Chemisorption on bimetallic NP-TiO_2 for CO oxidation catalyst: first principle and machine learning modeling

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The interaction between the nanoparticle (NP) and metal oxide (MOx) support is an important factor for the supported nanoparticle catalysts, especially for CO oxidation reaction [1]. One significant effect of interaction is the change of adsorption energy of small molecules on the surface. The interaction drastically affects the adsorption energies of small molecules. As the adsorption energy is a crucial factor of reaction barrier such as BEP relation [2], it is very important and helpful to understand the change of adsorption energy on the metal NP-MOx catalysts for the catalytic activity.

In this work, we tried to understand the interaction between NPs and support by the adsorption energies of oxygen atom and CO on the TiO_2 support using density functional theory (DFT) study. We modeled the metal NP-MOx catalysts by building 10-atom bimetallic A_9B_1 NPs on the (4×2) TiO_2 surface unit cell. For over several hundred kinds of bimetallic NPs on the TiO_2 support, the adsorption energies of oxygen atom and CO on the NP and TiO_2 support was calculated. It was possible to see the trend of adsorption energies in different bimetallic NP-TiO_2 support catalysts.

With the data from the DFT study, we did machine learning and predicted the adsorption energies of small molecules in different bimetallic NP-TiO_2 catalysts. Machine learning is an effective tool to predict the adsorption energy and even catalytic activity of catalysts [3]. From the linear regression to neural network, various machine learning algorithms have been tested. As a result, we could effectively capture the chemisorption of small molecules even with simpler features, like electronegativity or radius of atom.

For the verification of machine learning technique, we calculated the reaction barrier of CO oxidation at the interface site of bimetallic NP-TiO_2 catalyst using BEP relation. The results were quite similar with the reaction barrier calculated by common nudged elastic band method. From these results, we could verify the accuracy and usefulness of machine learning technique in the study of catalysts.

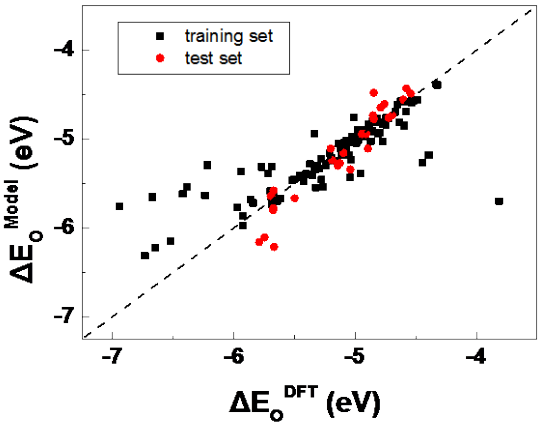

Fig.1 The adsorption energy of O atom on TiO_2 support predicted by ε-SVR machine learning algorithm.

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