Theoretical study on CO_2 capture in terms of structural characteristics of microporous carbon

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Rapidly increasing concentration of CO_2 in atmosphere is a major issue for climate change through greenhouse effect. In order to capture CO_2, activated carbon with large surface area and well-defined micropores is being widely studied. Considering that structural properties of microporous carbon could be changed by synthetic conditions, CO_2 capture performance was expected to be modulated. In this study, by using grand canonical Monte Carlo simulation and density functional theory calculation, we theoretically investigated the effect of pore size and functional groups on selective CO_2 adsorption from the mixtures with N_2 or CO gas. Among the pore size from 0.6 to 0.9 nm, the pore size of 0.7 nm showed the highest isosteric heat of CO_2 adsorption, and thus the highest CO_2 uptake. In terms of selectivity, the same size also showed better CO_2 selectivity compared to other similar pore size. Moreover, the isosteric heat of CO_2 adsorption in the OH-functionalized pore was significantly increased compared to the pristine system. Therefore, it was expected that the presence of the OH functional group would enhance the CO_2-selective adsorption capacity.