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A Study of F-center in the Ionic Crystal by Using The Quantum Dot Model Potential

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Abstract

This work presents a study of the electronic structure of F-center in the crystal of NaCl, CsCl and fluorite structure by using quantum dot model potential. This model employs the semi-continuum method due to Simpson and specifies the F-center as a quantum dot partially confined within finite potential. The energy levels and transition energy of the F-center are calculated analytically by using this new model potential and including the effect of continuum medium due to the coulomb tail and using the strong perturbation approach.

Keyword: F-Center, Color center, strong perturbation method, quantum dot

الخلاصة

يقدم هذا العمل دراسه التركيب الالكتروني للمراكز اللونية F−center في البلورات ذات تركيب NaCl, CsCl و الفلورايت باستخدام نموذج جهد النقطه الكميه . يستخدم هذا النموذج طريقة شبه الاستمراريه لسمبسون(Simpson) ويصف المراكزاللونية F−center كنقطه كميه محصورة بجهد محدد . مستويات الطاقه وطاقات الانتقال للمراكز اللونية F−center تحسب تحليليا باستخدام نموذج الجهد الجديد ويتم تضمين تاثير استمراريه الوسط من خلال ذيل كولومي واستخدام تقريب التصحيح القوي .

الكلمات المفتاحية: المركز اللوني، تقريب التصحيح القوي ، النقطة الكمية.

Introduction

The Importance of the color center studies stems from its ability to modify the optical and electrical properties of a material. Which result in new energy levels in the energy gap of that material. These levels are distinguished as the original levels of material.

The theoretical study of the color center usually consist of three parts. The structure of the defect and crystal, the model potential that approximate this structure. Besides the method of calculation. There are many models potential used to study different types of the color center. [Gourary (1957)] employed the PI model potential in the NaCl crystal structure .and utilized the vibrational method. [Bartram (1968)] devised modified PI called (BSG model potential) which exploits the PI models and pseudo potential method. In references [Matthe (1971), Kassim (1985), Kassim (1986), and Ya′koob (2009)] modified uses BSG model and a modified ion size effect. [Gash (2010)] using the norm conserving method and calculated the ion size coefficient. DFT are also used by many researcher to study this defect [Shi (2011), Qing, (2013) and Hepp (2014)]

In this work we will use a quantum dot model potential to specify the electronic structure for the F-center .and the strong perturbation method [Jiang (1987)] to compute the energy levels and wave function. This method proves useful and produces a good result [Uoda (2012) and Kassim (2007)]

Theory

Modal potential

According to the semi-continuum method by Simpson the confining potential of the F-center may be written as:

$$V(r) = \begin{cases} V_0 & if\ r < a \\ -\frac{2m}{r} & if\ r \geq a \end{cases} \qquad \dots\ (1)$$

Where

$$V_0 = -\frac{\alpha_m}{a} + \frac{1}{2a}(1 - \frac{1}{\epsilon}) \qquad \dots (2)$$

And

$$m = \frac{Z}{\epsilon} \qquad \dots (3)$$

Where a is the nearest neighbor and α_m is the Madelung constant. ϵ is the optical dielectric constant .

According to the potential form that is satisfied in equation (1) we can divide the potential into two parts the first is the square-like- potential which takes the form:

$$V_s(r) = \begin{cases} V_0 & if\ r < a \\ 0 & if\ r \geq a \end{cases} \qquad \dots (4)$$

And the second is the effect of the continuum medium as the Coulombian tail potential which take the form:

$$V_C(r) = \begin{cases} 0 & if\ r < a \\ -\frac{2m}{r} & if\ r \geq a \end{cases} \qquad \dots (5)$$

The first term can be solved directly while and for the second term we will employ the strong perturbation approach to solve it.

The square –well-like potential:

By using equation (4) the Schrödinger equation will take the form.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(r)\right]\psi(r,\vartheta,\varphi) = E\psi(r,\vartheta,\varphi) \qquad \dots (6)$$

Because the spherical symmetry of the potential the wave function $\psi(r,\vartheta,\varphi)$ can be written as:

$$\psi(r,\vartheta,\varphi) = \phi_{n,l}(r)Y_l^m(\vartheta,\varphi) \qquad \dots (7)$$

Where $\phi_{n,l}(r)$ is the radial part and $Y_l^m(\vartheta,\varphi)$is the angular part .As a result, the radial part of the Schrödinger equation will be:

$$\left[-\nabla_r^2 - \frac{l(l+1)}{r^2} + V_s(r)\right]\phi_{n,l}(r) = E_{nl}\phi_{n,l}(r) \qquad \dots (8)$$

The solution of this equation may be written as

$$\phi_{n,l}(r) = \begin{cases} Aj_l(k_{nl}r) & r<a \\ Bh_l^{(1)}(i\beta_{nl}r) & r>a \end{cases} \qquad \dots (9)$$

Where$j_l(k_{nl}r)$ is the spherical Bessel function and$h_l^{(1)}(i\beta_{nl}r)$ is the first type spherical Henkel function and k_{nl}, β_{nl} is the roots of the Bessel and Henkel function respectively given by:

$$k_{nl} = \sqrt{E_{nl} - V_0} \qquad \ldots(11)$$

$$\beta_{nl} = \sqrt{-E_{nl}} \qquad \ldots(12)$$

The wave function $\psi(r, \vartheta, \varphi)$ subject to continuity the continuum condition will take the form:

$$\psi_{nlm}(r, \vartheta, \varphi) = AY_{lm}(\vartheta, \varphi)\begin{cases} j_l(k_{nl}r) & if\ r \le a \\ \frac{j_l(k_{nl}a)}{h_l^{(1)}(i\beta_{nl}a)} h_l^{(1)}(i\beta_{nl}r) & if\ r > a \end{cases} \qquad \ldots(13)$$

Where A is the normalization constant and given in form:

$$|A|^2 = \int_0^a j_l^2\,(k_{nl}r)r^2dr + \left|\frac{j_l(k_{nl}a)}{h_l^{(1)}(i\beta_{nl}a)}\right|^2 \int_a^\infty \left|h_l^{(1)}(\beta_{nl}r)\right|^2 r^2dr \qquad \ldots(14)$$

The energy states will be calculated from numerical solution for following equation:

$$ik_{nl}h_l^{(1)}(i\beta_{nl}a)\mathrm{j}_{l-1}(k_{nl}a) + \beta_{nl}h_{l-1}^{(1)}(i\beta_{nl}a)\mathrm{j}_l(k_{nl}a) = 0 \qquad \ldots(15)$$

Table (1) the Energy Levels and Transition Energies (ΔE) of the F-Center in Crystal of NaCl Structure, were Calculated By Using the Simpson Semicontinuum Approach (with no coulombic tail). All Energies are in Ry Unit.

crystal	$-E_{1s}$	$-E_{2p}$	ΔE
LiF	0.404736	0.0548	0.349936
LiCl	0.337183	0.0998	0.237383
LiBr	0.318295	0.1064	0.211895
Lil	0.296156	0.1130	0.183156
NaF	0.394889	0.1070	0.287889
NaCl	0.333957	0.1269	0.207057
NaBr	0.316282	0.1290	0.187282
Nal	0.294479	0.1312	0.163279
KF	0.362955	0.1340	0.228955
KCl	0.319171	0.1454	0.173771
KBr	0.305228	0.1452	0.160028
KI	0.298889	0.1447	0.154189
RbF	0.349596	0.1395	0.210096
RbCl	0.310974	0.1497	0.161274
RbBr	0.280220	0.1335	0.146720
Rbl	0.278400	0.1456	0.132800

Table (2) the Energy Eevals and Transition Energy (ΔE) of the F-Center in Crystal of CsCl Structure, were Calculated By Using the Simpson Semicontinuum Approach (with no coulombic tail).. All Energies are in Ry Unit.

crystal	$-E_{1s}$	$-E_{2p}$	ΔE
CsCl	0.289202	0.136891	0.152311
CsBr	0.279091	0.138525	0.140566
Csl	0.264562	0.140184	0.124378

Table (3) the Energy Levals and Transition Energies (ΔE) of the F-Center in Crystal with Fluorite Structure, were Calculated By Using the Simpson Semicontinuum Approach (with no Coulombic tail).

crystal	$-E_{1s}$	$-E_{2p}$	ΔE
CaF_2	0.380520	0.103817	0.276703
SrF_2	0.369916	0.117825	0.252091
BaF_2	0.353798	0.127624	0.226174
PbF_2	0.336177	0.098360	0.237817
$SrCl_2$	0.317701	0.133072	0.184629
$BaCl_2$	0.303802	0.134608	0.169194

Table (4) Comparison of the F-center Transition Energies in Crystal with NaCl Structure with Experimental Values and Other Workers. All Energies in (eV) Unit.

crystal	ΔE(Present)	ΔE[Yakoob(2009)]	ΔE(exp.)
LiF	4.759	3.945	5.14
LiCl	3.228	3.234	3.304
LiBr	2.881	2.265	2.706
Lil	2.490	2.334	3.264
NaF	3.915	3.221	3.726
NaCl	2.815	2.559	2.774
NaBr	2.547	1.936	2.353
Nal	2.220	1.881	……
KF	3.113	2.476	2.802
KCl	2.363	2.428	2.339
KBr	2.176	1.942	2.081
KI	2.096	1.622	1.877
RbF	2.857	2.370	2.434
RbCl	2.193	2.271	2.026
RbBr	1.995	1.833	1.849
Rbl	1.806	1.519	1.713

Table (5) Comparison of the F-center Transition Energies in Crystal of CsCl Structure with Experimental Values and Other Workers. All Energies in (eV) Unit.

crystal	ΔE(Present)	ΔE[Yakoob(2009)]	ΔE(exp.)
CsCl	2.071	1.62	2.18
CsBr	1.911	1.52	1.94
Csl	1.691	1.37	1.68

Table (6) Comparison of the F-Center Transition Energies in Crystal of Fluorite Structure with Experimental Values and Other Workers.

crystal	ΔE(Present)	ΔE[H.S.Bennett(19	ΔE(exp.)
CaF_2	3.763	3.19	3.30
SrF_2	3.428	2.91	2.85
BaF_2	3.075	2.61	2.03
PbF_2	3.234	…	…
$SrCl_2$	2.510	…	…
$BaCl_2$	2.301	…	…

The effect of the Coulomb tail:

By using equation (5) the resulting nonlinear equation in strong perturbation theory takes the form:

$$|\nabla g|^2 - \nabla^2 g = \left.\frac{2m}{r}\right|_{r>a} \qquad \ldots(16)$$

Subjected to the boundary conditions imposed on (g): $g \to 0$ and $\nabla g \to 0$ when $r \to a$ or $Z \to 0$.which yields solution:

$$g = \frac{mr}{n'} \qquad \ldots(17)$$

Where n'=n+*l* and the Schrödinger equation will be reduced to the form:

$$f(h_0 + h')\psi_{nlm} = E_{nl} f \psi_{nlm} \qquad \ldots(18)$$

Where

$$f = e^{-g} \qquad \ldots(19)$$

$$h_0 = H_0 \qquad \ldots(20)$$

And

$$h' = \frac{2m}{n'}\frac{\partial}{\partial r} - \frac{2m}{r}\left(1 - \frac{1}{n'}\right) - \frac{m^2}{n'^2} \qquad \ldots(21)$$

The energy is corrected to the first order is given by:

$$E_{nl} = E_{nl}^{(0)} + E_{nl}^{(1)} \quad \text{… (22)}$$

Where $E_{nl}^{(0)}$is the zero order energy and it can be calculated from this equation:

$$E_{nl}^{(0)} = \langle \psi_{nlm} | h_0 | \psi_{nlm} \rangle = -\beta_{nl}^2 \quad \text{…(23)}$$

And $E_{nl}^{(1)}$ is the first order correction in energy (notice that $E_{nl}^{(1)}$ is not identical with that of the ordinary perturbation theory) which is given by:

$$E_{nl}^{(1)} = N^2 \int f^2 \psi_{nlm}^{*} (h' \psi_{nlm}) d\tau \quad \text{… (24)}$$

Where N is the normalization constant which may be computed from the following equation:

$$|N|^{-2} = \int f^2 |\psi_{nlm}|^2 d\tau \quad \text{… (25)}$$

Ground state

For the ground state (n'=1and *l*=0), the wavefunction (see equation (13)) will take the form:

$$\psi_{1s}(r, \vartheta, \varphi) = A Y_0^0(\vartheta, \varphi) \begin{cases} j_0(k_{10} r) & if\ r \le a \\ \frac{j_0(k_{10} a)}{h_0^{(1)}(i\beta_{10} a)} h_0^{(1)}(i\beta_{10} r) & if\ r > a \end{cases} \quad \text{… (26)}$$

Where

$$|A|^2 = \int_0^a j_0^2\,(k_{10} r) r^2 dr + \left| \frac{j_0(k_{10} a)}{h_0^{(1)}(i\beta_{10} a)} \right|^2 \int_a^{\infty} \left| h_0^{(1)}(\beta_{10} r) \right|^2 r^2 dr \quad \text{... (27)}$$

The substitution of the quantum number (n',l)in equation (21) yield :

$$h' = 2m \frac{\partial}{\partial r} - m^2 \quad \text{... (28)}$$

and by substituting equations (28)and (26) in equation (24) we obtain :

$$E_{1s}^{(1)} = N_{1s}^2 A^2 \left| \frac{j_0(k_{10} a)}{h_0^{(1)}(i\beta_{10} a)} \right|^2 \int_a^{\infty} h_0^{*(1)}(i\beta_{10} r) \left(2m \frac{\partial}{\partial r} - m^2 \right) h_0^{(1)}(i\beta_{10} r) r^2 e^{-2mr}\, dr \quad \text{…(29)}$$

Introducing the quantities I$_1$ and I$_2$ we get:

$$E_{1s}^{(1)} = N_{1s}^2 [2m I_1 - m^2 I_2] \quad \text{… (30)}$$

Substituting equation (26) in equation (25) will give:

$$N_{1s}^{-2} = A^2 \left[\int_0^a j_0^2\,(k_{10} r) r^2 dr \; + \; \left| \frac{j_0(k_{10} a)}{h_0^{(1)}(i\beta_{10} a)} \right|^2 \int_a^{\infty} \left| h_0^{(1)}(i\beta_{10} r) \right|^2 e^{-2mr}\, r^2 dr \right] \quad \text{…(31)}$$

$$N_{1s}^{-2} = J_1 + J_2 \quad \text{…(32)}$$

Using the following identity:

$$E_1(x) = \int_x^{\infty} \frac{e^{-\theta}}{\theta} d\theta = -\gamma - \ln x - \sum_{n=1}^{\infty} \frac{(-1)^n}{n\, n!}\, x^n \qquad \ldots (33)$$

We get:

$$I_1 = -\frac{D_0^2}{\beta_{10}^2} A^2 \left[\frac{\beta_{10}}{2(m+\beta_{10})} e^{-2(m+\beta_{10})a} + \mathrm{E}_1(2(m+\beta_{10})a)\right] \qquad \ldots(34)$$

$$I_2 = \frac{D_0^2 A^2}{2\beta_{10}^2(m+\beta_{10})} e^{-2(m+\beta_{10})a} \qquad \ldots(35)$$

$$J_1 = A^2 \int_0^a j_0^2\,(k_{10}r) r^2 dr \qquad \ldots(36)$$

and ;

$$J_2 = \frac{A^2 D_0^2}{2\beta_{10}^2(m+\beta_{10})} e^{-2(m+\beta_{10})a} \qquad \ldots(37)$$

Where

$$D_0^2 = \frac{\beta_{10}^2 \sin^2(x_{10})}{k_{10}^2} e^{2(\beta_{10})a} \qquad \ldots(38)$$

We can rewrite equations (30) and (32) in a more simplified form as:

$$E_{1s}^{(1)} = N_{1s}^2 A^2 \left[-2m\left(\frac{\beta_{10}\sin^2(x_{10})}{2k_{10}^2(1+\beta_{10})} e^{-2\mathrm{m}a} + \frac{\sin^2(x_{10})}{2k_{10}^2} e^{2a\beta_{10}}\, \mathrm{E}_1(2(m+\beta_{10})a)\right) \ldots \right.$$
$$\left. -m^2 \frac{\sin^2(x_{10})}{2k_{10}^2(1+\beta_{10})} e^{-2ma}\right] \qquad \ldots(39)$$

$$N_{1s}^{-2} = A^2 \left[\frac{1}{{k_{10}}^3} \int_0^{x_{10}} j_0(\rho)^2 \rho^2 e^{\frac{-2\rho}{k_{10}}}\, d\rho + \frac{\sin^2(x_{10})}{2k_{10}^2(1+\beta_{10})} e^{-2ma}\right] \qquad \ldots \qquad (40)$$

where

$$\rho = k_{10} r \qquad \ldots (41)$$

and x_{nl} are the roots of the Bessel function $x_{nl} = ak_{nl}$.

The total energy will be:

$$E_{1s} = -\beta_{10}^2 + E_{1s}^{(1)} \qquad \ldots(42)$$

First exited state

By following steps similar to those for the first exited state (n'=2and *l*=1), the wavefunction from equation (13) will take the form:

$$\psi_{2p}(r,\vartheta,\varphi) = AY_1^{0,\mp 1}(\vartheta,\varphi) \begin{cases} j_1(k_{11}r) & if\ r \leq a \\ \frac{j_1(k_{11}a)}{h_1^{(1)}(i\beta_{11}a)} h_1^{(1)}(i\beta_{11}r) & if\ r > a \end{cases}$$
… (43)

Where

$$|A|^2 = \int_0^a j_1^2\,(k_{11}r) r^2 dr + \left|\frac{j_1(k_{11}a)}{h_1^{(1)}(i\beta_{11}a)}\right|^2 \int_a^{\infty} \left|h_1^{(1)}(\beta_{11}r)\right|^2 r^2 dr \qquad \ldots (44)$$

Substituting the quantum number (n',l)in equation (21) we get :

$$h' = m\left(\frac{\partial}{\partial r} - \frac{1}{r}\right) - \frac{m^2}{4} \quad \text{... (45)}$$

By substituting equations (43) and (45) in equation (24) we get:

$$E_{2p}^{(1)} =$$

$$N_{2p}^2 A^2 \left|\frac{j_1(k_{11}a)}{h_1^{(1)}(i\beta_{11}a)}\right|^2 \int_a^\infty h_1^{*(1)}(i\beta_{11}r)\left[\left(m\left(\frac{\partial}{\partial r} - \frac{1}{r}\right) - \frac{m^2}{4}\right) h_1^{(1)}(i\beta_{11}r)\right] r^2 e^{-mr}\, d\backslash$$

$$\text{...(46)}$$

$$E_{2p}^{(1)} = N_{1s}^2\left[mI_1 - \frac{m^2}{4}I_2\right] \quad \text{...(47)}$$

By substituting equation (43) in equation (25),N$_{2p}$ will take the form :

$$N_{2p}^{-2} = A^2\left[\int_0^a j_1^2\,(k_{11}r)r^2dr + \left|\frac{j_1(k_{11}a)}{h_1^{(1)}(i\beta_{11}a)}\right|^2 \int_a^\infty \left|h_1^{(1)}(i\beta_{11}r)\right|^2 e^{-rm}\, r^2 dr\right] \quad \text{...(48)}$$

The above result can be writing in terms of two integrals J$_1$ and J$_2$ given:

$$N_{1s}^{-2} = J_1 + J_2 \quad \text{...(49)}$$

And by using the identity (33)

$$E_n(x) = \int_x^\infty \frac{e^{-tx}}{t^n}\,dt \quad \text{... (50)}$$

$$E_{n+1}(x) = \frac{1}{n}e^{-x} - \frac{x}{n}E_n(x) \quad \text{... (51)}$$

We get:

$$I_1 = \frac{-D_1^2}{\beta_{11}^2}A^2\left[\frac{\beta_{11}}{(m+2\beta_{11})}e^{-(m+2\beta_{11})a} + 4\mathrm{E}_1\big((m+2\beta_{11})a\big)\right.$$

$$\left. + \frac{6}{\beta_{11}\mathrm{a}}\mathrm{E}_1\big((m+2\beta_{11})a\big) + \frac{3}{(\beta_{11}\mathrm{a})^2}\mathrm{E}_3\big((m+2\beta_{11})a\big)\right] \quad \text{...(52)}$$

$$I_2 =$$

$$\frac{D_1^2}{\beta_{11}^3}A^2\left[\frac{\beta_{11}}{(m+2\beta_{11})}e^{-(m+2\beta_{11})a} + 2\mathrm{E}_1\big((m+2\beta_{11})a\big) + \right.$$

$$\left.\frac{1}{\beta_{11}\mathrm{a}}\mathrm{E}_1\big((m+2\beta_{11})a\big)\right] \quad \text{...(53)}$$

$$J_1 = A^2\int_0^a j_1^2\,(k_{11}r)r^2dr \quad \text{...(54)}$$

$$J_2 = \frac{D_1^2}{\beta_{11}^3}A^2\left[\frac{\beta_{11}}{(m+2\beta_{11})}e^{-(m+2\beta_{11})a} + 2\mathrm{E}_1\big((m+2\beta_{11})a\big) + \frac{1}{\beta_{11}\mathrm{a}}\mathrm{E}_1\big((m+2\beta_{11})a\big)\right] \quad \text{...(55)}$$

$$D_1^2 = \left|\frac{j_1(k_{11}a)}{h_1^{(1)}(i\beta_{11}a)}\right|^2 \quad \text{...(56)}$$

We can rewrite equations (47) and (49) in the following form:

$$E_{2p}^{(1)} = N_{2p}^{2}A^{2}\left[\frac{-m}{\beta_{11}^{2}}\,D_{1}^{2}\,\left(\frac{\beta_{11}}{(2\beta_{11}+m)}e^{-(2\beta_{11}+m)a} + 4\mathrm{E}_{1}\big((2\beta_{11}+m)a\big)\right.\right.$$

$$\left.+\frac{6}{\beta_{11}a}\mathrm{E}_{2}\big((2\beta_{11}+m)a\big)+\frac{3}{(\beta_{12}a)^{2}}\mathrm{E}_{3}\big((2\beta_{12}+m)a\big)\right)$$

$$-\frac{m^{2}}{4}\frac{D_{1}^{2}}{\beta_{11}^{3}}A^{2}\left[\frac{\beta_{11}}{(m+2\beta_{11})}e^{-(m+2\beta_{11})a} + 2\mathrm{E}_{1}\big((m+2\beta_{11})a\big)\right.$$

$$\left.\left.+\frac{1}{\beta_{11}\mathrm{a}}\mathrm{E}_{1}\big((m+2\beta_{11})a\big)\right]\right. \qquad \dots (57)$$

$$N_{2p}^{-2} = A^{2}\left[\frac{1}{{k_{11}}^{3}}\int_{0}^{x_{11}} j_{1}(\rho)^{2}\rho^{2}\,d\rho+\frac{1}{\beta_{11}^{3}}\,D_{1}^{2} \,*\right.$$

$$\left.\left(\frac{\beta_{11}}{(2\beta_{11}+m)}e^{-(2\beta_{11}+m)a}+2\mathrm{E}_{1}\big((2\beta_{11}+m)a\big)+\frac{1}{\beta_{11}a}\mathrm{E}_{2}\big((2\beta_{11}+\ m)a\big)\right)\right]$$

$$\dots (58)$$

And the total energy will be:

$$E_{2p} = -\beta_{11}^{2} + E_{2p}^{(1)} \qquad \dots (59)$$

These are our final analytical results

Table (7) the Effect of Colombian Tail Potential on Energy State and Transition Energies (ΔE) of the F-Center in Crystal with NaCl Structure, were Calculated By Using the Strong Perturbation Approach. All Energies are in Ry Unit

crystal	$-E_{1s}^{(1)}$	$-E_{2p}^{(1)}$	$(\Delta E)^{1}$
LiF	0.051685	0.108934	0.057249
LiCl	0.025431	0.048055	0.022624
LiBr	0.020156	0.036775	0.016619
Lil	0.014857	0.025942	0.011085
NaF	0.042891	0.089678	0.046787
NaCl	0.024331	0.047037	0.022706
NaBr	0.020085	0.037754	0.017669
Nal	0.015461	0.028019	0.012558
KF	0.031632	0.064395	0.032763
KCl	0.020826	0.040523	0.019697
KBr	0.017998	0.034334	0.016336
KI	0.014576	0.027061	0.012485
RbF	0.02795	0.056198	0.028248
RbCl	0.019166	0.037225	0.018059
RbBr	0.012901	0.022888	0.009987
Rbl	0.013279	0.024467	0.011188

Table (8) the Energy State and Transition Energies (ΔE) of the F-Center in Crystal with NaCl Structure, were Calculated By Using the Simpson Semicontinuum Approach and Strong Perturbation Approach. All Energies in Ry Unit

crystal	E_{1s}	E_{2p}	$(\Delta E)^1$
LiF	0.456674	0.163843	0.292831
LiCl	0.362819	0.147919	0.214900
LiBr	0.338644	0.143265	0.195379
Lil	0.311192	0.139054	0.172138
NaF	0.438006	0.196823	0.241183
NaCl	0.358478	0.174025	0.184453
NaBr	0.336548	0.166832	0.169716
Nal	0.310109	0.159355	0.150754
KF	0.394787	0.198558	0.196229
KCl	0.340170	0.186073	0.154097
KBr	0.323391	0.179630	0.143761
KI	0.301289	0.171854	0.129435
RbF	0.377737	0.195790	0.181947
RbCl	0.330306	0.187045	0.143261
RbBr	0.293288	0.156488	0.136800
Rbl	0.291829	0.170158	0.121671

Table (9) the Effect of Colombian Tail Potential on Energy State and Transition Energies (ΔE) of the F-Center in Crystal with CsCl Structure, were Calculated By Using the Strong Perturbation Approach. All Energies in Ry Unit

crystal	$-E_{1s}^{(1)}$	$-E_{2p}^{(1)}$	$(\Delta E)^1$
CsCl	0.014207	0.026328	0.012121
CsBr	0.012612	0.023055	0.010443
Csl	0.01053	0.018864	0.008334

Table (10) the Energy State and Transition Energies (ΔE) of the F-Center in Crystal with CsCl Structure, were Calculated By Using the Simpson Semicontinuum Approach and Strong Perturbation Approach. All Energies in Ry Unit

crystal	E_{1s}	E_{2p}	ΔE
CsCl	0.303409	0.175676	0.127733
CsBr	0.291703	0.171956	0.119747
Csl	0.275092	0.16658	0.108512

Table (11) the Effect of Colombian Tail Potential on Energy State and Transition Energies (ΔE) of the F-Center in Crystal with CaF_2 Structure , were Calculated By Using the Strong Perturbation Approach. All Energies in Ry Unit

crystal	$-E_{1s}^{(1)}$	$-E_{2p}^{(1)}$	$(\Delta E)^1$
CaF_2	0.037023	0.074776	0.037753
SrF_2	0.032708	0.065375	0.032667
BaF_2	0.027905	0.054842	0.026937
PbF_2	0.023241	0.042904	0.019663
$SrCl_2$	0.019111	0.035584	0.016473
$BaCl_2$	0.016218	0.029527	0.013309

Table (12) the Energy State and Transition Energies (ΔE) of the F-Center in Crystal with Fluorite Structure, were Calculated By Using the Simpson Semi Continuum Approach and Strong Perturbation Approach. All Energies in Ry Unit

crystal	E_{1s}	E_{2p}	ΔE
CaF_2	0.418836	0.178805	0.240031
SrF_2	0.402624	0.183221	0.219403
BaF_2	0.381703	0.182487	0.199216
PbF_2	0.359418	0.141285	0.218133
$SrCl_2$	0.336812	0.168675	0.168137
$BaCl_2$	0.32002	0.164153	0.155867

Table (13) Comparison of the F-Center Transition Energies in Crystal with NaCl Structure with Experimental Value and Results of Other Workers ΔE in the Present Calculation Includes Coulomb Tail Correction :

crystal	Present	ΔE[Yakoob(2009)]	ΔE(exp.)
LiF	3.982502	3.945	5.14
LiCl	2.92264	3.234	3.304
LiBr	2.657154	2.265	2.706
Lil	2.341077	2.334	3.264
NaF	3.280089	3.221	3.726
NaCl	2.508561	2.559	2.774
NaBr	2.308138	1.936	2.353
Nal	2.050254	1.881	……
KF	2.668714	2.476	2.802
KCl	2.095719	2.428	2.339
KBr	1.95515	1.942	2.081
KI	1.760316	1.622	1.877
RbF	2.474479	2.370	2.434
RbCl	1.94835	2.271	2.026
RbBr	1.86048	1.833	1.849
Rbl	1.654726	1.519	1.713

Table (14) Comparison of the F-Center Transition Energies in Crystal with CsCl Structure with Experimental Value and Result of Other Workers:

crystal	Present	ΔE[Yakoob(2009)]	ΔE(exp.)
CsCl	1.74	1.62	2.18
CsBr	1.63	1.52	1.94
Csl	1.48	1.37	1.68

Table (15) Comparison of the F-Center Transition Energies in Crystal with Fluorite Structure with Experimental Value and Result of Other Workers:

crystal	Present	ΔE[H.S.Bennett(19	ΔE(exp.)
CaF_2	3.264422	3.19	3.3
SrF_2	2.983881	2.91	2.85
BaF_2	2.709338	2.61	2.03
PbF_2	2.966609	…	…
$SrCl_2$	2.286663	…	…
$BaCl_2$	2.119791	…	…

Result and discussion

In tables (1) to (6) are listed the energy levels E_{1s} and E_{2p} and the transition energiesΔE. As a general trend, ΔE is governed by the nearest neighbor distance (a), this is in accord with Mellow-Ivey empirical law $\Delta E \sim a^n$ (n~1.8), in the fluorite structure however,the vacancy is doubly charged and accordingly the F-center electron is highly localized within the vacancy .The Mellow-Ivery empirical law still hold with 2p which is more localized as compared with the previous alkali-halides crystals . The short-coming of the square-well model is the ignorance of the detailed ionic arrangement in the vicinity of the defect, but the cancellation hidden in$(\Delta E)^1$ overshadow such effects.

Tables (7) to (12) list the energy levels of E_{1s} , E_{2p} and ΔE with the effect of Coulombic tail estimated by strong perturbation method . $(\Delta E)^1$ including the energy shift due to the Coulomic tail and is governed by three factors :(i) the nearest neighbor distance (ii)ϵ_∞ the optical dielectric constant and (iii)the charge of the vacancy . We notice that $(\Delta E)^1$ is larger in fluorite and chloride crystals as compared with NaCl structure crystals partly because of the vacancy charge and partly because of the different ϵ,but the general trend is in a accord with the Mellow-Ivey relation .

In tables (13) to (15) the comparison that we made between calculated $(\Delta E)$and the experimental values ΔE(exp) is compared with the calculation of other authors .It shows reasonable agreement, this would encourage one to peruse additional calculations to estimate theeffects of other environmental and local interactions.

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