NO$_x$ (x = 1,2) Adsorption on Alkaline Earth Metal Oxides and Transition Metals: A DFT Study

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The emissions of nitrogen oxides from automobiles cause air pollution such as acid rain. Selective Catalytic Reduction or Lean NOx Trap has been used to convert nitrogen oxides into harmless components such as N2 through the adsorption or the reduction of nitrogen oxides. NOx adsorbents mainly use the high cost noble metals. Thus, in order to develop more practical adsorbents, reducing the costs is inevitable. In this study, to explore good candidates of NOx adsorbents, we established the extensive database for the adsorption of nitrogen oxides on alkaline earth metal oxides and transition metals. The adsorbents with good performance should not be too strong nor too weak. If the interaction is weak, the adsorbate fails to bind to the catalyst and the reaction does not occur. On the other hand, if the interaction is strong, the product may not be separated after the reaction. Furthermore, understanding the adsorption energy of the molecules or atoms participating in the reaction plays an important role in predicting the activity of the conversion reaction. Focusing on these points, we will provide a useful insight for designing NOx adsorbents on metals or metal oxides.