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Experimental and Theoretical Investigation of Si(001)/Si (110) Junctions¹ ADRIAN CIUCIVARA, SACHIN JOSHI, B.R. SAHU, SANJAY BANERJEE, LEONARD KLEINMAN, University of Texas at Austin — We have observed large current asymmetries in Si(001)/Si(110) junctions where both sides are identical in all respects, except orientation. With a 280 atom GGA supercell calculation using the VASP ultrasoft pseudopotential code, we have obtained an adhesion energy of 110 meV/Å². The covalent and dangling bonds at the interface are displayed. The Si(110) potential averaged over a (110) interior unit cell was found to be 85 meV more negative (positive for holes) than the Si(001). This offset was used in a device simulator to simulate the behavior of the junction. Qualitative agreement with the experimental I-V characteristics was obtained. We will discuss possible errors introduced in the offset by the GGA energy gap error.

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Adrian Ciucivara
University of Texas at Austin

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