SAND2022-8472C

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# Quantum-dot-coupled Sn qubits in silicon: DFT analysis of coherent electronic shuttling

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## Introduction

- Quantum computing platforms leveraging homogeneous classical-quantum interfaces offer extraordinary engineering advantages.
- Kane's proposed architecture [1] based on donor nuclear spins *in silicon* was realized and it exhibits coherence times of $\mathcal{O}$*(seconds)* [2].
- Single-qubit gates can be precisely controlled using NMR, but Kane's exchange-coupled two-qubit gates are difficult to fabricate.
- Electron shuttling is a promising alternative, wherein two-qubit entanglement is established through the hyperfine interaction (HFI).
- Here an ancilla electron, initially entangled with one nuclear spin, is coherently transported to interact with a second nuclear spin.
- This is a feasible route toward nuclear-nuclear entanglement and coherence transfer fidelities of 99.4% were recently achieved [3].
- Donor defect sites over-bind electrons, causing electron shuttling to be intractable, so here we consider other candidate defects.
- Isoelectronic defects bind electrons loosely and their HFIs may be sufficiently strong for shuttling, as was recently shown for $^{29}$Si [4].
- As the HFI of $^{29}$Si is still quite small, in this work we explore the prospect of using other isoelectronic defects as nuclear spin qubits.

## Theory

- A *hyperfine interaction* (HFI) occurs when an unpaired electronic spin encounters a nucleus possessing a non-vanishing magnetic moment.
- The hyperfine Hamiltonian is written as $H_{\mathrm{hf}} = I \cdot A \cdot S$, with $I$ and $S$ the nuclear and electronic spin operators and $A$ the coupling tensor.
- When the electron is moved through electrostatic controls to maximize the HFI, $A$ is dominated by the *Fermi contact interaction* (FCI):

$$A \approx A_{\mathrm{FCI}} = \frac{8\pi}{3}\gamma_e\mu_e\gamma_I\mu_I|\Psi(R_I)|^2$$

- The *bunching factor*, or the electronic density enhancement at nuclear site $I$, was defined by Shulman and Wyluda [5] as $\eta = |\Psi(R_I)|^2/\langle\Psi^2\rangle_{\mathrm{Av}}$.
- Van de Waale et al. [6] later formulated $\eta$ using spin densities ($\rho_{\mathrm{spin}} = \rho_\uparrow - \rho_\downarrow$) while Assali et al. [7] outlined a DFT-based procedure to compute it for $^{29}$Si as

$$\eta = \frac{\rho_{\mathrm{spin}}(R_I)}{[\rho_{\mathrm{spin}}]_{\mathrm{Av}}}$$

- This may be computed using conventional Kohn-Sham (KS) DFT in 3 steps:

1) Introduce the defect and perform a structural optimization to relieve strain.
2) Converge the spin-polarized, spin-orbit SCF cycles for the neutral system.
3) Add an electron with a positive jellium background and solve KS equation.

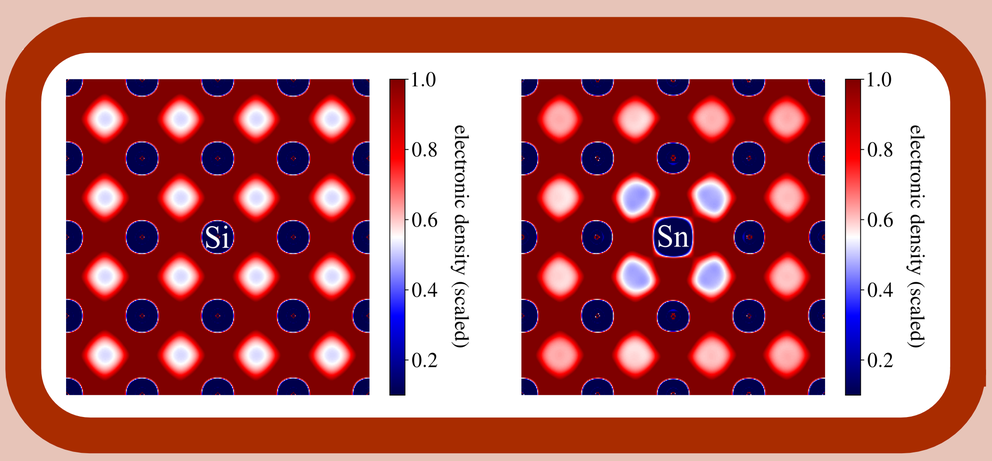
## Objective

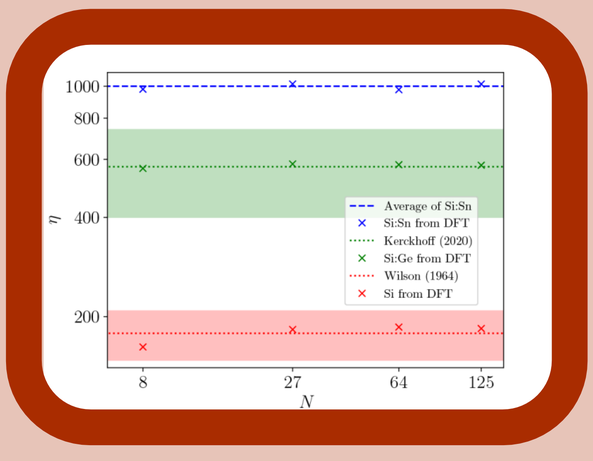
- Simulation can facilitate a high-throughput analysis of designer defects.
  We must first develop a method capable of predicting HFI strengths and then apply it to select the optimal isoelectronic defect in silicon.

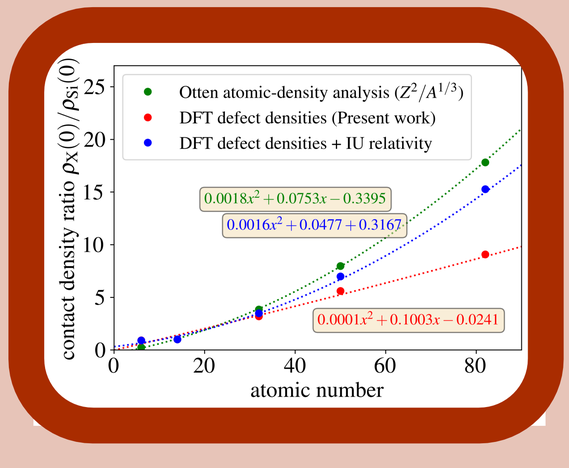
## Methods

- We performed full-potential spin-polarized DFT-PBE calculations using WIEN2k within a basis of linearized augmented plane waves plus local orbitals (LAPW+lo), while treating spin-orbit coupling in a separate variational optimization step.

## Results and discussion




- DFT-level computation of electron spin densities shows the conduction electron will bunch slightly at a Sn site, but localization is still very weak compared to the P donor.
- Meanwhile comparing to a Si nucleus in pristine bulk, the density at the Sn site is at least five times larger, which will conveniently distinguish it from the surrounding Si atoms.
- Thus the character of extrinsic isoelectronic defects looks promising, but why do we favor Sn over C, Ge, or Pb?

- Computed values for the hyperfine enhancement ($\eta$) of Si and Ge nuclei agree well with the experimental values of Wilson and Kerckhoff et al.
- $^{73}$Ge nuclei are spin-9/2, so we opt for the simpler ½ spins of $^{117}$Sn or $^{119}$Sn.
- The bunching factor ratio of $\eta_{\mathrm{Sn}}/\eta_{\mathrm{Si}} \sim 5$ translates to a hyperfine interaction enhancement for Sn of about 10 times with respect to the bath Si nuclei.
- Taking into account relativistic corrections to the Fermi contact interaction, the HFI enhancement for Sn grows to 13.7 times with respect to Si nuclei.

## Future work

- Nuclear flip-flop dynamics simulations of Sn in silicon are currently being planned. These will utilize in-house codes which have been in development for several years.
- Experimental fabrication and validation is also underway.

## References

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