Bioenergetics: Open Access

Short Communication Open Access

Metal-organic framework membranes for CO2 capture, biofuel purification and water desalination: A computational perspective

Jianwen Jiang

National University of Singapore, Singapore

Abstract

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 CO2CO2 emissions as a primary greenhouse gas that is contributing to climate change with higher than 1□C1□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. Monoethanolamine is the most common carbon sorbent; yet it requires a high regeneration energy of 3.5 GJ per tonne of CO2CO2. Alternatively, recent advances in sorbent technology reveal novel solvents such as a modulated amine blend with lower regeneration energy of 2.17 GJ per tonne of CO2CO2. Graphene-type materials show CO2CO2 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. CO2CO2 geosequestration provides an efficient and long-term strategy for storing the captured CO2CO2 in geological formations with a global storage capacity factor at a Gt-scale within operational timescales. Regarding the utilisation route, currently, the gross global utilisation of CO2CO2 is lower than 200 million tonnes per year, which is roughly negligible compared with the extent of global anthropogenic CO2CO2 emissions, which is higher than 32,000 million tonnes per year. Herein, we review different CO2CO2 utilisation methods such as direct routes, i.e. beverage carbonation, food packaging and oil recovery, chemical industries and fuelsThis 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. It includes theoretical, experimental, and combined approaches able to characterize the materials, investigate the adsorption/desorption/reaction properties of the adsorbates inside such environments, screen and design new materials, and analyze additional factors such as material regenerability, stability, effects of impurities, and cost among several factors that influence the effectiveness of the separations. CO2 adsorption, separations, and membranes are reviewed followed by an analysis of the effects of stability, impurities, and process operation conditions on practical applications. Fermentations provide an alternative to fossil fuels for accessing a number of biofuel and chemical products from a variety of renewable and waste substrates. 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. Membrane processes can provide a low energy aid/alternative for recovering these dilute fermentation products and reduce production costs. For these types of separations many current polymeric and inorganic membranes suffer from poor selectivity and high cost respectively. This paper reviews work in the production of novel mixed-matrix membranes (MMMs) for fermentative separations and those applicable to these separations. These membranes combine a trade-off of low-cost and processability of polymer membranes with the high selectivity of inorganic membranes. Work within the fields of nanofiltration, reverse osmosis and pervaporation has been discussed. The review shows that MMMs are currently providing some of the most high-performing membranes for these separations, with three areas for improvement identified: Further characterization and optimization of inorganic phase(s), Greater understanding of the compatibility between the polymer and inorganic phase(s), Improved methods for homogeneously dispersing the inorganic phase. Computational crystal construction algorithms were used to create twelve metal–organic frameworks containing a newly synthesized [2,2□-bithiazole]-5,5□-dicarboxylic acid (H2TzTz) spacer and assorted transition metal nodes. Among the twelve structures, the zirconium-based MOF of general formula [Zr6O4(OH)4(TzTz)6] (1) was found to be the best candidate for carbon dioxide uptake, as judged from the results of the grand canonical Monte Carlo (GCMC) simulations of CO2 adsorption isotherms. Guided by the simulation results, 1 was synthesized in the laboratory and thoroughly characterized.

Note: This work is partly presented at International Conference on Membrane Science and Technology September 11-12, 2017 | Paris, France