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The Electronic and Transport Properties of Si(111)-7×7 and Related Reconstructions[1] MANUEL SMEU, McGill University, WEI JI, Renmin University of China, ROBERT WOLKOW, National Institute for Nanotechnology, HONG GUO, McGill University — The 7×7 reconstruction of Si(111) has the interesting property of being metallic despite bulk Si being a semiconductor. This surface has a complex reconstruction that takes on a dimer-adatom stacking fault (DAS) structure composed of adatoms, rest atoms, and several other key features. It is believed that the conductivity occurs through the dangling bonds of the adatoms, and that it is entirely a surface effect. To elucidate the details of this mechanism, we have investigated a set of related Si(111) reconstructions of increasing complexity in order to resolve the effect of the different DAS features on the electronic and transport properties of the Si(111)-7×7 surface. Density functional theory (DFT) calculations have been carried out on the $\sqrt{3}\times\sqrt{3}$-$R30^\circ$, 2×2, 5×5, and 7×7 reconstructions of Si(111). Additionally, our work is extended to electron transport simulations employing the non-equilibrium Green's function technique coupled with DFT (NEGF-DFT) to calculate the conductance for these systems. Finally, the effect of atomic steps and adsorbates on the conductive properties will also be discussed.

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