World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:19, No:07, 2025

DFT Insights into CO_2 Capture Mechanisms and Kinetics in Diamine-Appended Grafted Mg_2 (dobpdc) Metal- Organic Frameworks

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Abstract : Climate change is widely recognized as a global crisis, with anthropogenic CO_2 emissions from fossil fuel combustion and industrial processes being major contributors. To address this challenge, carbon capture and sequestration (CCS) technology has emerged as a key strategy for selectively capturing CO_2 from flue gas streams. Among the various solid adsorbents, metal–organic frameworks (MOFs) are notable for their extensive surface area and controllable pore chemistry. The porous MOF structure is comprised of metal ions or clusters coordinated to organic linker compounds. In particular, the pore parameters of MOFs are readily tunable, making them promising materials for CO_2 capture applications. Among these, amine-functionalized MOFs have demonstrated exceptional CO_2 capture abilities because their high uptake capacity and selectivity. In this study, we have investigated the CO_2 capture abilities and adsorption mechanisms of the diamine-appended framework N-Ethylethylenediamine-Mg_2(4,4’-dioxidobiphenyl-3,3’-dicarboxylate) (e-2-Mg_2(dobpdc)) using density functional theory (DFT) calculations. Previous studies have suggested that CO_2 can be captured via both outer- and inner-amine binding sites. Our findings reveal that CO_2 adsorption at the outer amine site is kinetically more favorable compared to the inner amine site, with a lower energy barrier of 1.34 eV for CO_2 physisorption to chemisorption compared to the inner amine, which has an activation barrier of 1.60 eV. Furthermore, we find that CO_2 adsorption is significantly enhanced in an alkaline environment, as deprotonation of the diamine molecule reduces the energy barrier to 0.24 eV. This theoretical study provides detailed insights into CO_2 adsorption in diamine-appended e-2-Mg_2(dobpdc) MOF, offering a deeper understanding of CO_2 capture mechanisms and valuable information for the advancement of effective CO_2 sequestration technologies.

Keywords : DFT, MOFs, CO_2 capture, catalyst
Conference Title : ICCPE 2025 : International Conference on Chemical and Process Engineering
Conference Location : Tokyo, Japan
Conference Dates : July 22-23, 2025