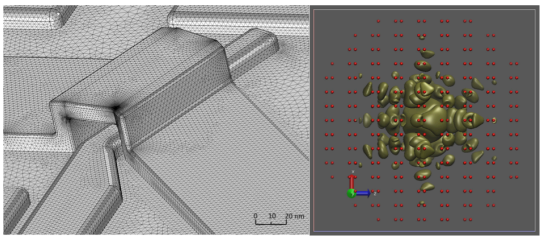
A Computational Workflow for Silicon Donor Qubits

Achievement: Demonstrated a unique computational workflow for characterizing the behavior of qubit developed from phosphorous-doped silicon devices.



(Left) Nanoscale electronic circuit to control a single phosphorous atom; (Right) electron spin density for phosphorous-doped nanocrystal

Significance and Impact: This work provides a first-in-kind tool for evaluating the influence of material properties on the quantum computing devices built using CMOS-compatible technology.

Research Details:

- A multi-staged computational workflow that can be used to design and characterize silicon donor qubit systems with modeling and simulation
- Show how atomistic details can be synthesized into an operational model for the logical gates

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Overview:

Developing devices that can reliably and accurately demonstrate the principles of superposition and entanglement is an on-going challenge for the quantum computing community. Modeling and simulation offer attractive means of testing early device designs and establishing expectations for operational performance. However, the complex integrated material systems required by quantum device designs are not captured by any single existing computational modeling method. We examine the development and analysis of a multi-staged computational workflow that can be used to design and characterize silicon donor qubit systems with modeling and simulation. Our approach integrates quantum chemistry calculations with electrostatic field solvers to perform detailed simulations of a phosphorus dopant in silicon. We show how atomistic details can be synthesized into an operational model for the logical gates that define quantum computation in this particular technology. The resulting computational workflow realizes a design tool for silicon donor qubits that can help verify and validate current and near-term experimental devices.