

Orientation Effect of DDR Zeolite Membrane for the Separation of CO<sub>2</sub> and H<sub>2</sub>이정현<sup>1,2</sup>, 김진철<sup>1</sup>, 김형준<sup>1</sup>, 김은주<sup>3</sup>, 최정규<sup>3</sup>, 곽상규<sup>1,†</sup><sup>1</sup>울산과학기술원; <sup>2</sup>에너지 및 화학공학부; <sup>3</sup>고려대학교(skkwak@unist.ac.kr<sup>†</sup>)

Zeolite is one of the most popular adsorbent due to its uniform pore structure as well as superior thermal, mechanical and chemical stabilities. In the separation of CO<sub>2</sub> and H<sub>2</sub> via membrane-based technology, since the kinetic diameter of H<sub>2</sub> is quite smaller than that of CO<sub>2</sub>, the adsorbent is required to have distinctive pore size and adsorptive property. DDR zeolite having 6 and 8-membered ring windows in different orientations could be employed for the separation of these gas molecules. In this study, the orientation effect of DDR zeolite membrane on CO<sub>2</sub> separation was investigated via molecular dynamics (MD) simulation and density functional theory (DFT) calculation. We considered two slab models, perpendicular to (001) and (101) surfaces, where adsorbed gas molecules pass through 6- and 8-membered ring windows. In the (001) slab model, both CO<sub>2</sub> and H<sub>2</sub> molecules undergo high-energy barrier, thereby impeded permeabilities. In contrast, in the (101) slab model, CO<sub>2</sub> was facilitatively diffused with good permeance, resulting in high H<sub>2</sub>/CO<sub>2</sub> separation performance. Through this study, the effectiveness of the oriented zeolite membrane in CO<sub>2</sub> separation was shown.