Decomposition of H_2S on Ni(100) and Ni_3Al(100): A first-principles study

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Spin-polarized density functional theory studies of H_2S decomposition on Ni(100) and Ni_3Al(100) surfaces were conducted to understand the aluminum(Al) alloying effect on the H_2S dissociation. We first determined the near surface structure of fully ordered Ni_3Al alloy along the [100] direction and examined the activation barriers for the H_2S and HS decomposition by using Climbing Image-Nudged Elastic Band method. We found that Al atom in bimetallic Ni_3Al(100) tends to exist in the first surface layer, rather than in the second or third layer, and the Ni_3Al (100) surface can substantially retard the H_2S decomposition by reducing the adsorption energy of sulfur compounds compared to the pure Ni(100) case. Furthermore, we found that the modification of surface Ni atoms by Ni-Al electronic (ligand) interaction and vertical location of Al in the Ni_3Al(100) slab, in particular, the alteration of the Ni *d* state induced by the first surface layer Al (rather than the second layer Al), serves an important role in reducing the adsorption energy of sulfur compounds.