[III-17]

Model-dependent electronic structure of the Si(111)2×1 surface

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We have used the pseudopotential density-functional total-energy scheme to study the atomic and electronic structure of the Si(111)2×1 surface: we examine and compare in detail both the standard Pandey's π-bonded chain (PC) model and the alternative three-bond scission (TBS) model including their variations. We find that while the PC model is acceptable both in energetics and in spectroscopic examination, the TBS model is energetically unfavored (0.25 eV/surface-atom higher in energy than the PC model) and doesn't agree in band structure with experiments. This differs from the result of the recent Hartree-Fock cluster calculations where the TBS model produces the experimental band structure. We also find that the reverse-buckled PC model is equally favored in energetics as the PC model, and its band structure is also compared well with experiments. The physical relevance of the reverse-buckled PC model and the TBS model is discussed in connection with some unresolved questions with this surface.