Orientation-dependent CO_2/H_2 permselectivity of highly aligned DDR zeolite membrane

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Zeolite membrane is one of potential candidates to replace energy-intensive separation methods such as distillation or absorption, due to its uniform pore structure and superior thermal stabilities. Until now, it has been believed that 6 membered ring (MR) in zeolite is effective for selective capture of H_2 over CO_2, considering the kinetic diameters of adsorbates and the size of 6MR pore aperture. However, experimentally synthesized c-oriented zeolite membrane, where the 6MR was preferentially aligned along the diffusion path, exhibited unexpected CO_2-permselectivity at room temperature. In this study, permeability of DDR membrane along particular orientation was investigated via non-equilibrium molecular dynamics simulation and density functional theory calculation. According to the simulation results, permeation rates of H_2 and CO_2 passing through 6MR was negligible, implying no intrinsic molecular sieving effect for H_2. In contrast, 8MR showed CO_2 and H_2 permselective at 30 and 200°C, respectively, due to competitive effects of thermodynamic interaction and kinetic size. Through this study, new insights for H_2/CO_2 permselectivity with aligned zeolite membrane was suggested.