

## Color centers envisioned as confined quantum systems: the case of F, F' and $F_2^+$ centers

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Color centers in alkali halides, as well as point defects with dimensions of a few nanometers, have been considered to be confined systems and were studied with a variational formalism within a semi-continuum model. This new approach was applied to the well-known F, F' and  $F_2^+$  centers, which are assumed to be cavities of a determined shape that can trap one or two electrons. Inside of the cavity, the electron is subject to a constant potential ( $V_0$ ) related to the Madelung energy and outside of it, the potential is Coulomb type due to a continuum polarizable medium. Because the F, F' and  $F_2^+$  confined systems were considered to be hydrogen-like, helium-like and  $H_2^+$ -like molecular ion systems, respectively, the *ansatz* functions were constructed from wave functions corresponding to these kinds of systems. For these systems, the energy transition ( $\Delta E$ ) from the ground state to the first excited state in KCl crystals was calculated and compared with experimental and calculated values obtained from the literature. The  $\Delta E$  behavior is shown for different values of  $V_0$ . It is worth mentioning that the formalism presented in this work would be useful for both graduate and undergraduate students embarking on the study of some properties of confined quantum systems, or some simple nanostructures as well.

*Keywords:* Color centers; semi-continuum model; variational method; confined systems.

Se presenta un estudio con un formalismo variacional dentro del modelo semicontinuo de centros de color en halogenuros alcalinos así como defectos puntuales con dimensiones nanométricas, los cuales fueron considerados como sistemas confinados. Este enfoque fue aplicado para los bien conocidos centros F, F' y  $F_2^+$ , los cuales fueron asumidos como una cavidad de forma específica que puede atrapar uno o dos electrones. Dentro de la cavidad el electrón “siente” un potencial constante  $V_0$  relacionado a la energía de Madelung, mientras que en la región exterior el potencial es de tipo Coulombiano debido al medio continuo polarizable. Las funciones correspondientes a los centros F, F' y  $F_2^+$  fueron construidas tomando en cuenta que estos sistemas fueron considerados como sistemas tipo hidrogenoide, helioide y ion molecular  $H_2^+$ , respectivamente. Así, para estos sistemas se calculó la energía de transición  $\Delta E$  del estado base al primer estado excitado en cristales KCl y se comparó con los valores experimentales, así como los calculados en otros trabajos. Se presenta también el comportamiento de  $\Delta E$  para diferentes valores de  $V_0$ . Es importante mencionar que el formalismo presentado en este trabajo puede ser útil para estudiantes de licenciatura o posgrado que deseen incursionar en el estudio de algunas propiedades de sistemas cuánticos confinados o algunas nanoestructuras sencillas.

*Descriptores:* Centros de color; modelo semicontinuo; método variacional; sistemas confinados.

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### 1. Introduction

In the last few years, the study of confined quantum systems has been one of the more active fields in physics. A great number of papers have been published regarding the so-called nanostructures. This trend could be explained if one considers the promising technological uses shown by these systems. Besides these important possibilities, the simplicity of these systems has made it possible to use them to verify many of the main quantum theoretical results.

Color centers (CC's) have been the object of research since the 40's, in the past century, until now because these defects induce some optical properties in materials that do not show any particular optical features in any other case. Extensive theoretical and experimental studies of CC's induced by radiation were carried out systematically in the 40's, 50's and 60's in the 20th century. Research on ionizing radiation damage has been connected with the purpose of finding mate-

rials and security criteria for storing radioactive wastes [1,2], and lately, in the 70's and 80's, other applications were developed [3,4]. Nowadays, the study of CC's is a timely research topic because of the various relevant roles that these defects have in different applications with new and unusual properties, particularly on a nanoscale dimension [5–7]. As is well known, in alkali halide (HA) crystals the main ionizing radiation effect is the production of Frenkel defects such as F and H centers through a primary process of electronic excitation; depending of radiation, energy and doses, F,  $F_2^+$ ,  $F_2^-$ ,  $F_3^-$  and  $F_3^+$  centers are formed. Laser emission in KCl:Li containing  $F_A$  centers [3] and LiF based on  $F_2^+$  and  $F_2^-$  centers [4] were reported in the 70's, and the research in this field is still a current problem, as shown in recent works about the potential development of lasers of LiF activated by  $F_2$ ,  $F_3^+$  [8,9] and  $F_2^+$  centers stabilized by anion and cation impurities and anion vacancies [10]. At present, the interest in developing miniaturized optical devices has al-

ready prompted research on novel techniques for the creation of low-dimensional structures and point defects ( $F_2$ ,  $F_3$ ,  $F_3^+$ , colloids, tracks) induced by irradiation with high energy particles [11–13]. Techniques such as soft X-rays and extreme UV light microprobes and electron-beam lithography have been used to produce luminescent nanostructures based on  $F_2$  and  $F_3^+$  centers in LiF crystals and films as well as miniaturized active channel waveguides [14–17].  $F_2$  and  $F_3^+$  centers could also be the basis for producing miniaturized build-in laser-active color centers and active waveguides by using a new interfered infrared femtosecond (fs) laser pulse technique in transparent materials such as LiF crystals [18]. A few years ago, the use of single color centers tightly confined was suggested as a possible solid-state structure for information processing and storage and computing applications based in quantum processes [19–21]. In particular, a single nitrogen F center [(nitrogen-vacancy, (NV)) on diamond nanocrystals and heterostructures has been proposed as a ‘qubit’ element [19,20].

As is well known, the F center consists of an electron trapped in an anion vacancy, and several models have been discussed in order to explain the general characteristics of its absorption and emission. In Ref. 22 and references therein, an exhaustive study is presented. Of all these models, the semi-continuum model has been the most successful because of the very good matching between the experimental and theoretical parameters. In this model, the crystal effect outside of the vacancy is considered by the introduction of a potential  $V_0$ , which contains the Madelung energy, the effective mass, the polarization energy and the electron affinity. More recently, the electronic structure of the F center in NaCl crystals was calculated from a NaCl cluster approach [23]. In this model, the clusters are embedded in a point charge field; different NaCl clusters with a  $Cl^-$  ion vacancy are studied using *ab initio* molecular orbital calculations. In the case of F center aggregates, many other theoretical studies using different approaches were conducted in the 50’s and 60’s, but most were a generalization of the F center case [24]. The  $F_2$  and  $F_2^+$  centers have been studied assuming the centers to be hydrogen molecules immersed in a medium of dielectric constant  $\kappa_0$  [25]. Alternatively, Nagamiya and Tatsuuma [26] have developed a model for the  $F_2$  center, as in the semi-continuum model. In this model the  $F_2$  center is considered to be two F centers separated by a potential which contains the interaction energy between the polarized lattice with the positive (vacancies) and negative (trapped electrons) charge, the electron interchange and the electrostatic interaction between vacancies and electrons. On the other hand in the qubit element case, the F center is assumed to be an electric dipole modelled in terms of an isotropic three-dimensional harmonic oscillator embedded in a dielectric. In the present work, a simple variational method within a semi-continuum model has been used to explore the connection between confined quantum systems and F,  $F'$  and  $F_2^+$  centers in alkali halide crystals. In this peculiar quantum system of nanometric dimensions, one or two electrons are trapped and the sur-

rounding material is considered to be a continuum polarizable medium. In doing so, we show that this approach constitutes an interesting alternative in the study of some properties of these kinds of defects, as was shown to be the case of other real systems [27–30].

## 2. Variational formalism to study confined quantum systems

In previous works [31–34], we proposed a simple variational approach to the study of confined quantum systems which is flexible enough to deal with impenetrable or penetrable boundaries as well as one or two electron systems. Since we shall mimic a real system, such as color centers, the most realistic confining boundaries would be the penetrable ones this means, in effective atomic units, the Hamiltonian associated with such a system can be written as:

$$H_i = -\frac{1}{2}\nabla_q^2 + V_i(q), \quad (q \in \Omega_i), \quad (1)$$

$$H_o = -\frac{1}{2}\nabla_q^2 + V_o(q), \quad (q \in \Omega_o), \quad (2)$$

where  $q$  is the set of generalized coordinates that generates the inner ( $\Omega_i$ ) and outer ( $\Omega_o$ ) regions, and  $V_{i(o)}$  is a potential associated with the defect.

According to the variational method, an upper bound to the energy of a particular state of the system may be found by requiring that:

$$\langle \varphi_i | H_i | \varphi_i \rangle_{\Omega_i} + \langle \varphi_o | H_o | \varphi_o \rangle_{\Omega_o} = \text{minimum}, \quad (3)$$

where  $\varphi_i$  ( $\varphi_o$ ) is the inner (outer) *ansatz* wave function.

In addition to Eqs. (1)-(3), we have also that

$$\langle \varphi_i | \varphi_i \rangle_{\Omega_i} + \langle \varphi_o | \varphi_o \rangle_{\Omega_o} = 1, \quad (4)$$

the normalization condition, and

$$\left. \frac{1}{\varphi_i} \frac{\partial \varphi_i}{\partial q} \right|_{q_0} = \left. \frac{1}{\varphi_o} \frac{\partial \varphi_o}{\partial q} \right|_{q_0}, \quad (5)$$

the continuity of the logarithmic derivatives of  $\varphi_i$  and  $\varphi_o$  at the boundary  $q = q_0$ , must be satisfied.

The inner *ansatz* wave function can be constructed as:

$$\varphi_i = \varphi_{0,i} f, \quad (6)$$

where  $\varphi_{0,i}$  is closely related to the wave function of the free system, and  $f$  is an auxiliary function that guarantees an adequate matching at the boundary with the exterior *ansatz* wave function  $\varphi_o$  which keeps the proper asymptotic behavior characteristic of the system under study. Furthermore, the choice of the auxiliary function  $f$ , must be such that it reduces to a cut-off function when the potential becomes infinite. In the latter case,  $f$  is simply the contour of the confining boundary. We shall use these ideas in the following sections to study three realistic systems, namely, the F center (one electron trapped in an anion vacancy), the  $F'$  center (two electrons trapped in an anion vacancy) and the  $F_2^+$  (one electron trapped in two contiguous anion vacancies) in order to explore the reliability of the formalism.

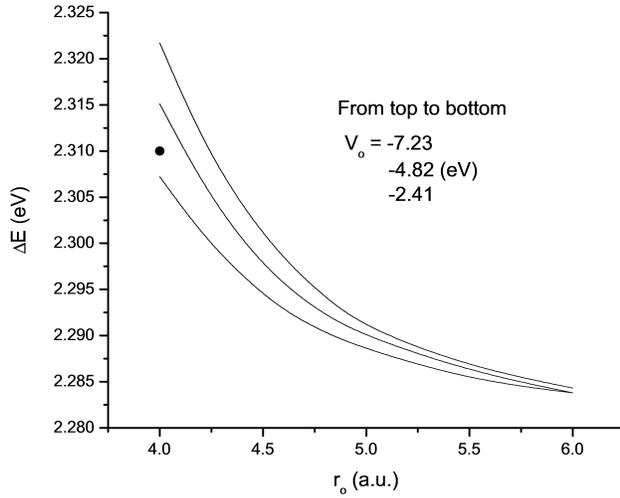


FIGURE 1. Behavior of  $\Delta E = E_{2p} - E_{1s}$  for the F center, as a function of the cavity radius  $r_0$  for various potential well depths. The filled circle represents the experimental value of  $\Delta E$  and the most used value of  $r_0$  for this defect. KCl was used as a generic example.

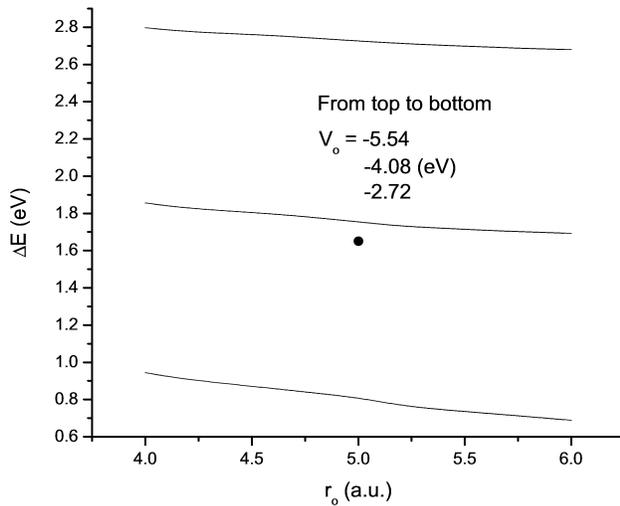


FIGURE 2. Behavior of  $\Delta E = -E_{1s}$  for the F' center, as a function of the cavity radius  $r_0$  for various potential well depths. The filled circle represents the experimentally measured  $\Delta E$  and a typical value of  $r_0$  used in other theoretical calculations for this defect. KCl was used as a generic example.

### 3. Application of formalism to color centers

The simplest defect in alkali halides is the F center, which is an electron trapped in a vacancy left by a missing halogen ion. For purposes of this work, we shall consider that the electron is trapped in a spherical cavity which is surrounded by a continuum polarizable medium that emulates the rest of the crystal in such a way that the potential felt by the electron is of the form:

$$V(r) = \begin{cases} -V_0, & 0 \leq r \leq r_0 \\ -\frac{1}{\kappa_0 r}, & r_0 \leq r < \infty \end{cases}, \quad (7)$$

where  $V_0$  is a constant related to the electrostatic energy needed to bring the electron from infinity and place it at the cavity (Madelung energy),  $r_0$  is the radius of the cavity and  $\kappa_0$  is the high frequency dielectric constant. In this system, the largest absorption band or F band would correspond to a transition from the ground state to the first excited state. Due to the spherical symmetry of the potential, this band would be related, within the present model, to a transition from a  $1s$ -like to a  $2p$ -like hydrogenic state. According to the previous section, the *ansatz* wave functions for these states can be written as:

$$\Psi_{1s}(\mathbf{r}) = \begin{cases} A(r_0 - \gamma r) \exp(-\alpha r), & 0 \leq r < r_0 \\ B \frac{1}{r} \exp(-\beta r), & r_0 < r < \infty \end{cases}, \quad (8)$$

and

$$\Psi_{2p}(\mathbf{r}) = \begin{cases} C(r_0 - \gamma r) r \cos \theta \exp(-\alpha r), & 0 \leq r < r_0 \\ D \frac{\cos \theta}{r} \exp(-\beta r), & r_0 < r < \infty \end{cases}, \quad (9)$$

where  $(A, B, C, D)$  are normalization constants and  $(\alpha, \beta, \gamma)$  variational parameters. With these functions, the energy functional can be constructed for each state, and its minimization gives the values of the variational parameters for which we have an upper bound for the energy. Note that the parameters  $(\alpha, \beta, \gamma)$  are not independent of each other but related through the condition given by Eq. (5), *i.e.* one of them can be expressed as a function of the rest and the minimization only involves two unknown parameters. In Fig. 1 we describe the behavior of the transition energy  $\Delta E_F = E_{2p} - E_{1s}$  as a function of  $r_0$  for different values of  $V_0$  (around the Madelung energy  $\alpha_M$ ) for a KCl crystal [22], as a generic example of a typical alkali halide. For purposes of comparison, the F band energy measured at 77 K is shown as a point in the same figure.

If we take as a reference the particle-in-a-box model for a given value of  $V_0$ , the energy levels become closer as  $r_0$  is increased, so that the difference between the ground state and the first excited state decreases and the position of the F-band ( $\Delta E$ ) is shifted to the red. Moreover, if we make use of the Hellman-Feynmann theorem, the force exerted by the spherical wall on the electron will be related to the derivative of the curves as it will exert a hydrostatic pressure on the crystal, so that this model predicts, at least qualitatively, a shift of the F-band to the blue because, when the crystal is under pressure, the cavity radius decreases. In the case of F-band energies, N. Singh and W. Joshi have reported a similar shift for several alkali halides under pressure [35, 36]. This shift is consistent with our model.

Now, let us consider that an additional electron is trapped in the vacancy or similarly, that an F center traps an electron, forming the so-called F' center. Taking atomic physics as a reference, the F center would represent a hydrogen-like system while the F' center would be a helium-like system. In

this case the potential can be modelled as

$$V(r_1, r_2) = \begin{cases} -V_0 + \frac{1}{r_{12}}, & 0 \leq r_1, r_2 \leq r_0 \\ -\frac{1}{\kappa_0} \left( \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} \right), & r_0 \leq r_1, r_2 < \infty \end{cases}. \quad (10)$$

Notice that in this case, the electron-electron interaction would decrease the depth of the well, an event that would shift the energy levels toward the ionization states or contin-

uum states since the well becomes shallow. Indeed, the corresponding absorption band for this center can be measured at low temperatures (liquid nitrogen temperature or lower). At room temperatures there is ionization of the center mainly due to the thermal vibration of the lattice.

As we have mentioned before, taking atomic physics as our reference, the *ansatz* wave function for this system can be constructed as a product of hydrogenic wave functions for each electron, that is

$$\Psi_{1s}(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} A(r_0 - \gamma r_1)(r_0 - \gamma r_2) \exp(-\alpha(r_1 + r_2)), & 0 \leq r_1, r_2 < r_0 \\ B \frac{1}{r_1 r_2} \exp(-\beta(r_1 + r_2)), & r_0 < r_1, r_2 < \infty \end{cases}, \quad (11)$$

and

$$\Psi_{2p}(\mathbf{r}) = \begin{cases} C(r_0 - \gamma r_1)(r_0 - \gamma r_2) r_1 r_2 \cos \theta_1 \cos \theta_2 \exp(-\alpha(r_1 + r_2)), & 0 \leq r_1, r_2 < r_0 \\ D \frac{\cos \theta_1 \cos \theta_2}{r_1 r_2} \exp(-\beta(r_1 + r_2)), & r_0 < r_1, r_2 < \infty \end{cases}. \quad (12)$$

Proceeding as in the previous case, it is possible to construct the energy functional for these states and minimize it with respect to the parameters involved to get an upper bound for their energy. Surprisingly, this model predicts just the  $1s$ -like bounded state, and no extremum for the  $2p$ -like state was found. So, in our model the  $F'$  band would be a transition from the ground state to the continuum, a closer picture to that observed experimentally. In Fig. 2 we depicted the energy associated with this transition, considering the bottom of the continuum to be a final state, that is  $\Delta E_{F'} = -E_{1s}$ , as a function of  $r_0$  for different values of  $V_0$ . For purposes of comparison, the experimental value measured at 77 K for the  $F'$  absorption band in KCl is also shown in Fig. 2.

The same observations made for the  $F$ -center can be applied to this center, the main difference being that, as the second electron is loosely bound, the shift to the red of its band is less pronounced, a result that is consistent with experimental observations regarding the broad band measured at low temperatures and the point that, at room temperatures, the center can not be observed since the second electron is thermally ionized.

To close this section, we shall study another defect in alkali halides whose symmetry is very different from that of

the previous ones. In this defect, two neighboring anion vacancies in the (110) direction trap an electron. This defect constitutes the so-called  $F_2^+$  center. If we now refer to molecular physics, it would be an  $H_2^+$ -like molecular ion; this similarity allows us to form an easy conception of the type of *ansatz* wave functions, which, according to the properties stated in Section 2, can be useful in obtaining the main features of at least the principal absorption band. As in the case of the molecular ion, the natural coordinates for this system are the prolate spheroidal coordinates  $(\xi, \eta, \varphi)$ , and the model potential would be as follows:

$$V(\xi, \eta, \varphi) = \begin{cases} -V_0, & 1 \leq \xi < \xi_0, \\ -\frac{1}{K_0} \left( \frac{1}{r_1} + \frac{1}{r_2} \right), & \xi_0 < \xi < \infty \end{cases}, \quad (13)$$

where now, for this symmetry, the 'size' of the confining region is associated with the 'radial' coordinate  $\xi$  in such a way that  $(\xi = \xi_0, -1 \leq \eta \leq 1, 0 \leq \varphi \leq 2\pi)$  is a spheroid of revolution around the  $z$ -axis. If we assume that this axis is the one where the neighboring anion vacancies are located, then we have a symmetry compatibility of both the defect and the system of coordinates. So, for this symmetry, the *ansatz* wave functions would be of the following form:

$$\Psi_{1s\sigma_g}(\xi, \eta, \varphi) = \begin{cases} A(\xi_0 - \gamma\xi) \exp(-\alpha(\xi + \eta)), & 1 \leq \xi < \xi_0 \\ B \exp(-\beta(\xi + \eta)), & \xi_0 < \xi < \infty \end{cases}, \quad (14)$$

and

$$\Psi_{2p\pi_u}(\xi, \eta, \varphi) = \begin{cases} C(\xi_0 - \gamma\xi) \sqrt{(\xi^2 - 1)(1 - \eta^2)} \exp(-\alpha(\xi + \eta)) \exp(i\varphi), & 1 \leq \xi < \xi_0 \\ D \sqrt{(\xi^2 - 1)(1 - \eta^2)} \exp(-\beta(\xi + \eta)) \exp(i\varphi), & \xi_0 < \xi < \infty \end{cases}. \quad (15)$$

TABLE I. Summary of the obtained results and the best calculated parameters for the studied centers and their comparison with experimental available data and other theoretical calculations. KCl was used as generic example.  $E_M = -(\alpha_M/a)$ , is the Madlung energy for a NaCl-type crystal (see for instance Ref. 19).

Center	$\Delta E$ (eV)	$\Delta E_{\text{exp}}$ (eV)	$r_0$ (a.u.)	$\xi_0$	$V_0$ (eV)	$E_M$ (eV)
F	2.29	2.31 <sup>a</sup>	4.0(3.98 <sup>b</sup> )	-	-6.0	-8.0
F'	1.62	1.65 <sup>a</sup>	5.0(5.18 <sup>c</sup> )	-	-3.9	-8.0
F <sub>2</sub> <sup>+</sup>	2.42	2.46 <sup>a</sup>	-	2.0 <sup>d</sup>	-4.7	-8.0

<sup>a</sup>From W.B. Fowler, *Physics of Color Centers* (Academic Press, New York, 1968).

<sup>b</sup>From G. Iadonisi and B. Preziosi, *Nuovo Cimento B* **48**, (1967) 92.

<sup>c</sup>From S.V. La and R.H. Bartram, *Phys. Rev.* **144**, (1966) 679.

<sup>d</sup>From the geometry of the defect and the interionic distance  $a$ .

In all cases  $a = 5.94$  (a.u.) and  $\kappa_0 = 2.19$ .

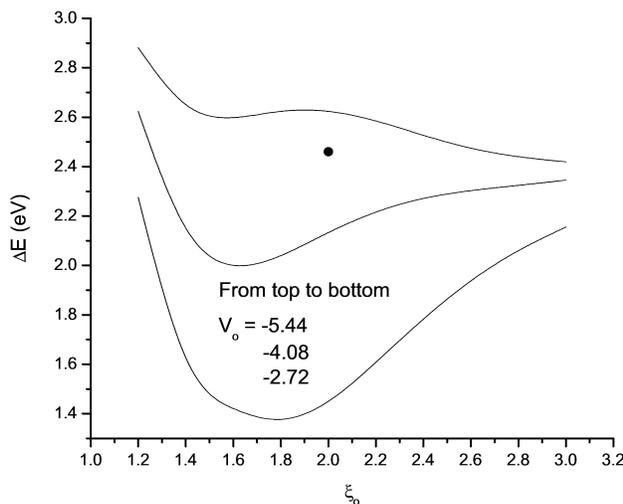


FIGURE 3. Behavior of  $\Delta E = E_{2p\pi_u} - E_{1s\sigma_g}$  for the F<sub>2</sub><sup>+</sup> center, as a function of the 'size' of the spheroid  $\xi_0$  and various potential well depths. The filled circle represents the experimentally measured  $\Delta E$  and the value of  $\xi_0$  consistent with the geometry and dimensions of the lattice. KCl was used as a generic example.

The choice of these functions is closely related to the form of the hydrogenic wave functions in prolate spheroidal coordinates, as reported by Coulson and Robinson [37, 38]. As before, we proceed to construct the corresponding energy functional and to find the energies of these bounded states. In Fig. 3, we plot the main absorption band of the F<sub>2</sub><sup>+</sup> center, defined as  $\Delta E = E_{2p\pi_u} - E_{1s\sigma_g}$ , as a function of  $\xi_0$ , for different values of  $V_0$  and the interfocal distance  $R \simeq \sqrt{2}a$  where  $a$  is the lattice constant for this type of crystal. We also include in this figure, for comparison purposes, the experimentally measured value  $\Delta E_{\text{exp}}$ .

The geometry of this defect is very different from the previous cases because when we choose a value for the interfocal distance  $R$ , we can have a variety of values of  $\xi_0$ , that is, the corresponding spheroid with a constant mayor axis would be flattened for  $\xi_0 \simeq 1$ , but could be almost a sphere when  $\xi_0 \gg 1$ ; in the middle there is a diversity of shapes, which would reflect the non-monotonic behavior of curves drawn in Fig. 3 and perhaps is a limitation of the model since the potential well assumed here is geometry independent. However,

a closer inspection of curves allows us to observe a  $V_0$  value between  $-5.54$  and  $-4.08$  eV, which shows a monotonic behavior close to the experimental value for the transition energy (the filled dot in this figure).

#### 4. Discussion and final remarks

The parameters used in calculations as well as the results for the best values of transition energies for the centers here considered are shown in Table I. For comparison purposes, the experimental values for the corresponding transitions energies are also included.

As the reader may notice, the free parameters involved such as the size of the confining region, or the depth of the potential well, have reasonable values compared with those used in similar studies [22, 39–42]. The latter fact constitutes a confirmation of the reliability of the model and a method of calculation, which make them amendable as a previous step for a more sophisticated calculation that would involve first principle calculations. It is also worth mentioning that the same formalism was used to study some properties of other real systems such as excitons in semiconductor crystallites or atoms trapped in solids, or to model atoms or molecules under high pressures. All these studies were fairly successful, in the light of experimental results.

In spite of its simple nature, the model proposed here can be useful in estimating some parameters associated with this kind of defect and would be, perhaps, a step leading to a more sophisticated calculation in order to study other properties. It is worth mentioning that there exist other formalisms used to study these defects, namely, the point ion and finite-size ion models (or pseudopotential); the main restriction underlying these models is that the polarization of the crystal cannot be accounted for properly, as it is by the semi-continuum approach. This matter was widely discussed for instance, in Refs. 22 and 39. Moreover, Fowler [43] and Georgiev [44] have shown that an improvement to the traditional semi-continuum model, can account, for instance, for Stokes shifts and vibronic coupling to the lattice of the states of F-center. The latter would represent an interesting topic for a future extension of the present model.

Finally, we would like to point out the crucial role played by hydrogen-like wave functions to construct the *ansatz* wave functions for all cases. Their flexibility is remarkable in our present calculations, as well as in atomic or molecular physics. Nowadays there exist more sophisticated tools for studying this type of system in a more complex fashion, but it seems that the use of this kind of function is still a very powerful tool in many fields of theoretical physics as are the harmonic oscillator wave functions [42]. This is one of the

legacies of Professor Carlos Ruiz-Mejía, regarding the theoretical study of this kind of defect in ionic crystals [45–49], to mention just one example.

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One of the authors (JLM) would like to dedicate this work to the memory of Professor Carlos Ruiz-Mejía, his former teacher and very close friend and colleague.

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