Metal–Organic Framework Materials for Energy-Efficient Ammonia Separation

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Alumina-based metal–organic framework materials (Al-based MOFs) were integrated into the ammonia (NH_3) synthesis process to achieve 1–5% NH_3 adsorptive separation at 25–100 °C and 1 bar (corresponding to an NH_3 partial pressure of 1–5 kPa), which can potentially enhance energy efficiency and reduce capital costs by minimizing processing steps. Monte Carlo simulation and temperature programmed analysis clarified the crucial role of functional groups on the pore surface and pore shape of Al-based MOFs and in influencing NH_3 interactions, which contrasts with the traditional focus on specific surface area. Among these Al-based MOFs, CAU-10-OH composed of octahedral Al species linked to 5-hydroxyisophthalic acid exhibited high NH_3 adsorption capacity (3.6–1.8 mmol g^{-1}) at 25–100 °C was stable for over 15 adsorption–desorption cycles (~180 h). This performance was comparable to that of microporous ZSM-5 zeolitic materials and significantly exceeded those of silica and activated carbon. NH_3 adsorption and desorption heat (60 kJ mol^{-1}) on CAU-10-OH with hydroxyl groups located in the cage-like pores (2.41 Å) were suitable for low-concentration, ambient-temperature NH_3 separation. Integrating CAU-10-OH at 25 °C downstream of a Ru-catalyzed mild NH_3 synthesis exhibited rapid NH_3 adsorption, proving its practical efficacy for synthesis and separation under mild conditions.