



Metal-organic Framework Membranes for CO₂ Capture, Biofuel Purification and Water Desalination: A Computational Perspective

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INTRODUCTION

As a unique class of hybrid nanoporous materials, Metal-Organic Frameworks (MOFs) have received tremendous interest over the last decade. The variation of metal oxides and the judicious choice of controllable organic linkers allow the pore size, volume and functionality to be tailored in a rational manner for designable architectures. MOFs thus provide a wealth of opportunities for engineering new membrane materials and have been considered as versatile candidates for many important potential applications. However, the number of MOFs synthesized to date is extremely large, thus experimental testing alone is economically expensive and practically formidable. With rapidly growing computational resources, molecular simulation has become an indispensable tool to characterize, screen, and design MOFs. Human activities have led to a massive increase in CO₂ emissions as a primary greenhouse gas that is contributing to climate change with higher than 1°C global warming than that of the pre-industrial level. We evaluate the three major technologies that are utilised for carbon capture: pre-combustion, post-combustion and oxyfuel combustion. We review the advances in carbon capture, storage and utilisation. We compare carbon uptake technologies with techniques of carbon dioxide separation. Monoethanol amine is the most common carbon sorbent; yet it

photographs inspire people to read it as well.

JMSP postlat I requires a high regeneration energy of 3.5GJ per tonne of CO₂. Alternatively, recent advances in sorbent technology reveal novel solvents such as a modulated amine blend with lower regeneration energy of .17 GJ per tonne of CO₂. Graphene- type materials show CO₂ adsorption capacity of 0.07 mol/g, which is 10 times higher than that of specific types of activated carbon, zeolites and metal-organic frameworks.

CO₂ geosequestration provides an efficient and long-term strategy for storing the captured CO₂ in geological formations with a global storage capacity factor at a Gt-scale within operational timescales. The recovery of these dilute fermentation products from the broth, however, can be incredibly energy intensive as a distillation process is generally involved and creates a barrier to commercialization. Regarding the utilisation route, currently, the gross global utilisation of CO₂ is lower than 200 million tonnes per year, which is roughly negligible compared with the extent of global anthropogenic CO₂ emissions, which is higher than 32,000 million tonnes per year. Herein, we view different CO₂ utilisation methods such as direct routes, *i.e.* beverage carbonation, food packaging and oil recovery, chemical industries and fuels. This Review focuses on research oriented toward elucidation of the various aspects that determine adsorption of CO₂ in metal-organic frameworks and its separation from gas mixtures found in industrial processes.

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