Modeling of charge stability diagrams and lead density of states fluctuations in donor-based (Si:P) quantum dot devices

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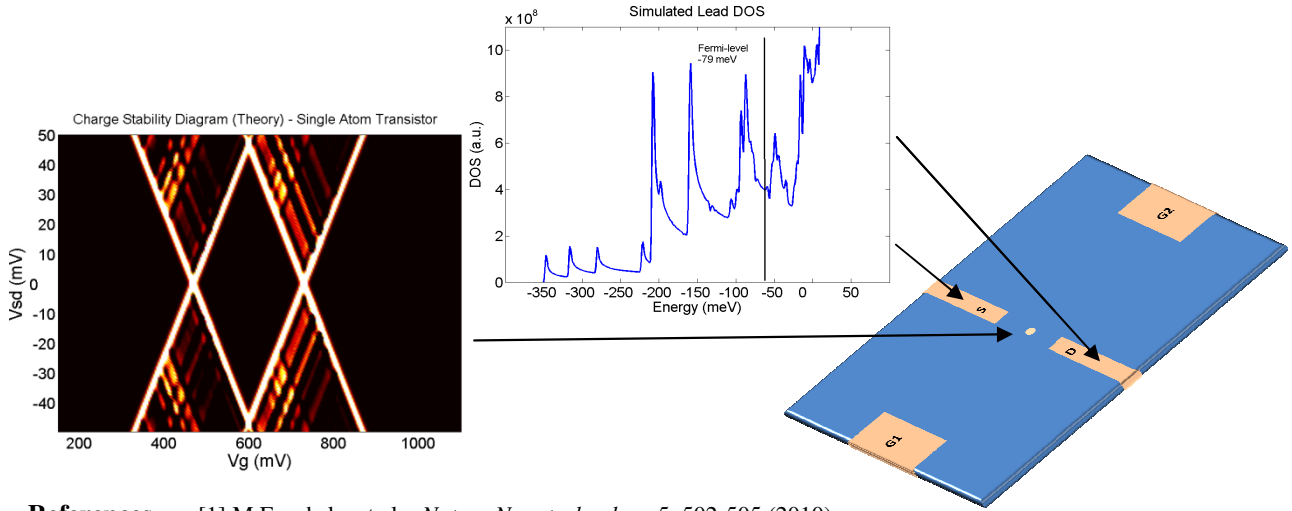
Quantum dot devices based on the deterministic placement of individual dopants have made considerable progress in recent years and usher device scaling into atomic-scale regimes. A few atom donor-based quantum dot (Si:P) with phosphorus doped gates has been reported as the world's to date smallest transistor in 2010 [1]. In a recent work (under review), M. Fuechsle et.al. report the realization of a fully gated single phosphorus donor quantum dot – the first single-atom transistor. In such atomic-scale devices the statistical nature of dopant placement begins to manifest itself in device behavior and new challenges arise as modern transistors push towards the ultimate scaling limit.

In this work, we present a hybrid modeling approach of semi-classical rate-equations [2] and atomistic multi-million atom simulations [3] to model the charge stability diagram of an experimental single phosphorus donor quantum dot device. We model, for the first time, the impact of the dopant distribution in the leads on the device characteristics of a single donor (Si:P) transistor. Our results show that 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 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. Furthermore, this work provides further insight into the effects of dopant placement on the device behavior of atomic-scale devices.



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