Study of adsorption and behavior of NO in Cu-SSZ-13

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Experimentally, Cu-exchanged SSZ-13 zeolite has been found to show excellent catalytic activity and high stability in the NOx reduction at high temperature. However, reaction mechanism and phenomena of NO in Cu-SSZ-13 are not fully uncovered in atomistic-level apect. Thus, we aim to study the adsorption and behavior of NO in Cu-SSZ-13 using molecular modeling and simulation methods, which are molecular dynamics (MD) and density functional theory (DFT). First, we checked the binding of NO with Cu2+ ions and calculated the binding and Gibbs free energy. Through this calculation, it was found that bonding of NO with both Cu2+ ion are possible also in six-membered ring but the more favorable binding site is eight-membered ring, which was shown by investigating transition states(TS). Secondly, to detect the molecular movement of adsorbed NO, MD simulation was performed by applying the stretching force of Cu-NO and the angle-bending force of ∠Cu-N-O in the zeolite, which were found from the DFT calculation. From this study, some of important characteristics of adsorbed NO in Cu-SSZ-13 have been revealed and compared with experimental results, which are in good agreement.