Supporting Information for Supression of Auger Processes in Confined Structures

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Solution of the Coupled, Two-band Kane Model

We seek a solution to the time-independent Schrödinger equation corresponding to the Hamiltonian of Eq. (3). Taking all energies on the scale of $\alpha_e \hbar^2/2m_0$, this Hamiltonian is expressed explicitly as

$$\hat{H} = \begin{pmatrix} -\frac{d^2}{dx^2} + \epsilon + U_e'(x) & -iP\frac{d}{dx} \\ -iP\frac{d}{dx} & \xi\frac{d^2}{dx^2} - \epsilon - U_h'(x) \end{pmatrix}. \tag{S-1}$$

In terms of the parameters in Eq. (3), we have defined $\epsilon = E_g m_0/(\alpha_e \hbar^2)$, $U_{e(h)}'(x) = 2U_{e(h)}(x)m_0/(\alpha_e\hbar^2)$, $\xi = \alpha_h/\alpha_e$ and $P = 2Km_0/(\alpha_e\hbar)$. Consider the system enclosed inside a large box of length $2L$. Provided that L is sufficiently larger than the confinement size a, the discretization imposed by introducing the impenetrable outer boundary does not significantly affect the results of the calculation.

To find the eigenvalues and eigenfunctions, we calculate the matrix form of $\hat{H}$ in the basis of the uncoupled problem:

$$\hat{H}_0 = \begin{pmatrix} -\frac{d^2}{dx^2} + \epsilon & 0 \\ 0 & \xi\frac{d^2}{dx^2} - \epsilon \end{pmatrix}, -L < x < L. \tag{S-2}$$

The normalized, two-component eigenfunctions of Hamiltonian (S-2) are given by

$$\varphi_n^{(even)}(x) = \frac{1}{\sqrt{L}}\begin{pmatrix} \cos(\sigma_n x) \\ 0 \end{pmatrix} \tag{S-3a}$$

$$\varphi_n^{(odd)}(x) = \frac{1}{\sqrt{L}}\begin{pmatrix} \sin(k_n x) \\ 0 \end{pmatrix} \tag{S-3b}$$

$$\eta_n^{(even)}(x) = \frac{1}{\sqrt{L}}\begin{pmatrix} 0 \\ \cos(\sigma_n x) \end{pmatrix} \tag{S-3c}$$

$$\eta_n^{(odd)}(x) = \frac{1}{\sqrt{L}}\begin{pmatrix} 0 \\ \sin(k_n x) \end{pmatrix} \tag{S-3d}$$

where the discrete wave numbers

$$\left.\begin{aligned} \sigma_n &= \left(n - \frac{1}{2}\right)\frac{\pi}{L} \\ k_n &= \frac{n\pi}{L} \end{aligned}\right., \quad n = 1, 2, 3\ldots, \tag{S-4}$$

enforce the boundary condition that demands the wave functions vanish at the impenetrable boundaries.

Assuming the potentials, $U_e'(x)$ and $U_h'(x)$, to be even, the nonvanishing matrix elements, H_{ij}, of the full Hamiltonian (S-1) can be expressed as

$$\begin{aligned}\langle\varphi_m^{(even)}|\hat{H}|\varphi_n^{(even)}\rangle &= H_{4m-3,4n-3}\\ &= (\sigma_n^2+\epsilon)\delta_{mn} + \frac{1}{L}\int_{-L}^{L} dx\, U_e'(x)\cos(\sigma_m x)\cos(\sigma_n x)\end{aligned} \tag{S-5a}$$

$$\begin{aligned}\langle\eta_m^{(even)}|\hat{H}|\eta_n^{(even)}\rangle &= H_{4m-2,4n-2}\\ &= -(\xi\sigma_n^2+\epsilon)\delta_{mn} - \frac{1}{L}\int_{-L}^{L} dx\, U_h'(x)\cos(\sigma_m x)\cos(\sigma_n x)\end{aligned} \tag{S-5b}$$

$$\begin{aligned}\langle\varphi_m^{(odd)}|\hat{H}|\varphi_n^{(odd)}\rangle &= H_{4m-1,4n-1}\\ &= (k_n^2+\epsilon)\delta_{mn} + \frac{1}{L}\int_{-L}^{L} dx\, U_e'(x)\sin(k_m x)\sin(k_n x)\end{aligned} \tag{S-5c}$$

$$\begin{aligned}\langle\eta_m^{(odd)}|\hat{H}|\eta_n^{(odd)}\rangle &= H_{4m,4n}\\ &= -(\xi k_n^2+\epsilon)\delta_{mn} - \frac{1}{L}\int_{-L}^{L} dx\, U_h'(x)\sin(k_m x)\sin(k_n x)\end{aligned} \tag{S-5d}$$

$$\begin{aligned}\langle\eta_m^{(odd)}|\hat{H}|\varphi_n^{(even)}\rangle &= H_{4m,4n-3} = H_{4m-1,4n-2} = H^*_{4n-3,4m} = H^*_{4n-2,4m-1}\\ &= (-1)^{m+n}\frac{2iP}{L}\frac{m(n-1/2)}{m^2-(n-1/2)^2}.\end{aligned} \tag{S-5e}$$

Taking an index range of $n, m = 1, 2, \ldots N$, we truncate the full Hamiltonian to a $4N\times 4N$ matrix, thus allowing standard numerical routines to be used in determining the eigenvalues and eigenvectors. Afterward, a check must be performed to assure that N was chosen large enough to have no significant effect on the result.

We label the eigenenergies both above and below the band gap by $j = 0, 1, \ldots N$, where each integer value corresponds either to a positive energy electron or to a negative energy hole. For example, $j = 0$ labels both the positive energy ground state above the band gap and the negative energy ground state below the band gap. Distinction between these cases is denoted in the eigenfunction by the appropriate e or h subscript. Expressed in the basis

(S-3), the eigenfunctions of the full Hamiltonian (S-1) are

$$\psi^j_{e(h)}(x) = \sum_{n=1}^{N} \left[A^j_{e(h)\,n}\, \varphi^{(even)}_n(x) + B^j_{e(h)\,n}\, \varphi^{(odd)}_n(x) + C^j_{e(h)\,n}\, \eta^{(even)}_n(x) + D^j_{e(h)\,n}\, \eta^{(odd)}_n(x) \right] , \tag{S-6}$$

where the expansion matrices, A, B, C and D, are obtained from numerical diagonalization. Finally, these single-particle wave functions are used to construct the initial and final state wave functions of Eqs. (4) and (5), respectively.

Auger Recombination Rate

In this section we deduce Eq. (8), thus showing that the Auger rate matrix element behaves like the Fourier transform of the hole ground state wave function evaluated at the wave number of the excited state. We consider the Auger process in which the ground state electron-hole pair annihilates then transfers its energy to an excess hole that is subsequently ejected into the continuum.

The Coulomb matrix element of Eq. (6) is

$$M_{if} = \sqrt{2} \int dx_1 dx_2\, \psi^0_h(x_1)^* \psi^0_h(x_2)^* \frac{e^2}{\kappa |x_1 - x_2| + \delta}\, \psi^0_e(x_1)^* \phi_f(x_2). \tag{S-7}$$

where $\psi^{0\,*}_e$ is really a hole wave function that is regarded as the complex conjugate of the electron ground state. Also, recall that a small parameter δ was introduced to keep the Coulomb interaction well-behaved at small distances. It is possible to simplify M_{if} by expressing the interaction as a Fourier integral

$$\frac{1}{|r| + \delta} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dq\, e^{-iqr} \tilde{V}(q)\,, \tag{S-8}$$

where

$$\begin{aligned} \tilde{V}(q) &= \int_{-\infty}^{\infty} dr\, e^{iqr} \frac{1}{|r| + \delta} \\ &= -\mathrm{Ei}(-iq\delta) \exp(iq\delta) - \mathrm{Ei}(iq\delta) \exp(-iq\delta)\,, \end{aligned} \tag{S-9}$$

$\mathrm{Ei}(x)$ is the exponential integral,[1] and $r = x_1 - x_2$. Substitution of (S-8) into (S-7) allows the spatial integrations to be separated

$$M_{if} = \frac{e^2}{\kappa} \frac{\sqrt{2}}{2\pi} \int_{-\infty}^{\infty} dq\, \tilde{V}(q) \int_{-\infty}^{\infty} dx_1\, e^{-iqx_1}\, \psi^0_h(x_1)^* \psi^0_e(x_1)^* \int_{-\infty}^{\infty} dx_2\, e^{iqx_2}\, \psi^0_h(x_2)^* \phi_f(x_2)\,. \tag{S-10}$$

Because the final state is a hole ejected into the continuum, we can approximate the corresponding wave function as a plane wave in a highly excited mode,

$$\phi_f(x_2) \sim e^{-ik_f x_2}. \tag{S-11}$$

Furthermore, the remaining wave functions in (S-10) are bound states which must decay rapidly outside the confinement, $|x_1|, |x_2| > a$. Since the two spatial integrals are Fourier transforms, it then follows that both have an approximate frequency cutoff of $\sim 1/a$. Moreover, $\tilde{V}(q)$ decays to zero as $|q| \to \infty$, thereby allowing the $1/a$ cutoff to be imposed on the integration variable q.

With these considerations, substituting (S-11) into (S-10) allows the matrix element to be approximated as

$$M_{if} \simeq \frac{e^2}{\kappa}\frac{\sqrt{2}}{2\pi}\int_{-1/a}^{1/a} dq\, \tilde{V}'(q)\, \tilde{\psi}_h^0(k_f - q)^*. \tag{S-12}$$

In addition to denoting the complex conjugate of the Fourier transform of the hole ground state by $\tilde{\psi}_h^{0\,*}$, we have defined

$$\tilde{V}'(q) = \tilde{V}(q) \int_{-\infty}^{\infty} dx_1\, e^{-iqx_1} \psi_h^0(x_1)^* \psi_e^0(x_1)^*. \tag{S-13}$$

If the excited state wave number is sufficiently larger than the cutoff, $k_f a \gg 1$, the matrix element becomes

$$M_{if} \simeq \frac{e^2}{\kappa}\frac{\sqrt{2}}{2\pi}\, \tilde{\psi}_h^0(k_f)^* \int_{-1/a}^{1/a} dq\, \tilde{V}'(q), \tag{S-14}$$

which is the desired result.

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[1] To express $\tilde{V}(q)$ in terms of the exponential integral, Ei, first split the integral into two parts, one for $r < 0$ and one for $r > 0$. The result will be a cosine integral which can be found in Gradshtein, I. S.; Ryzhik, I. M. *Table of Integrals, Series, and Products*; Academic Press: New York, 1980.