

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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Table of Contents Stream Of Consciousneb In Mordern Novel

1. Understanding the eBook Stream Of Consciousneb In Mordern Novel
 - The Rise of Digital Reading Stream Of Consciousneb In Mordern Novel
 - Advantages of eBooks Over Traditional Books
2. Identifying Stream Of Consciousneb In Mordern Novel
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Stream Of Consciousneb In Mordern Novel
 - User-Friendly Interface
4. Exploring eBook Recommendations from Stream Of Consciousneb In Mordern Novel
 - Personalized Recommendations
 - Stream Of Consciousneb In Mordern Novel User Reviews and Ratings
 - Stream Of Consciousneb In Mordern Novel and Bestseller Lists

5. Accessing Stream Of Consciousness In Modern Novel Free and Paid eBooks
 - Stream Of Consciousness In Modern Novel Public Domain eBooks
 - Stream Of Consciousness In Modern Novel eBook Subscription Services
 - Stream Of Consciousness In Modern Novel Budget-Friendly Options
6. Navigating Stream Of Consciousness In Modern Novel eBook Formats
 - ePub, PDF, MOBI, and More
 - Stream Of Consciousness In Modern Novel Compatibility with Devices
 - Stream Of Consciousness In Modern Novel Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Stream Of Consciousness In Modern Novel
 - Highlighting and Note-Taking Stream Of Consciousness In Modern Novel
 - Interactive Elements Stream Of Consciousness In Modern Novel
8. Staying Engaged with Stream Of Consciousness In Modern Novel
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Stream Of Consciousness In Modern Novel
9. Balancing eBooks and Physical Books Stream Of Consciousness In Modern Novel
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Stream Of Consciousness In Modern Novel
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Stream Of Consciousness In Modern Novel
 - Setting Reading Goals Stream Of Consciousness In Modern Novel
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Stream Of Consciousness In Modern Novel
 - Fact-Checking eBook Content of Stream Of Consciousness In Modern Novel
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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