

Abstract Submitted
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Size Limits on Doping Phosphorous into Silicon Nanocrystals¹

TZU-LIANG CHAN, MURILO L. TIAGO, University of Texas at Austin, EFTHIMIOS KAXIRAS, Harvard University, JAMES R. CHELIKOWSKY, University of Texas at Austin — The evolution of the semiconductor industry requires continued miniaturization. As this trend continues, devices will ultimately approach the nanometer-scale and it is expected that device construction based on macroscopic laws will start to fail. Using a real-space first-principles pseudopotential method, we study doping in the nano-regime using phosphorus-doped Si nanocrystals as the prototypical system. We simulate phosphorus-doped Si nanocrystals with diameter up to 6 nm and study the evolution of the defect state with the size of the nanocrystal. Our calculated size dependence of hyperfine splitting is in excellent agreement with experimental data. The effect of quantum confinement is also manifested in the higher binding energy of the dopant electron, we estimate that phosphorus in Si nanocrystals of less than 20 nm in diameter will not be a shallow donor. We also find that for Si nanocrystals smaller than 2 nm in diameter, the phosphorus atom will be energetically expelled to the surface, leading to a self-purification mechanism that hinders the incorporation of impurity atoms into nanocrystals.

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