# Supporting Information: Surface Dangling Bonds Are a Cause of B-Type Blinking in Si Nanoparticles

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## 1 Bulk Defect Structure

Figure 1 shows the ball and stick representation of the $P_b$ defect model in bulk silicon. This model is similar to the "A" center in bulk silicon, which is believed to be an oxygen-vacancy complex.[1–3]

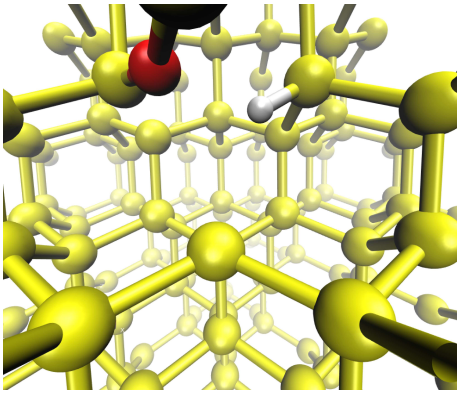

**Fig. 1** Model of the $P_b$ defect in bulk silicon. The defect was introduced within a 216 silicon atom supercell. Yellow, red and white spheres represent Si, oxygen and hydrogen atoms, respectively.

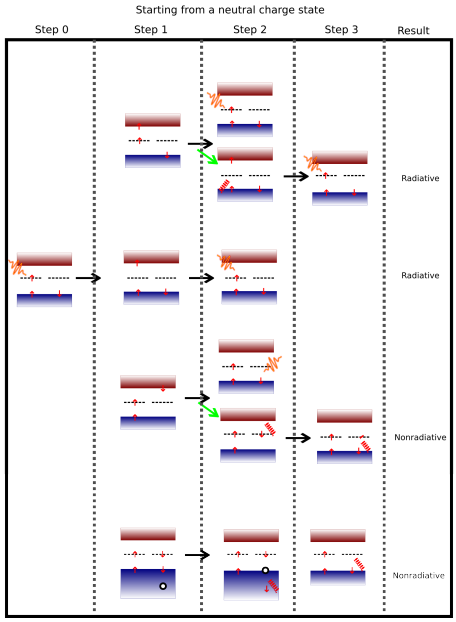


**Fig. 2** Possible decay dynamics of an excited neutral nanoparticle with a dangling bond to the ground state (see text).

## 2 Decay Dynamics

Figures 2-4 show possible channels for different initial charge states of a Si nanoparticle with a 1.3 nm diameter and an oxidized layer. The difference in the charge states can be caused by electron exchange with local defects in the surrounding oxide matrix. We assumed the additional holes/electrons were just spectators and do not change the rates. Furthermore, we assumed lifetimes were best represented by calculations where only atoms within the outer most hydrogen shell are relaxed. See figures 2, 3 and 4 below.

## 3 Estimation of Crossing Region

Using a single band effective mass approximation, we can write the activation energy as a function of NP size:

$$\begin{aligned} E_{act} &= \frac{(E_o - E_{FC})^2}{4E_{FC}} \\ &= \frac{(E_{Si,gap} - E_{FC} + E_c - E_{FC})^2}{4E_{FC}} \\ &= \frac{(E_{Si,gap} + \frac{\hbar^2\pi^2}{2m_c^* R^2} - 2E_{FC})^2}{4E_{FC}} \end{aligned}$$

where we have assumed $E_{FC}$ to be approximately equal to the energy of the defect state from the bulk valence band and independent of NP size. Using the following parameters:

- $m_c^*$=1.09 Ref.[4]
- $E_{Si,gap}$=1.1 eV
- $d_{FC}$=0.26 eV (from the $1P_b(r_{nn})$ calculation)

we find the nonradiative transition to be more efficient than the radiative for the $D^+ \rightarrow D^0$ process in NPs with diameters larger than 4 nm in diameter.

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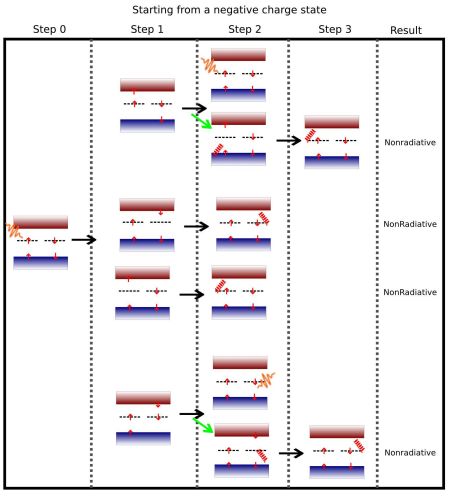


**Fig. 3** Possible decay dynamics a negative nanoparticle system.

## References


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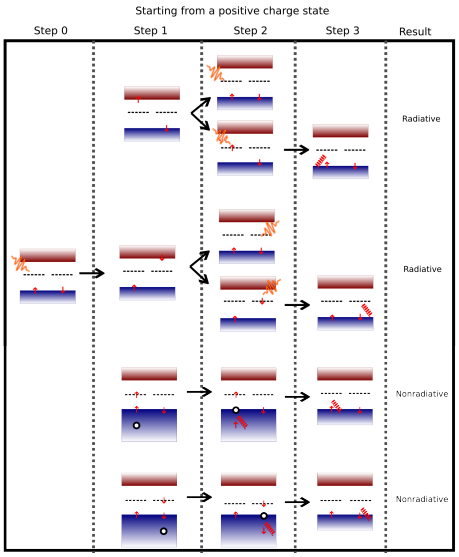


**Fig. 4** Possible decay dynamics a positive nanoparticle system.