Supporting Information

Mn^{2+}-doped CdSe/CdS Core/Multishell Colloidal Quantum Wells Enabling Tunable Carrier-Dopant Exchange Interactions

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Experimental Section

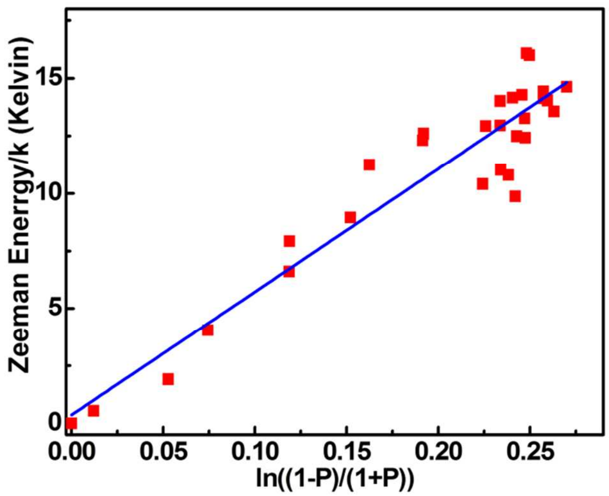

Figure S1. The plot of $\Delta E_{Zeeman}/k$ vs ln((1-P)/(1+P)) for sample 1. Blue line indicates the fitted line. The temperature derived from the slope of the line is equal to 53 K for the measurement performed at cryostat temperature of 7K.

Theoretical Section

Eigenenergies and Eigenfunctions

We consider the problem of a particle in a box; and the stationary Schrödinger equation is solved assuming the effective mass approximation. Under this assumption, the Schrödinger equation for the electron (hole) is given by

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V_z(z)\right]Z(z)=E_z Z(z) \tag{1}$$

where $V_z(z)$ is the electric potential.

Case I :

$$V(z)=\begin{cases} V_0 & -\frac{1}{2}L_2<z<-\frac{1}{2}L_1;\quad \frac{1}{2}L_1<z<\frac{1}{2}L_2 \\ 0 & -\frac{1}{2}L_1<z<\frac{1}{2}L_1 \\ \infty & \text{elsewhere} \end{cases} \tag{2}$$

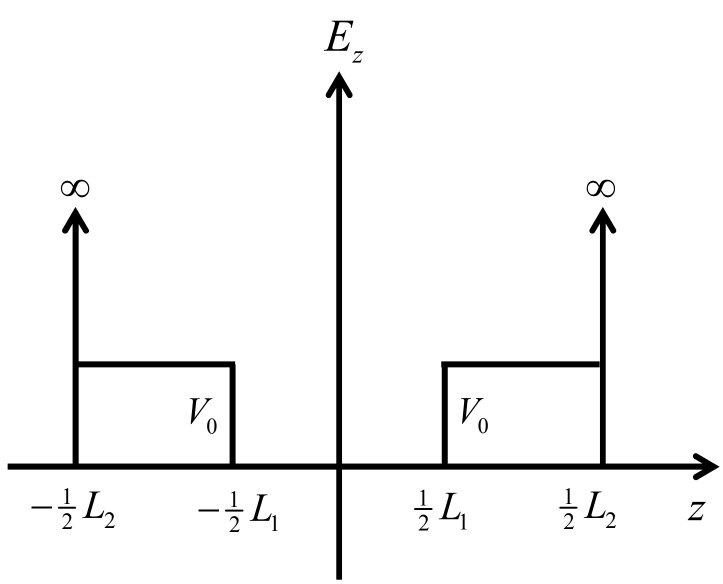

Figure S2: Energy diagram for particle in a box.

A) $E > V_0$ **:**

The solutions for this potential are of the form

$$Z(z) = \begin{cases} A_1 \cos[\alpha_1 z] + A_2 \sin[\alpha_1 z] & -\frac{1}{2}L_2 < z < -\frac{1}{2}L_1 \\ B_1 \cos[\alpha_2 z] + B_2 \sin[\alpha_2 z] & -\frac{1}{2}L_1 < z < \frac{1}{2}L_1 \\ C_1 \cos[\alpha_1 z] + C_2 \sin[\alpha_1 z] & \frac{1}{2}L_1 < z < \frac{1}{2}L_2 \end{cases} \tag{3}$$

with

$$\alpha_1(E) = \sqrt{\frac{2m_1}{\hbar^2}(E - V_0)} \tag{4}$$

$$\alpha_2(E) = \sqrt{\frac{2m_2}{\hbar^2}(E)} \tag{5}$$

The boundary conditions are given by:

$$Z_1\left(-\tfrac{1}{2}L_2\right) = 0 \tag{6}$$

$$Z_1\left(-\tfrac{1}{2}L_1\right) = Z_2\left(-\tfrac{1}{2}L_1\right) \tag{7}$$

$$Z_2\left(\tfrac{1}{2}L_1\right) = Z_3\left(\tfrac{1}{2}L_1\right) \tag{8}$$

$$Z_3\left(\tfrac{1}{2}L_2\right) = 0 \tag{9}$$

$$\frac{1}{m_1} Z'_1\left(-\tfrac{1}{2}L_1\right) = \frac{1}{m_2} Z'_2\left(-\tfrac{1}{2}L_1\right) \tag{10}$$

$$\frac{1}{m_2} Z'_2\left(\tfrac{1}{2}L_1\right) = \frac{1}{m_1} Z'_3\left(\tfrac{1}{2}L_1\right) \tag{11}$$

and normalization condition

$$\int_{-\frac{1}{2}L_2}^{-\frac{1}{2}L_1} Z_1(z) Z^*_1(z)\,dz + \int_{-\frac{1}{2}L_1}^{\frac{1}{2}L_1} Z_2(z) Z^*_2(z)\,dz + \int_{\frac{1}{2}L_1}^{\frac{1}{2}L_2} Z_3(z) Z^*_3(z)\,dz = 1 \tag{12}$$

From Eqs. (6) to (11), yield a set of linear equations, which depends only on energy, and it is given by

$$\mathbf{M}(E)\mathbf{Z} = \mathbf{0} \tag{13}$$

The non-trivial solution is given when the determinant is equal to zero, i.e.

$$\det\left|\mathbf{M}(E)\right| = 0 \tag{14}$$

Once the energy is found, coefficients A_1, A_2, B_1, B_2, C_1, and C_2 are found by Eq. (6) to (12).

B) $E < V_0$ **:**

The solutions for this potential are of the form

$$Z(z) = \begin{cases} A_1 \exp[\alpha_1 z] + A2 \exp[-\alpha_1 z] & -\dfrac{1}{2}L_2 < z < -\dfrac{1}{2}L_1 \\ B_1 \cos[\alpha_2 z] + B_2 \sin[\alpha_2 z] & -\dfrac{1}{2}L_1 < z < \dfrac{1}{2}L_1 \\ C_1 \exp[\alpha_1 z] + C_2 \exp[-\alpha_1 z] & \dfrac{1}{2}L_1 < z < \dfrac{1}{2}L_2 \end{cases} \tag{15}$$

with

$$\alpha_1(E) = \sqrt{\frac{2m_1}{\hbar^2}(V_0 - E)} \tag{16}$$

$$\alpha_2(E) = \sqrt{\frac{2m_2}{\hbar^2}(E)} \tag{17}$$

A_1**,** A_2**,** B_1**,** B_2, C_1, and C_2 can be found following the procedure presented in **Case I (A).**

Case II :

$$V(z) = \begin{cases} 0 & -\tfrac{1}{2}L_2 < z < -\tfrac{1}{2}L_1;\ \ \tfrac{1}{2}L_1 < z < \tfrac{1}{2}L_2 \\ V_0 & -\tfrac{1}{2}L_1 < z < \tfrac{1}{2}L_1 \\ \infty & \text{elsewhere} \end{cases} \tag{18}$$

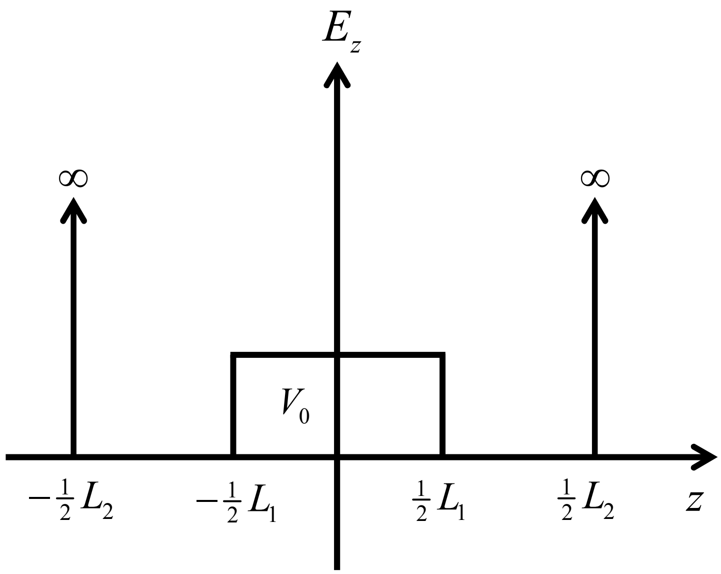

Figure S3: Energy diagram for particle in a box.

A) $E > V_0$***:***

The solutions for this potential are of the form

$$Z(z) = \begin{cases} A_1 \cos[\alpha_1 z] + A_2 \sin[\alpha_1 z] & -\frac{1}{2}L_2 < z < -\frac{1}{2}L_1 \\ B_1 \cos[\alpha_2 z] + B_2 \sin[\alpha_2 z] & -\frac{1}{2}L_1 < z < \frac{1}{2}L_1 \\ C_1 \cos[\alpha_1 z] + C_2 \sin[\alpha_1 z] & \frac{1}{2}L_1 < z < \frac{1}{2}L_2 \end{cases} \tag{19}$$

with

$$\alpha_1(E) = \sqrt{\frac{2m_1}{\hbar^2}(E)} \tag{20}$$

$$\alpha_2(E) = \sqrt{\frac{2m_2}{\hbar^2}(E - V_0)} \tag{21}$$

A_1, A_2, B_1, B_2, C_1, and C_2 can be found following the procedure presented in **Case I (A).**

B) $E < V_0$ ***:***

The solutions for this potential are of the form

$$Z(z) = \begin{cases} A_1 \cos[\alpha_1 z] + A_2 \sin[\alpha_1 z] & -\frac{1}{2}L_2 < z < -\frac{1}{2}L_1 \\ B_1 \exp[-\alpha_2 z] + B_2 \exp[\alpha_2 z] & -\frac{1}{2}L_1 < z < \frac{1}{2}L_1 \\ C_1 \cos[\alpha_1 z] + C_2 \sin[\alpha_1 z] & \frac{1}{2}L_1 < z < \frac{1}{2}L_2 \end{cases} \tag{22}$$

with

$$\alpha_1(E) = \sqrt{\frac{2m_1}{\hbar^2}(V_0 - E)} \tag{23}$$

$$\alpha_2(E) = \sqrt{\frac{2m_2}{\hbar^2}(E)} \tag{24}$$

A_1, A_2, B_1, B_2, C_1, and C_2 can be found following the procedure presented in **Case I (A).**

Numerical Results

We have studied five CdSe/CdS core-shell nanoplatelet samples in this work. In CdSe/CdS nanoplatelet the parameters used for our calculation are listed in Table 1. Important parameters of the calculation are the band offsets. Effective masses were calculated following the procedure of Ithurria et al.[1] In our system these offsets vary widely in the literature; ΔE_{CB} ranges from -0.3 eV to 0.3 eV[2-5] and ΔE_{VB} ranges from 0.4 eV to 0.8 eV.[6, 7] For this reason, we carried out the wave function calculations using the extreme values for the offsets.

Parameters	CdSe	CdS	Medium
High frequency dielectric constant	8.3	8.9	1.0
Energy gap	1.66 *eV*	2.40 *eV*	

Table 1: List of parameters for CdSe and CdS. Data was obtained from Ref 1.[1]

References

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