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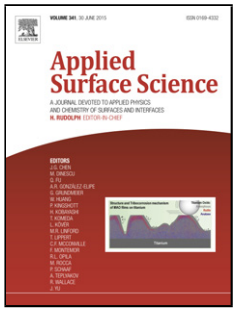

Title: Toward Improving CO_2 Dissociation and Conversion to Methanol via CO-Hydrogenation on Cu(100) Surface by Introducing Embedded Co Nanoclusters as Promoters: A DFT Study

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Toward Improving CO_2 Dissociation and Conversion to Methanol via CO-Hydrogenation on Cu(100) Surface by Introducing Embedded Co Nanoclusters as Promoters: A DFT Study

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Highlights

- Chemisorption behavior of CO_2 is sensitive to the amount of cobalt atoms, which are the sites to activate CO_2 on Cu(100) surface.
- A V-shaped variation of the energy barriers is predicted for the CO_2 dissociation on different Co_n/Cu(100) surfaces.
- The minimum energy barrier of CO_2 decomposition is obtained on the Co_4/Cu(100) bimetallic surface.
- Introducing Co clusters on Cu(100) surface can enhance the stability of key intermediates for methanol synthesis.

Abstract The dissociation and hydrogenation of CO_2 on Cu(100) surfaces that are modified by introducing Co nanoclusters with different size into the top layer have been investigated using density functional theory method. Our results show that on all surfaces the Co atoms are the sites for the adsorption of CO_2, and in the early stage of introducing Co dopant, the chemisorption behavior of CO_2 is sensitive to the amount of Co atom. According to the predicted pathways for the dissociation of CO_2 to CO, it is interesting that the energy barrier decreases first and then increases as more Co atoms are dispersed on the surface, forming a "V" shape. The minimum energy barrier of CO_2 decomposition is predicted on the Cu(100) surface that contains four Co atoms aggregated together on the top layer, namely Co_4/Cu(100) bimetallic surface. The most favorable reaction