

# Electron and hole addition energies in PbSe quantum dots

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## I. INTRODUCTION

Quantum dots (QDs) have attracted significant attention due to their unique electronic and optical properties. In this paper, we study the electron and hole addition energies in PbSe quantum dots. The addition energy is defined as the energy difference between two states with different numbers of electrons or holes. We use a tight-binding model to calculate the addition energies. The results show that the addition energies are strongly dependent on the size and shape of the quantum dot. For a spherical quantum dot, the addition energies increase with the size of the dot. For a cylindrical quantum dot, the addition energies are lower than those of a spherical dot of the same volume. The addition energies are also affected by the dielectric environment of the quantum dot. The addition energies are lower in a high-dielectric environment than in a low-dielectric environment.

The addition energies are important for understanding the electronic and optical properties of quantum dots. They determine the energy levels of the quantum dot and the energy of the emitted or absorbed photons. The addition energies are also important for the design of quantum dot devices, such as single-electron transistors and quantum dot lasers.

$$\mu(n) = \epsilon_y \mu(\infty) + \frac{e^2}{4\pi\epsilon_0\epsilon_y} \frac{1}{R} \quad (1)$$

where  $\mu(n)$  is the chemical potential of the quantum dot with  $n$  electrons,  $\epsilon_y$  is the dielectric constant of the quantum dot,  $\mu(\infty)$  is the chemical potential of the bulk material,  $e$  is the elementary charge,  $\epsilon_0$  is the permittivity of free space, and  $R$  is the radius of the quantum dot.

$$\Delta(n, n+1) = \mu(n+1) - \mu(n) \quad (2)$$

$$= \frac{e^2}{4\pi\epsilon_0\epsilon_y} \frac{1}{R} \quad (3)$$

where  $\Delta(n, n+1)$  is the addition energy. The addition energy is independent of the number of electrons in the quantum dot. This is because the addition energy is determined by the electrostatic energy of the quantum dot, which is independent of the number of electrons. The addition energy is also independent of the dielectric constant of the quantum dot, because the dielectric constant only affects the chemical potential of the quantum dot, which is subtracted out in the definition of the addition energy.

$$\epsilon(\mathbf{r}) = \sum_i \epsilon_i - \sum_i [\dots] \quad (1)$$

where  $\epsilon_i$  is the dielectric constant of the  $i$ -th component,  $\mathbf{r}$  is the position vector, and  $\mathbf{f}$  is the force vector. The term  $\sum_i [\dots]$  represents the contribution of the  $i$ -th component to the total dielectric constant.

$$\Phi_{iL}(\mathbf{r}) = \sum_{\sigma} \int \psi_i^*(\mathbf{r}, \sigma) \psi_i(\mathbf{r}, \sigma) \Phi_{iL}(\mathbf{r}) \mathbf{r} \quad (2)$$

where  $\{\psi_i(\mathbf{r}, \sigma)\}$  is the set of wave functions for the  $i$ -th component,  $\mathbf{r}$  is the position vector, and  $\Phi_{iL}(\mathbf{r})$  is the potential function.

$$\epsilon(\mathbf{r}) \nabla \Phi_{iL}(\mathbf{r}) = \pi \sum_{\sigma} \psi_i^*(\mathbf{r}, \sigma) \psi_i(\mathbf{r}, \sigma) \quad (3)$$

where  $\nabla$  is the gradient operator, and  $\pi$  is a constant. This equation relates the dielectric constant to the wave functions and the potential function.

$$\Sigma(\mathbf{r}) = \sum_i \Sigma_i - \sum_i [\dots] \quad (4)$$

where  $\Sigma_i$  is the surface energy of the  $i$ -th component, and  $\mathbf{r}$  is the position vector. The term  $\sum_i [\dots]$  represents the contribution of the  $i$ -th component to the total surface energy.

$$\Sigma_i = \sum_{\sigma} \int |\psi_i(\mathbf{r}, \sigma)|^2 \Sigma(\mathbf{r}) \mathbf{r} \quad (5)$$

where  $\Sigma(\mathbf{r})$  is the surface energy density, and  $\mathbf{r}$  is the position vector.

$$\Sigma(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{r}'} \{ \dots(\mathbf{r}, \mathbf{r}') \dots(\mathbf{r}, \mathbf{r}') \} \quad (6)$$

where  $V$  is the volume, and  $\mathbf{r}'$  is the position vector of the other end of the line element.

### C. Quasiparticle band gap

The quasiparticle band gap is defined as the energy difference between the upper and lower bands of the system. In the case of a band structure, the gap is the energy range where no states exist. The gap is determined by the energy levels of the system, which are given by the eigenvalues of the Hamiltonian operator. The energy levels are given by the equation  $E = \epsilon_0 + \epsilon_1$ , where  $\epsilon_0$  and  $\epsilon_1$  are the energy levels of the system.

$$\epsilon_1 = [\epsilon_2, \epsilon_3]$$

$\Sigma(\mathbf{r})$  is the total charge density,  $\mathbf{f}$  is the force density,  $\mathbf{f}_w$  is the force density due to the walls, and  $\mathbf{f}_e$  is the force density due to the electric field. The total force density is given by  $\mathbf{f} = \mathbf{f}_w + \mathbf{f}_e$ . The total charge density is given by  $\Sigma(\mathbf{r}) = \rho + \rho_w$ , where  $\rho$  is the charge density of the fluid and  $\rho_w$  is the charge density of the walls. The total force density is given by  $\mathbf{f} = \mathbf{f}_w + \mathbf{f}_e$ . The total charge density is given by  $\Sigma(\mathbf{r}) = \rho + \rho_w$ .

**B. Charge distribution of the injected carriers**

The charge distribution of the injected carriers is determined by the continuity equation and the Poisson equation. The continuity equation is given by  $\nabla \cdot \mathbf{j} + \partial \rho / \partial t = 0$ , where  $\mathbf{j}$  is the current density and  $\rho$  is the charge density. The Poisson equation is given by  $\nabla \cdot \mathbf{E} = \rho$ , where  $\mathbf{E}$  is the electric field. The total charge density is given by  $\Sigma(\mathbf{r}) = \rho + \rho_w$ . The total force density is given by  $\mathbf{f} = \mathbf{f}_w + \mathbf{f}_e$ .

**C. Charging spectrum and addition energies**

The charging spectrum and addition energies are determined by the total energy of the system. The total energy is given by  $E = E_{kin} + E_{pot} + E_{int}$ , where  $E_{kin}$  is the kinetic energy,  $E_{pot}$  is the potential energy, and  $E_{int}$  is the internal energy. The charging spectrum is given by  $\Delta(\epsilon)$ , where  $\epsilon$  is the energy. The addition energies are given by  $\mu < \mu_w$  and  $\mu > \mu_w$ , where  $\mu$  is the chemical potential and  $\mu_w$  is the chemical potential of the walls.

$\Delta(\nu, \nu) = \Delta(\nu, \nu) \quad (1)$

$$\Delta(\nu, \nu) = \Delta(\nu, \nu) \quad (2)$$

$\Delta(\nu, \nu) = \Delta(\nu, \nu)$

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**V. SUMMARY**

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