Multi-scale modelling of STM devices with in-plane degenerately doped contacts

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Atomic fabrication of phosphorus doped silicon devices using scanning tunneling microscope (STM) has shown great prospect in the pathway to manufacture a scalable quantum computer [1]. The precision placed donor quantum dots are tuned and modulated using degenerately phosphorus doped, in-plane metallic contacts [2, 3]. Here we demonstrate a comprehensive study including the effect of the leads onto the donor dots. The impact on the donor dots are strongly correlated with the geometry, orientation and the electrostatic properties of the delta-doped contacts. In this work, we have investigated the characteristics of the leads using an atomistic $sp^3d^5s^*$ nearest neighbour tight-binding model coupled with a Poisson solver which enables us to explore band gap narrowing due to heavy doping and the extent of the confinement of electrons in the leads accurately. We have integrated the effect of leads on the central donor dots by calculating a 3D electrostatic potential profile using an iterative non-linear poisson solver considering the properties of the leads at millikelvin temperature and the corresponding boundary conditions. The potential profile under different applied bias enables us to calculate the charging energy, and the D^0 and D^- charge transitions of electrons in a single phosphorus donor atom using the tight-binding approach. The results show excellent agreement with the experimental data [2] . This methodology involves multi-scale modelling under realistic device conditions which can be useful in predicting the charge transitions, lever arms and transport properties of the 2D and 3D STM devices[3, 4].

[1] He, Yu, et al. "A two-qubit gate between phosphorus donor electrons in silicon." Nature 571.7765 (2019): 371-375.

[2] Fuechsle, Martin, et al. "A single-atom transistor." Nature nanotechnology 7.4 (2012): 242-246.

[3] Hill, Charles D., et al. "A surface code quantum computer in silicon." Science advances 1.9 (2015): e1500707.

[4] Donnelly, Matthew B., et al. "Monolithic Three-Dimensional Tuning of an Atomically Defined Silicon Tunnel Junction." Nano Letters 21.23 (2021): 10092-10098.