

Abstract Submitted
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Hydrogen adsorption on Al (100) facilitated by surface alloying with Sc FENG ZHANG, YAN WANG, M. Y. CHOU — We report first-principles investigations of hydrogen adsorption on the Al (100) surface modified by alloying with Sc, as the first step to understand the catalytic role of scandium in the hydrogenation process in Sc-doped NaAlH₄. Sc prefers to stay at subsurface sites with or without adsorbed hydrogen. The adsorption energy on the Sc-modified surface is 0.5 eV/H₂ lower than that on the pure Al surface, while the dissociation barrier of H₂ is similar for the two systems. The structure with two H atoms adsorbed on two nearest-neighbor bridge sites is at least 0.3 eV more stable than other structures; but no additional activation energy is required for H to diffuse among these structures. Electronic structures are also examined to explain these alloying-induced effects.

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