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Electronic structure of Si:P delta doped layer CHIN-YI CHEN, Purdue University, Indiana, US, FEDERICO MAZZOLA, JUSTIN W. WELLS, Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway, RAJIB RAHMAN, Purdue University, Indiana, US — Densely doped Si:P delta layers are used to form many of the electronic components of qubit devices patterned by Scanning Tunneling Microscope (STM) lithography. A variety of methods, ranging from ab-initio to empirical and from atomistic to continuum, has been used to compute the band structures of such Si:P layers. However, the vastly varying results from these methods have not been verified by experiments. Here, we compare atomistic tight-binding (TB) calculations of band structures of Si:P layers with angle resolved photoemission spectroscopy (ARPES) measurements. The experimental data portrays a second set of gamma bands, in addition to the two typically predicted valley split gamma bands, separated by around 215 meVs. Our calculations show that the existence of these additional gamma bands can be explained by an increase of the effective dielectric constant to about 20. In addition, we study the non-parabolicity of the bands and spin splittings due to spin-orbit coupling.

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