Abstract Submitted
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Effect of substrate-catalyst interaction on Spin-dependent chemical reactions: CO oxidation[1] SHUNFANG LI, Department of Materials Science and Engineering, University of Tennessee; School of Physics, Zhengzhou University, China, YANFEI GAO, Department of Materials Science and Engineering, University of Tennessee; Materials Science and Technology Division, ORNL, ZHENYU ZHANG, Department of Physics and Astronomy, University of Tennessee; ICQD, University of Science and Technology of China, Hefei, Anhui, China — First-principles calculations have been performed to investigate and compare the catalytic reactivity of Ni(Pd)$_1$/TiO$_2$(110) and Ni(Pd)$_2$/TiO$_2$, for CO oxidation. A recent experiment showed that the catalysis of small Ni(Pd)$_2$ clusters deposited on rutile TiO$_2$(110) surface exhibit very different performance for CO oxidation, compared with the single atom cases, Ni(Pd)/TiO$_2$(110). However, the underlying mechanism of this interesting phenomenon is still unclear. Our calculations show that the catalyst-substrate interaction plays a key role in both the thermodynamic and kinetic process of the catalytic reactions. Particularly, the spin degree of freedom of the complex oxide is found to dominate the reaction rate. Essentially, the oxidation of CO on the single atom cases is a spin-forbidden reaction, while it is spin-permitting for the dimer cases. This work provides valuable guidance for high efficient catalyst design at the atomic scale.

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