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Diffusivity Investigation of Hydrogen Isotopes in Flexible MOFs by Quasi-Elastic Neutron Scattering

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Kinetic-quantum-sieving-assisted H2:D2 separation in flexible porous materials is more effective than the currently used energy-intensive cryogenic distillation and girdle-sulfide processes for isotope separation. It is believed that material flexibility results in a pore-breathing phenomenon under the influence of external stimuli, which helps in adjusting the pore size and gives rise to the optimum quantum-sieving phenomenon at each stage of gas separation. However, only a few studies have investigated kinetic-quantum-sieving-assisted isotope separation using flexible porous materials. Here, we present the quasi-elastic neutron scattering (QENS) data showing a significantly faster diffusion of deuterium than hydrogen in a flexible pore structure, even at high temperatures. Unlike rigid structures, the extracted diffusion dynamics of hydrogen isotopes within flexible frameworks show that the diffusion difference between the isotopes increases with an increase in temperature confirmed by measured QENS data. Owing to this unique inverse trend, a new strategy can be proposed for achieving higher operating temperatures for efficient isotope separation utilizing a flexible metal-organic framework system.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Advanced Materials & Processing