Reconciling the contradicting picture of the band structure of Si:P δ-layers

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Atomically precise lithography of phosphorus δ-layers in silicon has led to the fabrication of functional atomic-scale devices [1,2]. Motivated by the successful fabrication of these atomic-scale devices, the morphology of Si:P δ-layers have been studied down to the atomic limit by scanning tunnelling microscopy [3], and their band structure thoroughly investigated by different theoretical methods [4]. Calculations predict that confinement of the P dopants to a single atomic plane beneath the Si surface leads to a lowering and discretization of the conduction band (CB) resulting in two parabolic-like states dispersing across the Fermi level, which are referred to as 1Γ and 2Γ. These states give the Si:P δ-layers metallic character, and are responsible for the transport properties observed in atomic-scale devices. Angle-resolved photoemission spectroscopy (ARPES) measurements can provide direct access to the band structure of these Si:P δ-layers [5]. Our ARPES measurements reveal a surprising result: a third parabolic-like state at the Fermi level. We find that the origin of this third state is related to an underestimation of the theoretical strength of the material's dielectric constant. This result allows us to reconcile an apparently contradicting picture of the physics of Si:P δ-layers. We are able to make a crucial revision of the electronic structure of these systems, and provide a more accurate description of the states involved in the transport properties of atomic-scale devices.

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