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Theoretical analysis of chemisorption properties of atomic hydrogen on the Ag(111) surface.

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Adsorption of hydrogen on metallic surfaces has been studied extensively because it provides basic concepts for the interaction between the adsorbate and the metal surface. In this study, we have investigated the adsorption properties of atomic hydrogen on the Ag(111) surface using the fist-principles density functional calculations. The computed binding energies (with respect to the H_2 molecular energy) on the surface at 1/4, /12, and 1.0 monolayers are -0.21, -0.15, and -0.40 eV, respectively. These values are much smaller than those on the other metal surfaces such as Ni and Cu. The electronic structures of the H/Ag(111) surfaces clearly show the occupied bonding and anti-bonding states of covalent interaction of Ag 4*d* bands with the H 1*s* state. The occupation of the anti-bonding states gives rise to the weak chemisorption energy of H on the Ag(111) surface. The results of H on the Ag surface will be compared to the those on other metal surfaces as well as those of photoemission studies.