COMPUTATIONAL AND THEORETICAL STUDIES ON ZnS_xSe_{1-x} $(0 \leq x \leq 1)$

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ABSTRACT

The aim of this work is to study a theory of the energy band gap of ZnS_xSe_{1-x} ($0 \leq x \leq 1$) materials, and to obtain the density of states (DOS) in a quantizing magnetic field. From $\vec{k}.\vec{p}$ perturbation theory, momentum matrix elements and energy eigenvalue of the Zn-S-Se alloy are derived. An empirical relationship $\frac{\mu^*}{m_c} = \left(0.124Eg_0\right)^{1.76}$ *where* $(\mu^*)^{-1}=(m_c)^{-1}+(m_v)^{-1}$, *and* m_c, m_v *are the electron and hole rest masses respectively, is incorporated in the derivation of the energy gap equation*

$$Eg = Eg_0 + \frac{2\hbar^2\pi^2}{m_c D^2\left(\left(0.124Eg_0\right)^{1.76}\right)}$$

The $\vec{k}.\vec{p}$ *perturbation theory is also extended to include the spin-orbit interaction leading to a different expression for the energy gap*

$$Eg = Eg_0 + \frac{2\hbar^2\pi^2}{D^2\left(\left(0.124Eg_0\right)^{1.76}\right)m_c}\frac{\left(Eg_0+\Delta\right)}{\left(Eg_0+\frac{2}{3}\Delta\right)}$$

Third, the density of states (DOS) for ZnS_xSe_{1-x} in a quantizing magnetic field has been determined by the E-k relation. The energy gap calculated from CASTEP is considered the unperturbed energy gap, Eg_0. The actual energy Eg is related to Eg_0 and results obtained are in reasonable agreement with published results obtained from literature. Energy gap with spin-orbit interaction is higher than the values calculated using energy gap equation without spin.

The DOS $$N(E) = \frac{1}{4\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}\frac{\hbar eB}{m_c}\left[E - \left(\left(0.124Eg_0\right)^{1.76}\right)\frac{\left(l+(1/2)\right)\hbar eB}{\mu^*}\right]^{1/2}$$

is shown to depend on the electron energy and the magnetic field. Fermi level is modified by the magnetic field.

ABSTRAK

Tujuan kerja ini adalah untuk membangunkan teori jurang jalur tenaga bahan-bahan ZnS_xSe_{1-x} *(*$o \le x \le 1$*), dan untuk mendapatkan ketumpatan keadaan (DOS) dalam medan magnet pengkuantuman. Menurut teori pertubasi* $\vec{k}.\vec{p}$*, matriks momentum unsur-unsur dan nilai tenaga eigen aloi Zn-S-Se diperolehi. Hubungan empirikal di mana* $(\mu^*)^{-1} = (mc)^{-1} + (mv)^{-1}$*, dengan* m_c *dan* m_v *masing-masing adalah jisim elektron dan jisim lohong dimuatkan dalam menerbitkan persamaan jurang tenaga.*

$$Eg = Eg_0 + \frac{2\hbar^2\pi^2}{m_c D^2\left(\left(0.124Eg_0\right)^{1.76}\right)}$$

Teori pertubasi $\vec{k}.\vec{p}$ *juga diperluaskan kepada interaksi spin-orbit yang membawa kepada ungkapan yang berlainan bagi persamaan jurang tenaga*

$$Eg = Eg_0 + \frac{2\hbar^2\pi^2}{D^2\left(\left(0.124Eg_0\right)^{1.76}\right)m_c}\frac{\left(Eg_0+\Delta\right)}{\left(Eg_0+\frac{2}{3}\Delta\right)}$$

Ketiga, ketumpatan keadaan (DOS) untuk ZnS_xSe_{1-x} *dalam medan magnet pengkuantuman telah ditentukan oleh hubungan E-k. Jurang tenaga yang ditaksir dari CASTEP dianggap jurang tenaga tidak terusik,* Eg_0*. Tenaga jalur tidak terusik adalah berkaitan dengan* Eg_0 *dan keputusan yang diperolehi adalah munasabah dengan hasil yang telah diterbitkan dalam jurnal. Jurang tenaga dengan interaksi spin-orbit adalah lebih tinggi daripada nilai-nilai dikira menggunakan persamaan jurang tenaga tanpa spin-orbit.*

DOS

$$N(E) = \frac{1}{4\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}\frac{\hbar eB}{m_c}\left[E - \left(\left(0.124Eg_0\right)^{1.76}\right)\frac{\left(l+(1/2)\right)\hbar eB}{\mu^*}\right]^{1/2}$$

ditunjukkan bergantung kepada tenaga elektron dan medan magnet. Aras Fermi diubahsuai oleh medan magnet.

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CONTENTS

LIST OF FIGURES

LIST OF TABLES