

Multiscale high-throughput computational screening of nanoporous materials for Xe/Kr adsorption separation

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Xe and Kr gases, are needed in many applications such as illumination, narcotic, and inert probe for nuclear magnetic resonance (NMR). Currently, the pressure swing adsorption (PSA) is considered the most promising separation method because it could greatly reduce the cost and energy consumption of the separation compared to the cryogenic distillation. In this work, based on the CoRE MOFs 2019 and C.U.R.A.T.E.D COFs v9 databases to find high-performing nanoporous materials that can efficiently perform the separation. More than 140 high-performing nanoporous materials identified from molecular simulations were subsequently evaluated based on the ideal adsorption process simulations to evaluate their final performance in the actual process settings.