## Technology Computer-Aided Design Simulations of Hole Spin Qubits In Gated Double Quantum Dots

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Fig. 1. (a) Scanning electron micrograph of the gate layout of the double quantum dot device. (b) Barrier-gate control of the tunnel coupling 2t of the double quantum dot. Ground-state hole density at: (c) strong tunnel coupling, (d) weak tunnel coupling. (e) Exchange-driven Rabi oscillations between  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$  heavy-hole spin states in the double quantum dot under dephasing and relaxation noise from hyperfine coupling to nuclear spins and phonon-induced relaxation.

The design and engineering of classical semiconductor chips often relies on a mature set of computational tools. Among these tools are technology computer-aided design (TCAD) software which are used to predict device performance and trends before fabrication. As we move toward using semiconductors for quantum technologies in the form of, e.g., spin qubits, it seems plausible that we will need to adopt best practices employed for classical semiconductor systems. However, because of the fundamental differences in operating principles between classical and quantum hardware, specialized quantum TCAD tools must be developed for quantum systems.

Recently, a hole double quantum dot device in a GaAs/AlGaAs heterostructure was studied experimen-

tally by the NRC [1] and considered for the realization of a quantum repeater for long-range quantum communication [2]. GaAs is a promising material for quantum-repeater applications because of its direct bandgap enabling photon-to-spin conversion. In addition, because of the *p*-like nature of the heavy-hole orbitals, hole spins are expected to be less sensitive than electron spins to dephasing from hyperfine interactions with the nuclear spins in the GaAs/AlGaAs lattice [3], which may enable high-fidelity entangling-gate operations that are needed to distribute entanglement across quantum-repeater nodes.

In this work, we use the spin-qubit device modeling software package QTCAD [4] to perform TCAD simulations of the NRC's hole double-dot device. Starting from the gate layout of the device, we build a 3D TCAD model of the structure and go through a complete workflow that includes the simulation of device electrostatics, quantum-well physics, hole charge stability diagrams, double-quantum-dot tunneling rates, exchange energies, exchange-driven Rabi oscillations between two-qubit states, and the calculation of a  $\sqrt{SWAP}$  gate fidelity. These results showcase how 3D TCAD simulations of hole spin qubits can help steer the design of quantum hardware used in both quantum-computing and quantum-communication applications. References

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