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Differences in the surface electronic structure of Ge(001) and Si(001) from angle-resolved photoemission spectroscopy and *ab-initio* theory RICHARD C. HATCH, HOSUNG SEO, PATRICK PONATH, MIRI CHOI, AGHAM B. POSADAS, ALEXANDER A. DEMKOV, Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA — Using high-resolution angle-resolved photoemission spectroscopy (ARPES) we compare the surface electronic structure of both Ge(001) and Si(001) surfaces. Unlike previous ARPES experiments, where the Ge(001) surfaces were prepared using cycles of ion sputtering and annealing, our Ge(001) surfaces were prepared using a combination of wet etching and oxygen plasma cleaning. This new technique has the advantage that it avoids the incomplete healing of surface roughening associated with sputtering and annealing cycles. The ARPES data show that the dimer-derived surface state that determines the charge neutrality level, and thus the Schottky barrier height in Si, is actually a surface resonance in Ge, and the highest occupied state is a bulk state. In order to avoid theory predicting an overlap of the valence and conduction bands, we employed first-principles, hybrid density functional theory (DFT). This theory effectively explains the presence of a number of photoemission features in both Si and Ge. We found it is necessary to incorporate spin-orbit interaction in the hybrid DFT calculations for Ge in order to model ARPES data, and we found a spin-orbit splitting of 0.28 eV both experimentally and theoretically.

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