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Initial Processes of Hydrogen Adsorption on Si(100) Surface

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Abstract: The adsorption of one monolayer H atoms on an ideal Si(100) surface is studied by using the self-consistent tight binding linear muffin-tin orbital method. Energies of adsorption systems of H atoms on different sites are calculated. It is found that the adsorbed H atoms are more favorable on B1 site (bridge site) with a distance 0.056 nm above the Si surface. There does not exist reaction barrier at the Si surface. The layer projected density states are calculated and compared with those of the clean surface. The charge transfers are also investigated.

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