潘艳秋（教授） 赞741 同专业博导 同专业硕导 个人学术主页
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教授 博士生导师 硕士生导师
任职：化工学院教学指导委员会主任

论文成果

Molecular simulation and optimization on the microporous structure in carbon molecular sieve membrane for CO2/CH4 separation

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第一作者：He, Liu
通讯作者：Pan, YQ (reprint author), Dalian Univ Technol, Sch Chem Engn, Dalian 116024, Peoples R China.; Wang, TH (reprint author), Dalian Univ Technol, Sch Chem Engn, Grp Carbon Membranes & Porous Mat, State Key Lab Fine Chem, Dalian 116024, Peoples R China.
合写作者：Pan, Yanqiu,Wang, Tonghua,Yu, Lu
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摘要：Zigzag-type pore model with a modified structure was proposed to evaluate the effect of micropore structure on the gas separation performance of carbon molecular sieve membranes (CMSM). Molecular simulation was applied to investigate the adsorption and diffusion of equimolar CO2/CH4 mixture in the micropores of CMSM and the separation performance. Results showed that the simulated isotherms of CO2 and CH4 were consistent with the experimental ones at pore size of 0.54 nm. The separation performance of CO2/CH4 mixture would be the largest at pore size of 0.6 nm under bending cell length of 3.767 nm and bending angle of 150 degrees.

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