Computational screening of all-Silica Zeolites for simultaneous H_2S and CO_2 adsorptive separation

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Natural gas is composed of most of methane and ethane, but the Hydrogen sulfide (H_2S) and Carbon dioxide (CO_2) also included. H_2S is highly toxic, corrosive, and flammable in nature. CO_2 is common greenhouse gas and rapid increase of atmospheric CO_2 concentrations threaten human society and the natural environment. The adsorption separation is economical method rather than conventional distillation separation. For the adsorption separation, there were many studies and solutions for capturing H_2S and CO_2 individually, but there were no tries to separate H_2S and CO_2 from natural gas simultaneously. We carried out high-throughput screening on experimentally reported all-silica zeolite database to find top-performing materials for simultaneous H_2S and CO_2 separation for adsorption separation. Breakthrough curve study for the promising zeolites to check out the performance at pressure-swing adsorption process level.