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Differences in the surface electronic structure of Ge(001) and Si(001) from hybrid density functional theory and angle-resolved photoemission spectroscopy HOSUNG SEO, RICHARD C. HATCH, PATRICK PONATH, MIRI CHOI, AGHAM B. POSADAS, ALEXANDER A. DEMKOV, Department of Physics, The University of Texas at Austin — Even with renewed interest in Ge as a competitor to Si in field effect transistors, several key features of the surface electronic structure of Ge(001) have remained controversial. Notably, the character of the valence band top of Ge(001) has been heavily debated. Using first-principles hybrid density functional theory and angle-resolved photoemission spectroscopy, we unambiguously establish the critical differences between the electronic structure of the Si and Ge (001) surfaces. In order to avoid the problems associated with the band gap underestimation in LDA and GGA, we utilized the screened Hartree-Fock hybrid exchange correlation density functional due to Heyd, Scuseria, and Ernzerhof (HSE06). We explicitly show that the surface state that determines the charge neutrality level, and thus the Schottky barrier height in Si, is actually a surface resonance in Ge. Our results strongly suggest that the recently observed strong Fermi level pining in Ge/metal junctions comes from the evanescent states. Additionally, using surface resonance calculations and bulk HSE06 calculations with the spin-orbit coupling, we identify the origin of a number of highly debated ARPES features for Ge(001) and Si(001).

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