Theoretical study of NO adsorption in 6MR/8MR of Cu(I)/Cu(II)-SSZ-13 zeolite

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Metal-exchanged-zeolites have been commercialized in consideration of the emission control. In particular, Cu-exchanged SSZ-13 zeolite with a chabazite (CHA) structure having good hydrothermal stability exhibited superior activity to remove NO_x compounds. Cu-SSZ-13 zeolite has the 4-, 6- and 8-membered rings (4, 6, and 8 MRs). Cu (I, II) ions, which can be located on the faces of those rings, serve a role of active sites for the NO_x adsorption. 8-MR was known energetically favorable NO adsorption site while 4- , 6-MRs were known for unstable NO adsorption sites. However, based on our calculations of binding energy, activation energy and Gibbs free energy using density functional theory (DFT) calculations we conjecture that NO adsorption is possible when Cu ion (I) is located on the face of 6 MR. This theoretical result showed a possible proof to increase, maximally up to twice as much as NO in the adsorbent.