

RESEARCH ARTICLE

Development of a novel Cu (I) π -complexation adsorbent for ultra-deep desulfurization from a carbon dioxide stream

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Abstract

Desulfurization technology is rather difficult and urgently needed for carbon dioxide (CO₂) utilization in industry. A new Cu(I)-based adsorbent was synthesized and examined for the capacity of removing carbonyl sulfide (COS) from a CO₂ stream in an effort to solve the competitive adsorption between CO₂ and COS and to seek opportunity to advance adsorption capacity. A wide range of characterization techniques were used to investigate the physicochemical properties of the synthesized Cu(I) adsorbent featuring π -complexation and their correlations with the adsorption performance. Meanwhile, the first principal calculation software CP2K was used to develop an understanding of the adsorption mechanism, which can offer useful guidance for the adsorbent regeneration. The synthesized Cu(I) adsorbent, prepared by using copper citrate and citric acid on the ZSM-5 (SiO₂/Al₂O₃ = 25) carrier, outperformed other adsorbents with varying formulations and carriers in adsorption capacities. Through optimization of the preparation and adsorption conditions for various adsorbents, the breakthrough adsorption capacity (Q_b) for COS was further enhanced from 2.19 mg/g to 15.36 mg/g. The formed stable π -complex bonds between COS and Cu(I), as confirmed by density functional theory calculations, were verified by the significant improvement in the adsorption capacity after regeneration at 600°C. The above advantages render the novel synthesized Cu(I) adsorbent a promising candidate featuring cost-effectiveness, high efficacy and good regenerability for desulfurization from a CO₂ stream.

KEYWORDS

π -complexed adsorption, carbonyl sulfide, CO₂ purification, Cu(I) adsorbent, desulfurization

1 | INTRODUCTION

As the major component of greenhouse gas, carbon dioxide (CO₂) emissions are considered a primary contributor to the global climate change, which accounts for roughly 66% of the global warming caused by anthropogenic activities.^[1]

The Paris Agreement was signed to commit to combat climate change through global efforts.^[2] To limit or even reduce the CO₂ emissions, carbon capture, utilization, and storage (CCUS) technologies have been extensively studied and developed in the past decades to provide efficient and cost-effective solutions.^[3,4] In the coal chemical industry, a

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