Role of Interface for the Water-Gas Shift Reaction over Size-Controlled Supported Metal Catalysts: A Combined Theoretical and Experimental Study

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Water-gas shift reaction (WGSR) is industrially vital since it converts CO into CO_2 by adding H_2O to produce H_2, which can be used as a fuel and further used for ammonia (NH_3) synthesis. Thus, design of an efficient catalyst for WGSR is essential. Supported noble metal catalyst has been widely studied because it can maximize the utility of the noble metal by increasing the dispersion. However, role of the metal-support interface during WGSR has not yet been clearly revealed and is still elusive. For a model system of Pd/Co_3O_4 catalyst, the role of interface for improved WGS reactivity and the atomistic origin of the activity improved by metal-support interaction were studied using density functional theory (DFT) calculations, combined with genetic algorithm. The results from the DFT calculations are further experimentally validated using size-controlled Pd catalysts. The theoretical insights on the role of interface presented here are believed to provide valuable knowledge to design efficient supported metal catalysts for WGSR.