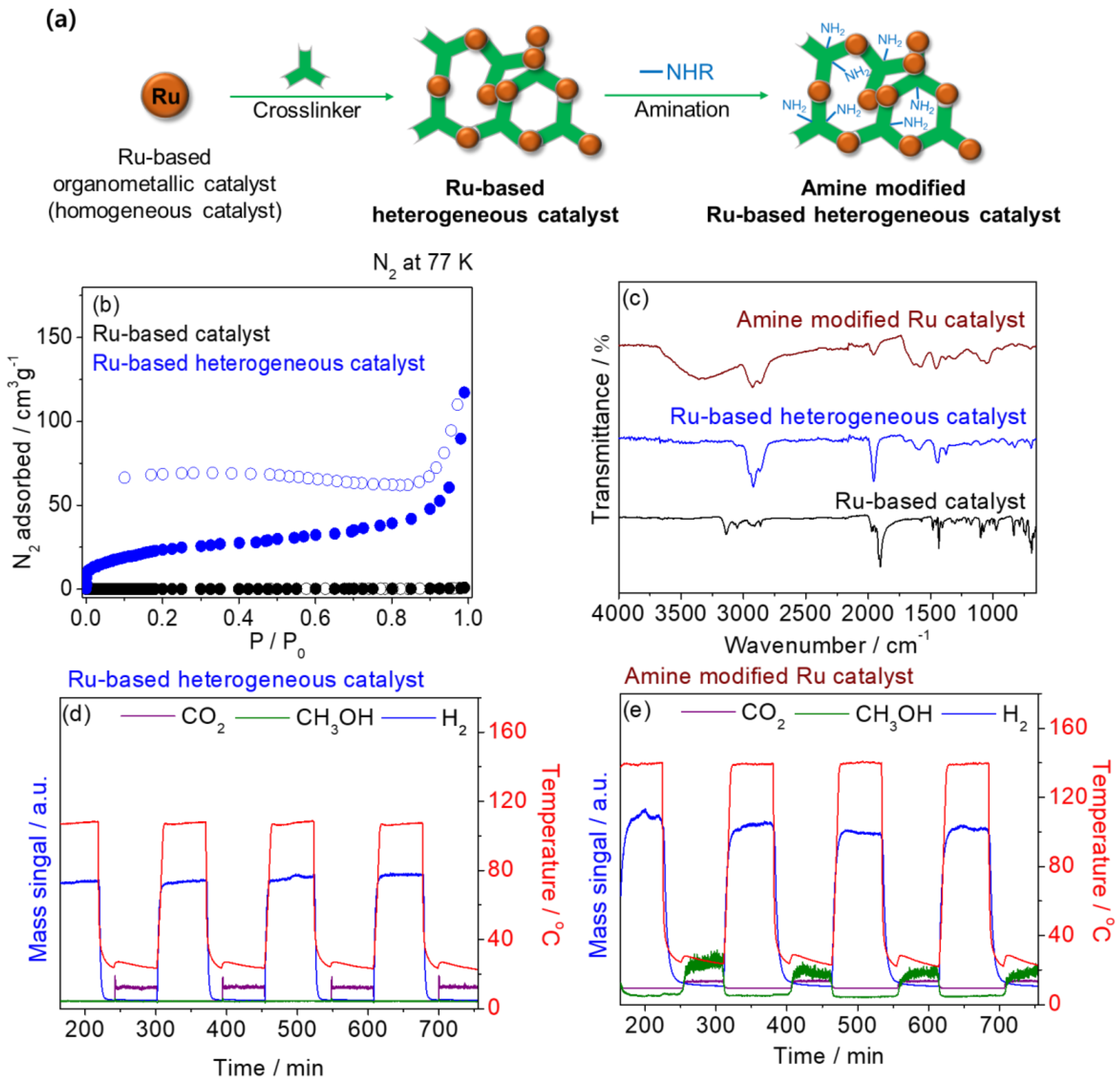

Figure 1. (a) Polymerization of the Ru-based catalyst and subsequent amine functionalization. (b) N_2 adsorption at 77 K for the samples. (c) IR spectra of the samples. (d-e) CO_2-to-methanol conversion tests for the Ru-based catalyst and the amine-functionalized Ru-based catalyst.

References

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3. *Omodolor, I. S. et al. Ind. Eng. Chem. Res.* **2020**, *59, 17612*