Tight-binding Simulations on a Deterministic Single Atom Transistor

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In this work, we study the electronic and transport properties of a single phosphorus atom donor device embedded in host Si bulk constituting a quantum dot. Using the recently fabricated deterministic single donor device as a target of modeling [1], we represent the electronic structure of the single donor device atomistically with the $sp^3d^5s^*$ tight-binding (TB) band model [2], and simulate the gate-modulation of channel confinement using a 3-D Schrödinger solver coupled to a self-consistent charge-potential [3]. We also model the charge stability diagram using the rate-equation method [4], to explain the resonances observed at the edges of the Coulomb diamonds. The calculated charging energy, gate-controllability, and the shape of calculated stability diagram establish very strong connections to the experimental results. We therefore claim that the fabricated device indeed contains a single phosphorous atom in the channel, which is a real single atom transistor representing the ultimate limit of device downscaling. This work can be highlighted as the first modeling of a realistically extended single atom transistor via 3-D simulations in a fully atomistic TB approach.

References

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