

Abstract Submitted
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Electronic properties of phosphorous δ -doped silicon¹ GEFEI QIAN, YIA-CHUNG CHANG, JOHN R. TUCKER, University of Illinois at Urbana-Champaign — We present a comprehensive theoretical study of phosphorous δ -doped silicon (a candidate material for quantum computation) with doping density up to $3.4 \times 10^{14} \text{cm}^{-2}$ (which corresponds to 1/2 monolayer of doping). A microscopic model based on empirical pseudopotentials and planar Wannier orbital basis is used to calculate the delta-doped system. 1000 monolayers of silicon is included to minimize the boundary confinement effect. Self-consistent potential as well as the exchange-correlation effects due to the doping electrons have been taken into account. It is shown that the 2D band structure of the delta-doped system can be reasonably approximated by an effective mass model over a large range of doping density. However, for ultra-high doping ($> 2 \times 10^{14} \text{cm}^{-2}$), which reaches the experiment limit, the band-structure is significantly deformed, as a result of the strong confinement from the V-shape self-consistent potential. The Fermi level (relative to the conduction band minimum) as a function of the doping density is studied and its implication on the transport properties will be discussed.

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