

Ab initio structure and electronic properties of Si(100) using ACRES

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We apply the recently developed ACRES method (Adaptive Coordinate Real-space Electronic Structure), [1] to study the structural and electronic properties of various reconstructions of the (100) surface of Silicon. In this electronic structure approach, based on Density Functional Theory, a finite (curvilinear, in general) grid is used for representing the charge density and the Kohn-Sham wavefunctions, and a real-space integration of the quasiparticle Schrödinger equation is performed.

We performed calculations for almost all known surface reconstructions of the Si(100), including (2×1) , (2×2) , $p(2 \times 2)$, $c(2 \times 2)$, $c(4 \times 2)$, $c(4 \times 4)$, plus a missing dimer model. We discuss the atomistic features, such as bond lengths and angles, and various aspects of the electronic structure of these surfaces, such as electron density contour plots, simulated STM images and surface band structures. These studies reveal how the wavefunctions and energies of the surface states depend on the underlying atomic arrangement.

References

- [1] N. A. Modine, G. Zumbach, and E. Kaxiras, Phys. Rev. B **55**, 10289 (1997).