Modeling of charge stability diagrams and lead density of states fluctuations in a single phosphorus donor transistor

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A hybrid modeling approach of atomistic multi-million atom simulations [1,2] and semi-classical rate-equations is presented [3] to quantitatively model the experimental charge stability diagram of a single phosphorus donor quantum dot device. This work aims to provide further insight into the effects of dopant placement on the device behavior of atomic-scale devices. The impact of the dopant distribution in the leads [4] on the device characteristics is studied for the first time for a single donor (Si:P) transistor. The individual distribution of dopants in atomic-scale devices causes considerable density of states (DOS) fluctuations in the leads. Although the effects of DOS fluctuations are clearly identifiable in the charge stability characteristics of the device, we can confirm that transistor functionalities of the single donor device are still preserved. Our results support the experimental claims of the first successful realization of a gated and deterministic single-atom transistor.

References

[1] Sunhee Lee, Hoon Ryu, Huw Campbell, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, "Electronic structure of realistically extended, atomistically resolved disordered Si:P δ-doped layers", Phys. Rev. B 84, 205309 (2011)

[2] H Ryu, S Lee, Y H M Tan, G Klimeck, M Fuechsle, J Miwa, S Mahapatra, M Y Simmons, L Hollenberg, *Toward single atom transistors: A tight-binding study on single donor quantum dots* (to be submitted)

[3] G Klimeck, R Lake, S Datta, Vol. 50 Nr. 8 1994 *Physical Review B*

[4] Bent Weber, Suddhasatta Mahapatra, Hoon Ryu, Sunhee Lee, A. Fuhrer, T. Reusch, D. Thompson, W. C. T. Lee, Gerhard Klimeck, Lloyd Hollenberg, Michelle Simmons, "Ohm's Law Survives to the Atomic Scale", Science 335, 64 (2012);doi: 10.1126/science.1214319