

## Atomic and electronic structure of the Pb/Si(111)- $\sqrt{7}\times\sqrt{3}$ surface: DFT calculations

정성철, 강명호

포항공과대학교 물리학과

The atomic and electronic structure of the Pb adsorbed Si(111)-( $\sqrt{7}\times\sqrt{3}$ ) surface has been studied by density-functional theory (DFT) calculations. We examined two structural models: One is the 1.0 ML trimer model proposed by a STM experiment [1], and the other is the 1.2 ML triangular model, characterized by a Y-shape arrangement of four Pb atoms, proposed by a X-ray experiment [2]. We find that while the 1.0 ML trimer model is locally unstable, the 1.2 ML triangular model is stable, which is consistent with a previous DFT study [3]. The triangular model was found to reproduce the experimental Y-shape STM images. This structure shows metallic band structure, the surface-state bands of which have free-electron-like parabolic dispersions. These characters are in agreement with the band structure reported by a recent ARPES experiment [4]. Our calculations, however, do not reproduce some of the experimental bands. The origin of this discrepancy will be discussed in connection with the triple-domain LEED pattern reported in the ARPES experiment.

[참고문헌]

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