Spin relaxation and donor-acceptor recombination of Se$^+$ in 28-silicon:

Supplementary material

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I. OBTAINING THE SELENIUM IMPURITY CONCENTRATION

The concentration of selenium impurities of the samples used in this work was determined by Hall effect measurements at room temperature using the van der Pauw method [1]. The measurements were carried out under a static magnetic field of 1 T and a constant current of 100 mA and the resulting free electron concentration was determined to be $n_c = 1.1 \times 10^{15} \text{ cm}^{-3}$.

Due to high ionisation energy, selenium donors are in general not fully ionised at room temperature. Therefore a simulation was carried out to relate the concentration of donors with the measured concentration of free carriers. The thermal equilibrium population of the donor levels was then calculated by applying Fermi-Dirac statistics for double donors and solving a balance equation for the chemical potential $\mu$ [2]. Under boron compensation (see main text), the balance equation reads:

$$n_c + n_{\text{Se}} = 2[\text{Se}] - [\text{B}] + p_v + p_B$$

where $n_{\text{Se}}$ is the concentration of electrons bound the selenium donor, $n_B$ is the concentration of holes bound boron, $n_c$ and $p_v$ are the free carriers and $[\text{Se}]$ and $[\text{B}]$ are the impurity concentrations. The solution of this equation is determined by including the explicit dependence of $n_c$, $p_v$, $p_B$ and $n_{\text{Se}}$ with the chemical potential. In order to take into account the fact that selenium is a double donor, the average number of electrons bound to each impurity can be written as

$$n_{\text{Se}} = 2(\text{Se}^0) + (\text{Se}^+)$$

and the population of each donor charge state can be calculated using the Fermi-Dirac distribution. By solving Eq. 1 at room temperature using the measured concentration of free carriers $n_c$, a concentration of selenium impurities $[\text{Se}] \approx 5 \times 10^{15} \text{ cm}^{-3}$ was determined.

II. TEMPERATURE DEPENDENCE OF ELECTRON SPIN $T_2$

Figure 1 shows example $T_2$ and $T_1$ measurements of the Se$^+$ donor electron spin, made using the Hahn echo and inversion recovery sequences, respectively [3]. We attribute the observed temperature dependence of $T_2$ (see Figure 3 of the main text) to the combination of three different mechanisms [3]: i) spin relaxation of the central spin, yielding an echo decay of...
FIG. 1: Experimental relaxation times of $^{77}\text{Se}^+$ at 15 K and relative pulse sequences used to measured $T_1$ (a) and $T_2$ (b).

The form $\exp[-(2\tau/T_1)]$; ii) a temperature-independent process of the form $\exp[-(2\tau/T_{2,\text{lim}})]$ with $T_{2,\text{lim}} = 80$ ms; and iii) a spectral diffusion process caused by spin relaxation of nearest neighbours, of the form $\exp[-(2\tau/T_{SD})^2]$, such that the overall echo decay follows:

$$V(2\tau) = \exp\left[-\frac{2\tau}{T_1}\right] \exp\left[-\frac{(2\tau)^2}{T_{SD}^2}\right] \exp\left[-\frac{2\tau}{T_{2,\text{lim}}}\right].$$

(3)

The spectral diffusion process, which results in a Gaussian, decay has a characteristic time:

$$T_{SD}^2 = \frac{18\sqrt{3}}{\gamma^2} \frac{\mu_0}{\gamma^2} \frac{T_1}{[\text{Se}^+]}$$

(4)

where $T_1$ is the electron spin relaxation, $[\text{Se}^+]$ is the concentration of $\text{Se}^+$, $\mu_0$ is the vacuum permeability, $\gamma$ is electron gyromagnetic ratio [5, 6].

When different mechanisms contribute simultaneously to overall spin echo decay the coherence time ($T_2$) can be defined as the time at which the echo intensity falls to $1/e$ of its maximum value. We then define $T_2$ with the solution of the equation

$$T_2 \frac{1}{T_{SD}^2} + T_2 \left(\frac{1}{T_1} + \frac{1}{T_{2,\text{lim}}}\right) - 1 = 0.$$ 

(5)

Figure 3 in the main text gives the temperature dependence of $T_2$ of the sample measured in the main text together with the with contributions of the different mechanisms, as described above. Because the spectral diffusion is never the dominant decoherence mechanism, we do not directly observe any non-exponential decay of the spin echo. However, this mechanism
still has a small contribution that has to be considered in order to understand the temperature dependence of $T_2$. This dependence is obtained by solving Eq. 5 using the measured values of $[\text{Se}^+]$ and $T_1$ and with $T_{2,\text{lim}}$ as the only fitting parameter, to give the limit of $T_2$ at low temperature.

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