Integrated Material and Process Multi-Scale Evaluation of Metal-organic Frameworks Database for Energy-efficient SF_6/N_2 Separation

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The high dielectric strength of SF_6 makes the gas useful in gas-insulated switchgear, where SF_6 is typically mixed with relatively cheap N_2. However, SF_6 has been identified as one of the main greenhouse gases due to its high global warming potential (GWP: 22,800 - 23,900). We proposed multi-scale screening, which employs both molecular and process-level methods, to identify high-performing MOFs for energy efficient separation of SF_6 and N_2 mixture. Grand canonical Monte Carlo (GCMC) simulations were combined with ideal adsorption process simulation to computationally screen 2,890 metal-organic frameworks (MOFs). 78 MOFs selected for the VSA conditions were able to achieve the 90 % target purity level of SF6, but 62 top-performing MOFs selected for the PSA condition could not reach the purity level with a single train PSA configuration. Cascade PSA configuration was proposed and adopted to improve the purity level. Finally, the process-level performance of top-performing MOFs (HKST-1, UiO-67) was evaluated on the basis of the experimental isotherms obtained from the literature and compared with the other materials reported in the literature (MIL-100(Fe), UiO-66, and zeolite 13X).