

Adsorption of Fe on GaAs (100) Surface

WEI Shu-Yi, MA Li, WANG Jian-Guang, and WANG Tian-Xing

College of Physics & Information Engineering, Henan Normal University, Xinxiang 453002, China
(Received: 2002-7-4; Revised: 2002-9-29)

Abstract: The adsorption of one monolayer Fe atoms on an ideal GaAs (100) surface is studied by using the self-consistent tight-binding linear muffin-tin orbital method. The Fe adatom chemisorption on Ga- and As-terminated surface are considered separately. A monolayer of S atoms is used to saturate the dangling bonds on one of the supercell surfaces. Energies of adsorption systems of an Fe atom on different sites are calculated, and the charge transfers are investigated. It is found that Fe-As interaction is stronger than Fe-Ga interaction and Fe atoms prefer to be adsorbed on the As-terminated surface. It is possible for the adsorbed Fe atoms to sit below the As-terminated surface resulting in an Fe-Ga-As mixed layer. The layer projected density states are calculated and compared with that of the clean surface.

PACS: 73.20.At

Key words: chemisorption, supercell, interaction, low index single crystal surfaces

[\[Full text: PDF\]](#)

Close