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The Dependence of Electronic Structure and Optical Absorption Coefficient on the Size and Mass of the Wurtzite ZnS Quantum Dot

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Abstract—The density functional theory is used to analyze the electronic band structures of various atoms and molecules. The effect of quantum confinement on the electronic and exciton band structures is taken into account, which optical properties are insensitive to light polarization. The effective mass approximation, the valance band degeneracy, and the reduced effective mass in the parallel and perpendicular directions of the electrons and holes are also taken into account. The dispersion relation, quantum confinement effects, joint density of states, refractive index, and absorption coefficient are calculated and discussed, which gives good agreement with the theoretical calculations and experimental measurements.

Keywords: quantum dot, effective mass, quantum confinement, optical absorption

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INTRODUCTION

The potential energy of an electron in a crystal is known to be periodic in space, but the most important is the energy spectrum, which is divided into allowed and forbidden energy bands. For allowed bands, the energy spectrum is determined by the dependence of energy on the quasi-momentum, $E(p)$. A certain number of allowed bands with the lowest energy are completely filled with electrons in insulators and semiconductors at zero temperature (according to the Pauli principle), while bands with a higher energy are empty. In the case of semiconductors, the energy band gap varies from zero (the so-called gapless semiconductor, such as HgTe) to 3 eV. The number of free carriers (electrons in the conduction band or holes in the valence band), which is an important property of semiconductors, is always small compared to the number of atoms. Carriers are formed either by doping or by thermal excitation, in which the number of electrons is equal to the number of holes. In the case when the carrier concentration never exceeds 10^{20} cm^{-3}, the number of states per 1 cm^{-3} in this band is about 10^{22}, i.e., typical electrons occupy only a very small fraction of the valence band. In the center of the Brillouin zone ($p = 0$, as in the case of GaAs) and for a small momentum p, the function $E(p)$ should be parabolic.

The electronic bands of semiconductors (wurtzite type) near the center of the Brillouin zone (in the directions parallel and perpendicular to the c*-axis of the reciprocal space) are defined as [1]:

$$E_e = E_g + \frac{\hbar^2 k^2}{2m_e^*}, \tag{1}$$

$$E_A(\mathrm{HH}) = -\frac{\hbar^2 k^2}{2m_{\mathrm{HH}}^*}, \tag{2}$$

$$E_B(\mathrm{LH}) = -\frac{\hbar^2 k^2}{2m_{\mathrm{LH}}^*} - \Delta_{\mathrm{CF}}, \tag{3}$$

$$E_C(\mathrm{SO}) = -\frac{\hbar^2 k^2}{2m_{\mathrm{SO}}^*} - \Delta_{\mathrm{CF}} - \Delta_{\mathrm{SO}}, \tag{4}$$

because the valence bands are split into three subbands in the center of the Brillouin zone due to the Δ_{CF} crystal field and Δ_{SO} spin orbit interaction. The effective mass may be anisotropic, i.e., have different values for different directions in the crystal, m_e^* is the electron effective mass, and m_{HH}^*, m_{LH}^*, m_{SO}^* are the hole effective masses (heavy-hole (HH), light-hole (LH), and split-off (SO) bands). From the above equations we obtain the general expression for the effective mass [1]:

$$m^* = \hbar^2 \left(\frac{d^2 E(k)}{dk^2} \right)^{-1}. \tag{5}$$

EFFECTIVE MASS APPROXIMATION

Using the principles of quantum mechanics for a particle in a potential box and the effective masses of electron and holes in terms of kinetic energy, by means of effective mass approximation we can calculate the energy band gap depending on the size of the quantum dot [2]. The effective mass approximation is a single-