High-throughput computational screening of porous polymer networks for natural gas sweetening based on neural network

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Abstract

17,846 PPNs with the diamond-like topology were computationally screened to identify the optimal adsorbents for the removal of H2S and CO2 from humid natural gas based on the combination of molecular simulation and machine learning algorithms. The top-performing PPNs with the highest adsorption performance scores (APS) were identified based on their adsorption capacities and selectivity for H2S and CO2. The strong affinity between water molecules and the framework atoms has a significant impact on the adsorption selectivity of acid gases. We proposed two main design paths (LCD [?] 4.648 , Vf [?] 0.035, PLD [?] 3.889 or 4.648 [?] LCD [?] 5.959 , ρ [?] 837 kg·m-3) of high-performing PPNs. We also found that artificial neural network (ANN) could accurately predict the APS of PPNs. N-rich organic linkers and highest isosteric adsorption heat of H2S and CO2 are main factors that could enhance natural gas sweetening performance.

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