Computational Screening of Pure-Silica Zeolites for Carbon Capture under Humid Conditions

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CO_2 capture using promising porous materials such as zeolites and metal-organic frameworks could be one of the viable options to deploy carbon capture and sequestration (CCS) in large-scale fossil fuel power plants. However, it has been reported that widely used or best-performing porous materials showed significant decrease in CO_2 adsorption capacity at realistic flue gas conditions containing 5~8% water vapor. To understand underlying mechanisms and to find the optimal zeolites under humid conditions, a computational screening of hundreds of pure-silica zeolites has been conducted. Grand canonical Monte Carlo (GCMC) simulations have been utilized to calculate CO_2 adsorption isotherms in both dry and humid conditions. From the screening studies, we have identified several zeolite materials that show enhancement in CO_2 uptake in presence of water. The mechanism for enhancement/deterioration of CO_2 adsorption at humid conditions has been analyzed.