Atom-scale view of Ni_2 Cluster Catalyst for CO_2 Low-temperature Dissociation by STM and AFM

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Single clusters with well-defined compositions and structures are gaining significant attention for their remarkable efficiency and tunable configurations. However, achieving precise synthesis, particularly for heteronuclear clusters, remains a considerable challenge. In this study, we introduce a stepwise kinetic regulation strategy to successfully synthesize two distinct types of bimetallic clusters. The orthogonal M_a/O-M_b clusters, with M_a and M_b linked by oxygen in a nearly perpendicular orientation, contrast with the linear M_a-O-M_b clusters, where M_a and M_b are connected in a linear arrangement. These clusters exhibit notably different Catalytic Properties. For example, the Ni_2 clusters possess an excellent low-temperature CO_2 dissociation activity, as revealed by combined techniques including scanning tunneling microscopy (STM), noncontact atomic force microscopy (nc-AFM), Kelvin probe force microscopy (KPFM), and infrared reflection absorption spectroscopy (IRAS). Density functional theory (DFT) calculations have shown that the Ni_2 cluster significantly alters the spatial symmetry of its frontier orbital to adapt to the molecular orbital requirement for subsequent CO_2 dissociation.

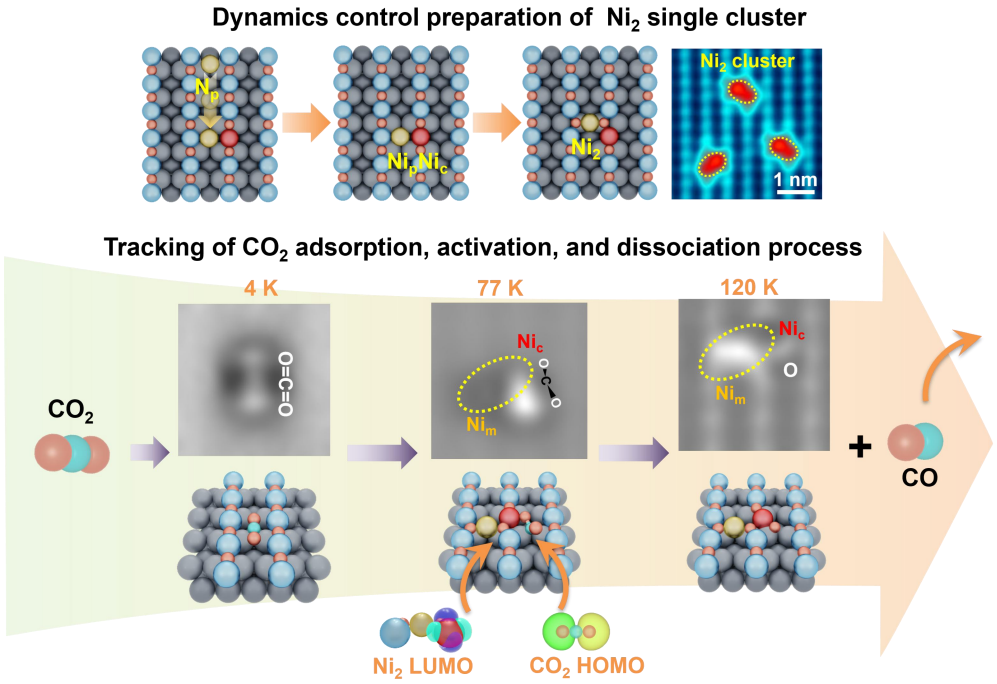

Figure 1. Preparation of Ni_2 catalysts with CO_2 low-temperature dissociation.

Reference

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