

HIGH-THROUGHPUT DISCOVERY OF ADSORBENT FOR ETHANE/ETHYLENE SEPARATION: MOLECULAR/PROCESS SIMULATION AND EXPERIMENTAL VALIDATION

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As an important process for essential feedstocks of industries, economic ways of ethylene production have been broadly studied. For energy-efficient separation of the ethylene, various areas have worked with adsorptive separation processes, whose key materials are adsorbents. In this work, we include both Grand canonical Monte Carlo (GCMC) and adsorptive process simulations in the high-throughput computational screening work to explore more than 14,000 metal-organic framework (MOFs) in the CoRE MOF 2019 database. Their results show that top three MOFs have superior ethylene recovery. The discovered MOFs were synthesized for testing its feasibility, which leads to Ni(IN)₂ that survived due to the stability issue. Moreover, the potential energy surface analysis, adsorption energy distribution and DFT optimized configuration results illustrate the underlying mechanism of ethane-selective adsorption in Ni(IN)₂. The process level evaluation shows that Ni(IN)₂ is superior to many of the adsorbent materials reported to date for ethane/ethylene separation.