High-throughput, Multiscale Computational Screening of Metal-organic Frameworks for Energy-efficient SF_6/N_2 Separation

차재훈, 정용철[1,†], 가성빈[2]
부산대학교; [1]Pusan National University; [2]Pusan Natinal University
(drygchung@gmail.com[†])

We combined high-throughput molecular simulation with process-level simulation to computationally screen CoRE MOF database 2019 with the aim of high-performing materials for SF_6/N_2 separation. The top 3 materials are finally selected as the promising adsorbents based on the energy consumption evaluation in each VSA and PSA cases. For the PSA simulation, ideal PSA cascade simulation is suggested to boost the SF_6 maximum purity. The relations between the structural properties of MOF, the adsorption isotherm shapes of the top materials, and the adsorption process performance is analyzed looking at the top 10 screened adsorbents.