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Optical Responses in Biofunctionalized Spherical Semiconductor Quantum Dots

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Abstract

We explore the impact of a biomaterial shell and diatomic confining potential on GaAs/AlGaAs/Bioshell spherical quantum dots. Using effective mass and parabolic band approximations, we solve the Schrödinger equation via finite element method (FEM). Our results show that varying core, shell, and confinement parameters significantly affects electron energies and optical absorption. Diatomic confinement allows precise control over quantum dot properties, promising tailored performance in biosensing.

Model

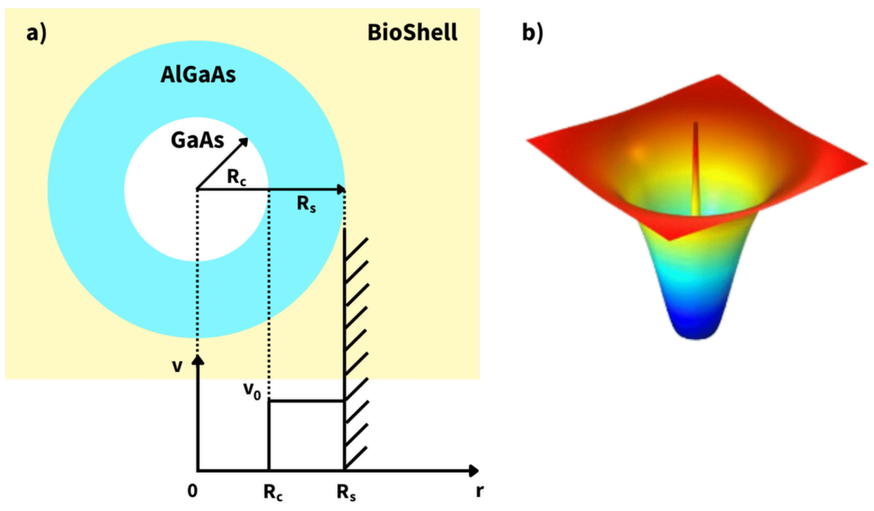

Figure 1: (a) GaAs/AlGaAs/Bioshell spherical quantum dots. (b) Diatomic potential.

Theoretical framework

For the electronic structure and optical properties of the system with fields electric in direction z, the Hamiltonian to be solved is:

$$H = -\frac{\hbar^2}{2}\nabla\left(\frac{1}{m_j^*}\nabla\right) + V(r), \tag{1}$$

The effective mass is: $m_c^* = 0.067\, m_0$ in GaAs, $m_s^* = 0.093\, m_0$ in AlGaAs.

$$V(r) = V_0\left(1 - \frac{e^{z_0/\rho_0}+1}{e^{r/\rho_0}+1}\right)^2, \tag{2}$$

$$V_0 = V(x) + \sum(R_s) \;\text{ and }\; V(x) = 1.155x + 0.37x^2, \tag{3}$$

Where x is the Aluminium concentration. $V(r)$ is the effective potential in AlGaAs shell and zero potential in GaAs core, infinite potential in bioshell. $\sum$ is the self-energy term due to the polarization induced by charging the QD with dielectric environment. The analytical expression of the self-energy is:

$$\sum(R_s) \approx \frac{e^2}{2R_s}\left(\frac{1}{\varepsilon_{\text{BS}}} - \frac{1}{\varepsilon_{\text{in}}}\right) + 0.47\left(\frac{e^2}{2R_s\varepsilon_{\text{in}}}\cdot\frac{\varepsilon_{\text{in}} - \varepsilon_{\text{BS}}}{\varepsilon_{\text{in}} + \varepsilon_{\text{BS}}}\right), \tag{4}$$

$\varepsilon_{in} = \sqrt{\varepsilon_c\,\varepsilon_s}$ and ε_{BS} represents the dielectric constants of the dot and the bioshell materials: $\varepsilon_{PEG} = 14.1$, $\varepsilon_{ChOx} = 3.5$ and $\varepsilon_{Streptavidin} = 2.1$ respectively.

Nonlinear Optical Absorption

The dipole matrix elements, with polarization in $\xi = z$ and $\xi = r$:

$$M_{if} = \int \psi_f^*(r)\, e\, \xi\, \psi_i(r)\, dV, \tag{5}$$

The nonlinear optical absorption coefficients are:

$$\alpha^{(1)}(\omega) = \omega\, e^2 \sqrt{\frac{\mu_0}{\varepsilon_0\,\varepsilon_{in}}}\left[\frac{\rho\,\hbar\,\Gamma_{if}|M_{if}|^2}{(E_{if} - \hbar\,\omega)^2 + (\hbar\,\Gamma_{if})^2}\right], \tag{6}$$

$$\alpha^{(3)}(\omega, I) = -\sqrt{\frac{\mu 0}{\varepsilon_0\varepsilon_{in}}}\left(\frac{\omega\, I}{2n_r\varepsilon_0 c}\right)\frac{4\rho\,\hbar\Gamma_{if}|M_{if}|^4}{\left[(E_{if} - \hbar\omega)^2 + (\hbar\Gamma_{if})^2\right]^2}, \tag{7}$$

Where μ_0 and ε_0 are the magnetic permeability and dielectric permittivity in vacuum. c is the speed of light, ε_{in} the dielectric permittivity of the semiconductor, ρ is the electron density. The damping term is $\Gamma_{if} = 1/\tau_{if}$ y ω is the frequency of incident photons.

Results

Electron energy levels, dipoles and nonlinerar optical absorption coefficients.

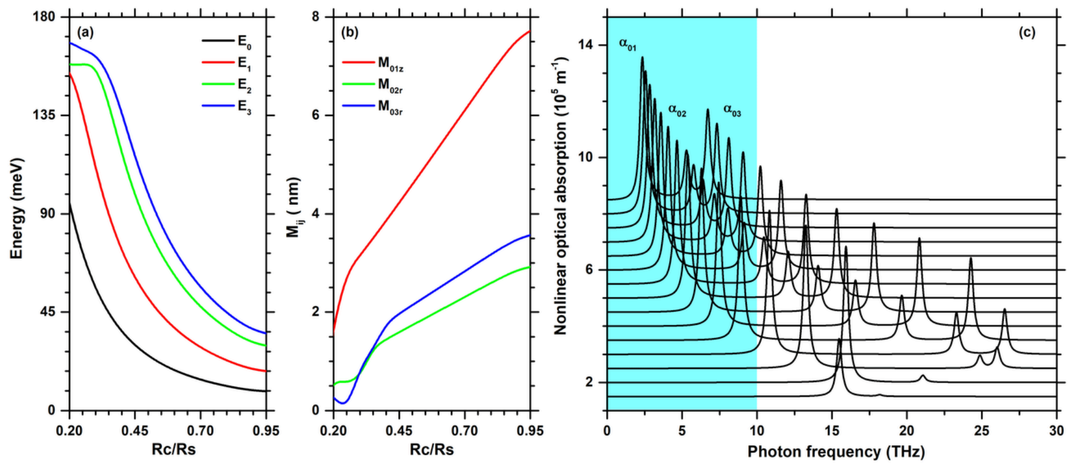

Figure 2: Dielectric environment PEG bioshell, with $x = 0.2$ and $R_s = 25$ nm.

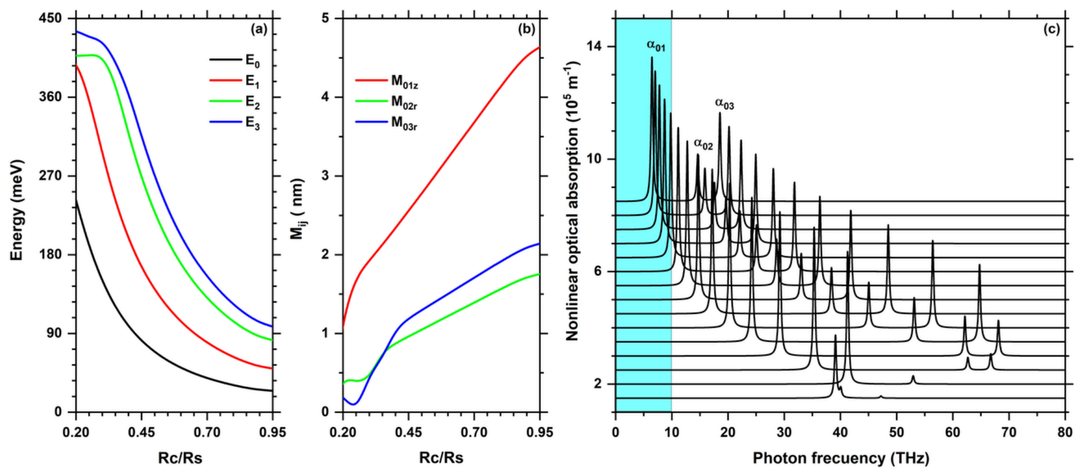

Figure 3: Dielectric environment Streptavidin, with $x = 0.45$ and $R_s = 15$ nm.

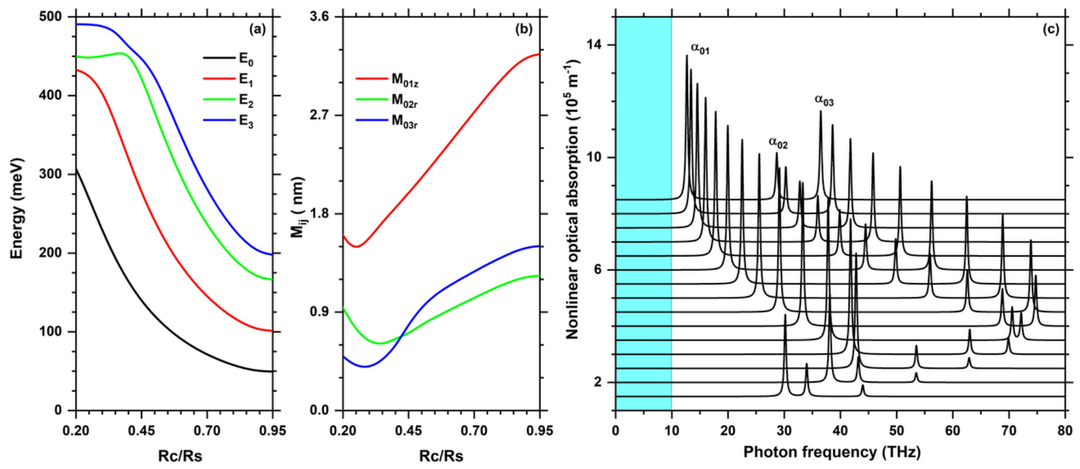

Figure 4: Dielectric environment ChOx bioshell, with $x = 0.45$ and $R_s = 10.5$ nm.

Conclusions

We conclude that the diatomic confinement potential parameters enable adjustment of both ground and excited state energies, thereby modulating the amplitudes and positions of peaks in the obtained optical properties. This nuanced control over the quantum dot properties holds promise for tailoring device performance in optical biosensing applications. By enhancing sensitivity and specificity in detecting biomolecules, such devices could revolutionize biomedical diagnostics, offering rapid and accurate detection of diseases or biomarkers.

Acknowledgements

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