High-Throughput Screening of CoRE MOFs for Biogas Purification

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NMGC Abstract

The increased usage of fossil fuels causes environmental and human health problems since most of the fossil fuel combustion products are toxic. Another challenge about fossil fuels is their non-renewable nature and, in the long term, they possess the risk of depletion unless new, very large fields of fossil fuel resources are discovered. Owing to these reasons, cleaner and renewable energy resources have attracted much interest. Biogas, where methane is the major constituent, is one of the renewable energy resources whose use would generate less pollutants, and CO_2 than fossil fuels if it can be effectively separated. The biogas content is primarily composed of CH_4 and CO_2, however, it also involves other gases such as N_2, H_2S and NH_3 which should be separated before biomethane is used. Metal-organic frameworks (MOFs) have been recently shown to be useful for many gas separation applications due to their advantageous properties such as high pore volume, chemical and structural diversity etc. This work focuses on the identification of MOFs that can selectively capture contaminants in the biogas over methane using a multi-stage approach. The set of MOFs that are screened belongs to computation-ready experimental MOFs (CoRE MOFs) with a pore limiting diameter higher than 3 Å. Using Grand Canonical Monte Carlo (GCMC) simulations, firstly, gas pair (CH_4/CO_2, CH_4/N_2, CH_4/H_2S, and CH_4/NH_3) separation performances of MOFs are evaluated at 298 K, 1 bar. In the second stage, MOFs that are selective towards the contaminants are picked from the first stage and GCMC simulations have been performed for them using a five-component gas mixture (50% CH_4, 45% CO_2, 3% N_2, 1% H_2S, 1% NH_3). Finally, the top performing MOFs that can selectively capture CO_2, N_2, H_2S, and NH_3 from biogas mixture are determined using several metrics.