Porous M_6L_3 Type Metallocage for High CO_2 Adsorption Selectivity: A Molecular Simulation Study

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The metallocage, UMC-1, has a trigonal bipyramid inter-cage composed of Zr-cationic cluster and organic linker containing SO_2 group suitable for CO_2 adsorption. Based on experimental observation, UMC-1 shows a very high selectivity of 150 for CO_2/N_2. Thus, computational approach using GCMC and DFT calculations were adopted to figure out the cause of high selectivity to CO_2. For accurate GCMC calculation, we modified the forcefield parameters, which could reproduce the experimental CO_2 adsorption isotherm. DFT was used to further optimize the adsorption structures observed at previous step, confirming stable adsorption structure and adsorption energy. Importantly, the site of CO_2 adsorption in UMC-1 is mainly classified into three types. Site 1, which is the most stable site for adsorption, is a place where Cl ion and hydroxyl groups act as Brønsted acidic sites for CO_2, site 2 was a place where CO_2 adsorbed on the pore window and interacted with neighboring SO_2. Lastly, site 3 enabled stable CO_2 adsorption due to the weak interactions of Cp located outside the cage. Based on these findings, it was possible to suggest the cause of the strong adsorption energy of CO_2 in UMC-1.