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Structural and Optical Response of Complex Mixed Gas Dynamics in Rare Earth Metal-Organic Frameworks

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Rare Earth-DOBDC metal organic frameworks (RE-MOFs) have demonstrated responses to the presence of acid gases (SO_2, NO_2, H_2O). Density functional theory and ab initio molecular dynamics (AIMD) were used to investigate mechanisms of acid gas interactions in the RE-MOF framework. The calculated binding energies of individual gases highlight unique interaction types in the RE-MOF framework and indicate binding site selectivity. The AIMD trajectories elucidate direct competitive adsorption within the pore structure and identified varying reactions and binding strengths in the MOF, with implications for acid gas separation. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.