Exploiting unexplored adsorption and diffusion mechanisms for molecular separations in zeolites and metal-organic frameworks

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Separation processes play a major role in the chemical and petrochemical industry. Adsorptive separations can have larger cost and energy efficiency than conventional distillation techniques. The present work provides additional insights in various largely unexplored adsorptive separation mechanisms such as the chain length dependent adsorption, gate-opening, breathing, selective stacking and the molecular trapdoor mechanism. Therefore, a combination of diverse experimental (static and dynamic adsorption experiments in gas, vapor and liquid phase) and modeling techniques (breakthrough simulations, pressure swing adsorption simulations) were used. Different types of nanoporous adsorbents, such as zeolitic materials (KFI, SAPO-34) and metal-organic frameworks (MIL-47, MIL-53, ZIF-8, Mg-MOF-74), were studied in various industrially relevant separation processes such as the recovery of the bio-butanol, separation of xylenes and ethylbenzene (EB), and the separation of EB from styrene. In addition, CO_2 separations were studied in the 8 membered-ring zeolite KFI to investigate the (potential) presence and impact of different separative effects (equilibrium, kinetic, molecular trapdoor). Finally, the performance of one of the most promising metal-organic frameworks (Mg-MOF-74) in the field of CO_2 separations was compared to zeolites.