

Light Hole Spins Confined in Germanium

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Hole spins in group IV semiconductor quantum wells (QW) are promising candidates for reliable and scalable qubits. Besides their compatibility with Si, group IV semiconductors provide a vast playground for engineering hole spins by leveraging their wide span in lattice parameter and bandgap energies. Moreover, group IV semiconductors can be isotopically purified to remove spin-full nuclei within the lattice, which significantly increases spin coherence times. Holes also take advantage of the large spin-orbit coupling of their host crystal, enabling fast and efficient spin manipulating schemes such as electric-dipole-spin-resonance (EDSR) and g -tensor modulation.

Although Ge has recently been at the core of numerous achievements towards scalable hole spin qubits and has been the subject of many theoretical investigations, research in this area focuses mostly on heavy hole (HH) spin systems. This is mostly attributed to material limitations, as Ge is usually subject to compressive epitaxial strain caused by combining it with $\text{Si}_{1-y}\text{Ge}_y$, a smaller lattice parameter material. This strain lifts the degeneracy at the top of the valence band and promotes HHs to the ground state.

On the other hand, combining Ge with the larger lattice parameter material $\text{Ge}_{1-x}\text{Sn}_x$ creates a significant amount of tensile strain in Ge, which if large enough can push LHs to the ground state (Fig. 1a, right panel). To achieve this, we propose the heterostructure displayed in Fig. 1b, where a thick and graded buffer of $\text{Ge}_{1-x}\text{Sn}_x$ with increasing Sn concentration is grown on top of a Ge virtual substrate (VS). [1] Sn concentrations reaching $x \approx 0.13$ just below the Ge QW layer is expected to produce enough tensile strain to create a LH ground state within the well (Fig. 1c). A LH qubit would inherit many qualities from its HH counterpart, but with a significantly larger in-plane g -tensor component. LHs are also expected to couple more efficiently with proximity-induced superconductivity.

This work investigates the properties of LH spins confined in $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}/\text{Ge}_{1-x}\text{Sn}_x$ QWs using $k \cdot p$ theory. [2] We first establish the conditions required to confine a LH in Ge, before delving into the peculiar confinement properties of the $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}/\text{Ge}_{1-x}\text{Sn}_x$ QW system. We evaluate important LH characteristics such as their effective masses and their effective g -tensor for various Sn concentrations and well thicknesses. Large in-plane g -factors (~ 10) are reported, as well as sizable linear-in- k Rashba couplings. The magnitude of the two cubic-in- k Rashba couplings $\beta_{2,3}$ are shown to be reversed with respect to HHs, with the EDSR-relevant β_3 being one order of magnitude larger for LHs. [2-3] We also discuss the effects of strain and well thickness on LH-HH mixing. Our calculations explicitly take in account the hole wavefunctions spreading across interfaces, as well as the large number of HH levels located within the $\text{Ge}_{1-x}\text{Sn}_x$ barriers.

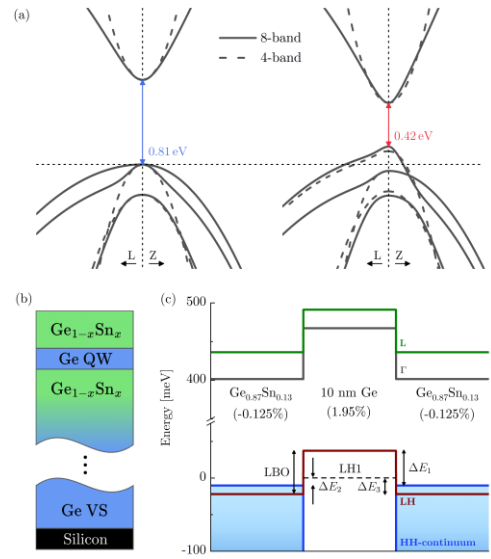


Fig.1. (a) Bulk $E(k)$ dispersion near the Γ point of relaxed Ge (left) and biaxially tensile strained Ge (right). In the right panel, the strain tensor components $\epsilon_{xx} = \epsilon_{yy} = +2\%$ and $\epsilon_{zz} = -1.3\%$. (b) Schematic of a tensile strained Ge QW on $\text{Ge}_{1-x}\text{Sn}_x$ barriers. (c) Band alignment profile of a Ge QW on $\text{Ge}_{0.87}\text{Sn}_{0.13}$.

References

- [1] S. Assali *et al.* Adv. Mater. **34**, 2201192 (2022)
- [2] P. Del Vecchio *et al.* arXiv:2402.10449
- [3] P. Del Vecchio *et al.* Phys. Rev. B **107**, L161406 (2023)