Hydrogenation of aluminium hexamer: ab initio molecular orbital theory and density functional theory study.

Autorzy

Jerzy Moc

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Streszczenie

The detailed mechanism of the reaction of aluminium hexamer with H_2 molecule to form a dihydride has been studied using ab initio molecular orbital theory and density functional theory. For the bare Al_6 cluster, the singlet state distorted octahedron (D_{3d}) is found to be the ground-state structure. The hydrogenation reaction of the singlet state Al_6 cluster is described by the lack of activation barrier for H_2 cleavage, consistent with experiment. The most stable product isomer involves two H bridges on the Al–Al edges of the same Al–Al–Al face of the Al_6 octahedron and its formation is exothermic by about 30 kcal/mol.

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