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Comparison of simulation methods for studying CO■ storage in mining waste

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Introduction

New decarbonization technologies are urgently needed to address global warming and reduce the occurrence of extreme weather events driven by climate change. Carbon capture and storage (CCS) is one of the technological solutions aimed at mitigating these impacts. This practice involves capturing CO_2 from industrial or atmospheric sources and storing it safely and efficiently over the long term, either in geological reservoirs or in materials capable of adsorbing or retaining it. Mining, on the other hand, is a sector that generates large volumes of waste during mineral processing, known as mining waste. This waste requires extensive disposal areas and may pose environmental liabilities if not properly managed. However, depending on their characteristics, mining wastes can be reused and recycled, presenting an opportunity to address two environmental challenges simultaneously: CO_2 storage and waste disposal. Mining residues such as coal and limestone waste have properties that can be exploited for CO_2 capture. In the case of coal waste, CO_2 adsorption on their surface is possible. For limestone waste, chemical reactions with CO_2 can lead to mineralization, forming stable carbonate compounds. Utilizing this mining waste not only offers an environmental solution for residue disposal but also contributes significantly to climate change mitigation efforts, creating a virtuous cycle of waste utilization and carbon emission reduction. To assess the efficiency of CO_2 storage in mining waste, it is essential to understand the molecular mechanisms governing both CO_2 adsorption in coal waste and the chemical reactions involved in the mineralization of limestone waste.

Method and Theory

Several computational methods are available for simulating atomic- and molecular-level systems: Grand Canonical Monte Carlo (GCMC), Molecular Dynamics (MD) simulations, Density Functional Theory (DFT), and Artificial Neural Network (ANN) models. The Monte Carlo (MC) algorithm is a stochastic computational method based on statistical principles, using numerous data samples to generate random outputs. GCMC is a widely used approach in MC simulations, particularly for studying gas adsorption in coal. MD simulations are based on Newton's laws of motion. DFT is a quantum mechanical method used to study the electronic structure of multi-electron systems. An ANN is a type of machine learning algorithm inspired by the structure and function of biological neural networks in the brain. ANNs are computational models composed of interconnected nodes, known as artificial neurons, that process information in a way similar to biological brains. In this context, the present work aims to compare these different methods, through literature review and preliminary simulations, to define the most suitable computational approaches for simulating CO_2 storage in mining waste — both for adsorption and reaction processes — providing a detailed theoretical perspective of the mechanisms involved.

Results and Conclusions

Preliminary results, based on bibliographic review and initial computational model development, indicate that all previously mentioned methods are appropriate tools for theoretically evaluating CO_2 storage in mining waste. This study is expected to lay the groundwork for future practical applications, contributing to the development of solutions and climate change mitigation.