Development of a general evaluation metric for rapid screening of adsorbent materials for post-combustion CO_2 capture

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Molecular simulations are combined with macroscopic pressure swing adsorption (PSA) modelling and process optimization to screen more than 5,000 metal-organic frameworks (MOFs) for their suitability in separating CO_2 from N_2 under conditions of interest in post-combustion CO_2 capture. The hierarchical screening process eliminates MOFs based on metal price, new heuristics based on the heats of adsorption, full PSA modelling and optimization, and other factors. Based on PSA modelling of 190 materials, a general evaluation metric (GEM) is developed that can rank the performance of adsorbent materials as defined by the lowest cost for post-combustion CO_2 capture. The metric requires only isotherm data and the N_2 internal energy of adsorption. The N_2 working capacity is the most important component of the metric, followed by the CO_2 working capacity, the CO_2/N_2 selectivity at desorption conditions, and the N_2 internal energy of adsorption.