

Transport in Hierarchical Zeolites with Micro- and Mesopores

Scientific Achievement

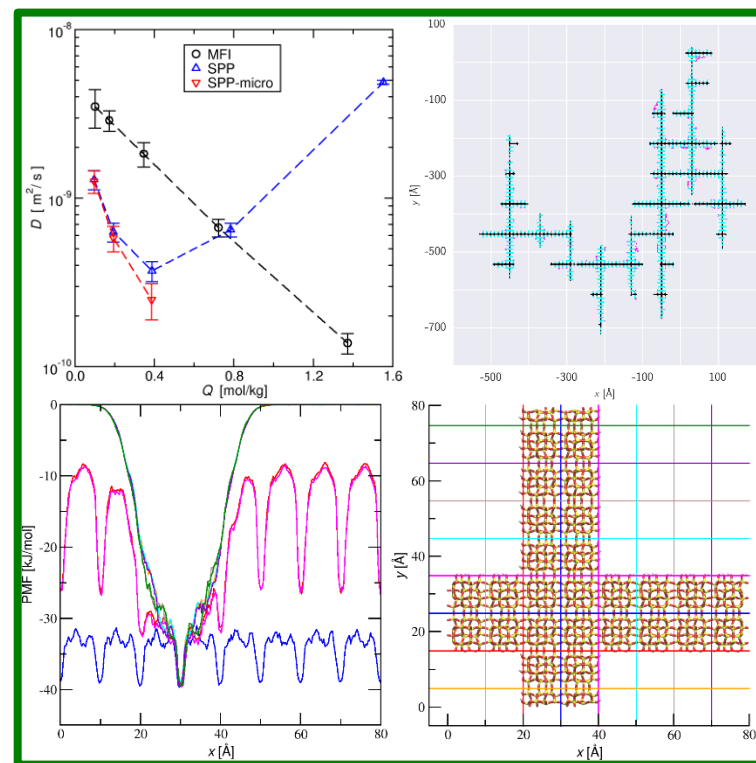
A type of diffusive barrier unrelated to structural defects is elucidated and explained in terms of the intrinsic thermodynamics of materials with nanoscale dimensions. Regimes where the novel class of hierarchical nanoporous zeolites out-perform conventional materials are identified.

Significance and Impact

- Materials with ultra-thin microporous regimes can have much faster uptake and greatly improved utilization while maintaining high selectivity.
- Knowledge of the mechanisms of transport barrier can aid process design and optimizations.

Research Details

- Diffusion of *n*-hexane is slower in a hierarchical zeolite than in a conventional material with the same micropore structure at low *T* and loadings, but much faster at high *T* or loadings.
- Free-energy profiles indicate a large, enthalpic penalty for molecules to escape from the micropores into mesopore channels.
- Equilibrium preference of sorbates towards micropores leads to a dynamic behavior characterized by tortuous diffusion pathways in the microporous domains.



P. Bai, E. Haldoupis, P. J. Dauenhauer, M. Tsapatsis, and J. I. Siepmann, *ACS Nano*. **2016**, 10, 7612—7618