Machine Learning approach to the inverse problem in STM imaging of dopant-based quantum devices

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Atomic-scale solid-state qubits could be implemented using scanned-probe lithography to place two or more phosphorus dopants in silicon close to each other. Scanning tunnelling microscopy (STM) has been used to image individual dopants and to find dopant positions in the host silicon lattice based on that image. Determining the geometry of two-dopant qubits will be an essential step in device fabrication, however, double dopant-based devices will lead to a more challenging problem due to the complicated inter-valley wave-function interference patterns.

Here we propose a theoretical solution to that problem. We utilize a multi-million atom tight-binding method, accounting for d-orbitals, surface passivation and surface reconstruction. Further, we use a machine learning approach to determine the positions of both dopants based on STM images generated with tight-binding simulations. Together with a possible calibration with experimental data, the proposed method forms a practical scheme for analysing multi-dopant experimental STM images.

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