

하이브리드 분자 동적 모사 방법을 이용한 무기막 투과 현상 관찰

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In this research, gas permeation through inorganic membrane is observed using hybrid molecular dynamics simulation. The molecular flows near the system boundaries are described through the hybrid molecular simulation method, which is a combination of molecular dynamics simulation and grand canonical Monte Carlo simulation.

In the present study, helium and nitrogen gases are used to investigate the permeation phenomena. The number of permeated molecules is counted to calculate the membrane permeability. Also, the permeability is estimated for various conditions using hybrid molecular simulation. It is compared with the experimental data. The separation mechanism is analyzed for the simulation results.