

Single adatom adsorption and diffusion on Si(111)-(7×7) surfaces

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The study of the initial stages of adatom adsorption on semiconductor surfaces is of both fundamental and technological importance. Information on the stable adsorption sites, the diffusion pathway, and the activation energy barrier are expected from a detailed study at an atomic scale.

We have studied the adsorption and diffusion of a single lead adatom on the Si(111)-(7×7) surface by combining scanning tunneling microscopy (STM) experiments and first-principles electronic structure calculations. The STM data, measured at low temperature, have allowed the determination of three preferential adsorption zones in each (7×7) half-cell, the so-called basins of attraction¹. Diffusion events between these zones have been observed in real time, and the energy barrier for inter-basins diffusion have been measured. The identification of the lowest energy adsorption sites have been made possible by means of the *ab initio* calculation, and the comparison between experimental and simulated STM images. The energy barrier for intra and inter basins diffusion have also been calculated. We find an excellent agreement between calculations and experiments.

¹ K. Cho et al., *Europhys. Lett.* **39**, 287 (1997)