

# Multireference configuration interaction potential curve and analytical potential energy function of the ground and low-lying excited states of CdSe\*

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(Received 22 November 2006; revised manuscript received 15 May 2007)

The potential energy curves (PECs) of the ground state ( $^3\Pi$ ) and three low-lying excited states ( $^1\Sigma$ ,  $^3\Sigma$ ,  $^1\Pi$ ) of CdSe dimer have been studied by employing quasirelativistic effective core potentials on the basis of the complete active space self-consistent field method followed by multireference configuration interaction calculation. The four PECs are fitted to analytical potential energy functions using the Murrell-Sorbie potential function. Based on the PECs, the vibrational levels of the four states are determined by solving the Schrödinger equation of nuclear motion, and corresponding spectroscopic constants are accurately calculated. The equilibrium positions as well as the spectroscopic constants and the vibrational levels are reported. By our analysis, the  $^3\Pi$  state, of which the dissociation asymptote is Cd( $^1S$ ) + Se( $^3P$ ), is identified as a ground state of CdSe dimer, and the corresponding dissociation energy is estimated to be 0.39 eV. However, the first excited state is only 1132.49 cm<sup>-1</sup> above the ground state and the  $^3\Sigma$  state is the highest in the four calculated states.

**Keywords:** potential energy curve, multireference configuration interaction, spectroscopic constants, vibrational levels

**PACC:** 3420, 3180, 3150

## 1. Introduction

II-VI semiconductors, owing to their special structures, are technologically important materials. The recent fabrication of the blue-green laser diode based on these compounds has renewed interest in their physical properties. Among these compounds, the cadmium chalcogenides (CdS, CdSe, and CdTe) have attracted special attention in recent years from both experimental<sup>[1-6]</sup> and theoretical<sup>[7-17]</sup> points of view (the listed references are only a part of representative studies). The *ab initio* calculations, as well as others, have been extensively carried out to study the structural, electronic, elastic, thermodynamic and lattice dynamical properties for cadmium chalcogenides.<sup>[18]</sup> However, these studies mainly concentrate on the solid properties of bulk materials of CdSe, and as far as we know, there exist almost no calculations on the micro-clusters or molecules of CdSe dimer, which have very special properties. To fill in the gap, we carry out high-level *ab initio* calculations for the potential en-

ergy curves (PECs) of the four existed states of the CdSe dimer, identify the ground state, and induce the analytical potential energy functions (APEFs).<sup>[19]</sup> Based on these, we can determine the spectroscopic constants and vibrational energy levels of the four calculated states. The spectroscopic properties and vibrational levels can give a reference to the experimental observation, and the APEFs can be used for dynamical calculations or constructing many-body APEF to optimize more complex clusters.

## 2. Computational approach

*Ab initio* calculations were performed on the CdSe dimer with the internally contracted multireference configuration interaction method (MRCI)<sup>[20,21]</sup> for the ground and three low-lying excited states. The MRCI is a way to systematically include those configuration state functions (CSFs) that contribute most significantly to the correlation energy, and it is accu-

\*Project supported by the national Natural Science Foundation of China (Grant No 10674114).

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rate in treating small systems, especially dimers. In the process of our calculation, the MRCI calculation was preceded by complete active space self-consistent field (CASSCF) calculation,<sup>[22,23]</sup> in which all valence molecular orbitals were optimized. Molecules containing transition-metal atoms, particularly their excited states, are often difficult to treat using *ab initio* calculations. Generally, the basis sets must be chosen carefully and the configuration of molecular orbitals must be constructed elaborately.<sup>[24]</sup> As Cd belongs to transition metal, it needs treating carefully: the basis set for it should contain more active electrons. At the same time, it is nowadays universally received that the accurate *ab initio* electronic structure calculation for systems with heavy elements requires the inclusion of relativistic effects, and even for systems with elements in the second row a relativistic effective core potential study may be more accurate than a non-relativistic all-electron investigation.<sup>[25]</sup> On the other hand, the heavy atoms contain more electrons, so the computational consumption will become very great if a large basis set including all-electrons and relativistic effect is employed. Considering both the relativistic effects and the CPU time, we employed ECP28MWB for both atoms Cd and Se, which is a quasi-relativistic effective core potential. For atom Cd, it means that the inner 28 electrons are replaced by the effective potentials, while the remainder are treated as active ones. At the same time, the valence orbitals of Cd are expanded on (8s7p6d2f1g) primitive Gaussian functions, contracted to [6s5p3d2f1g]. For the atom Se, the ECP28MWB describes the inner 28 core electrons with a pseudopotential and the 4s<sup>2</sup>p<sup>4</sup> electrons with a (4s5p) primitive Gaussian functions are contracted to [2s3p]. It is well known that in the configuration interaction calculation for excited states the same molecular orbitals as the ground state should be used in order to compare the energies of the considered states and identify the ground state accurately, so we calculate the four states together, i.e. all the four states are optimized together using the CASSCF method, and the obtained wavefunction is used to carry out the MRCI calculation. In order to increase the accuracy of the results, we increase the reference configurations by adding virtual orbitals to the active space (two virtual orbitals are added to the A1 symmetry). Then the number of corresponding configuration state functions of the MRCI calculation is 348. Through the CASSCF calculation, the number of the closed shell orbitals is 4 (2110), and the number of active orbitals

is 11 (6221), while the number of active electrons is 18.

The *ab initio* calculations are performed with the MOLPRO program package<sup>[26]</sup> running on the Dawning-4000A<sup>[27]</sup> computer at Ludong university. APEFs are deduced by using the Murrell–Sorbie potential function and least square fitting method, while the spectroscopic constants are determined by using the relationship between the APEF and them. Based on the APEFs, the vibrational levels are determined by solving the Schrödinger equation of nuclear motion, and these calculations are carried out with the program LEVEL 7.5.<sup>[28]</sup>

### 3. Analytical potential energy function and spectroscopic parameters

Among the functions that proposed to fit APEFs of diatomic molecules, the Murrell–Sorbie (MS) potential energy function seems to be best. It can accurately reproduce interaction potential energies of many neutral and cationic diatomic molecules, and we have successfully tried it in deducing APEFs for many molecules.<sup>[29–45]</sup> The general MS function is<sup>[46]</sup>

$$V(\rho) = -D_e \left( 1 + \sum_{i=1}^n a_i \rho^i \right) \exp(-a_1 \rho), \quad (1)$$

where  $\rho = R - R_e$ , with  $R$  and  $R_e$  being the internuclear distance and equilibrium bond length respectively;  $D_e$  is the dissociation energy. The parameters  $a_i$  and  $D_e$  can be determined by fitting. In many cases satisfactory results can be obtained when  $n$  equals 3, while sometimes  $n$  equals 4 the result is better, in other cases more terms are needed. After trying a series of fittings, we find that for the CdSe dimer, reasonable APEFs of the singlet states (<sup>1</sup>Σ, <sup>1</sup>Π) can be obtained when  $n$  equals 9. While for the triplet states (<sup>3</sup>Σ, <sup>3</sup>Π), 8 is available.

It is significant to note that during the fitting process,  $R_e$  is also treated as a fitting parameter. The spectroscopic parameters can be calculated based on the APEFs. First, the force constants can be determined from the parameters of the APEFs as follows:

$$f_2 = D_e(a_1^2 - 2a_2), \quad (2)$$

$$f_3 = 6D_e \left( a_1 a_2 - a_3 - \frac{a_1^3}{3} \right), \quad (3)$$

$$f_4 = D_e(3a_1^4 - 12a_1^2a_2 + 24a_1a_3 - 24a_4), \quad (4)$$

where  $f_2$ ,  $f_3$ ,  $f_4$  are quadratic, cubic and quartic force constants respectively. And then, the spectroscopic parameters are

$$B_e = \frac{h}{8\pi^2 c \mu R_e^2}, \quad (5)$$

$$\omega_e = \sqrt{\frac{f_2}{4\pi^2 \mu c^2}}, \quad (6)$$

$$\alpha_e = -\frac{6B_e^2}{\omega_e} \left( \frac{f_3 R_e}{3f_2} + 1 \right), \quad (7)$$

$$\omega_e \chi_e = \frac{B_e}{8} \left[ \frac{-f_4 R_e^2}{f_2} + 15 \left( 1 + \frac{\omega_e \alpha_e}{6B_e^2} \right)^2 \right], \quad (8)$$

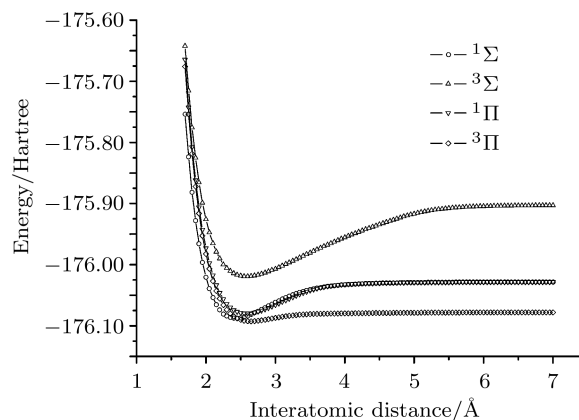
$$D_{\text{rot}} = \frac{4B_e^2}{\omega_e^2}, \quad (9)$$

where  $\mu$  is the reduced mass of atoms Cd and Se, and  $c$  is the speed of light in vacuum. In the above equations,  $B_e$  is the rigid-rotational factor, while  $a_e$  is the nonrigid-rotational factor.  $\omega_e$  is the harmonic vibrational frequency,  $\omega_e \chi_e$  is the inharmonic vibrational factor, and  $D_{\text{rot}}$  is the rotational constant.

## 4. Results and discussion

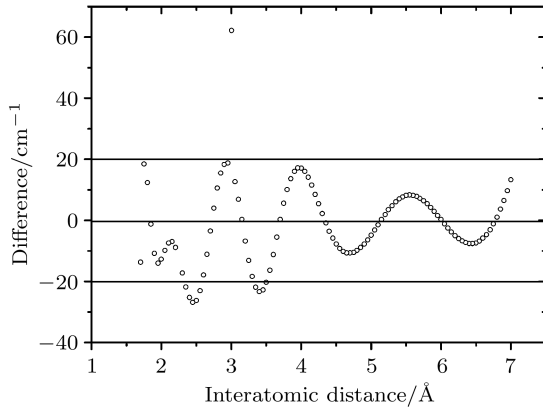
The ground state of the CdSe molecule should be the  $^3\Pi$  state if the two atoms stay separately in their atomic ground state, i.e. in Cd( $^1S$ ) and Se( $^3P$ ). However, when the CdSe molecule is formed, Se atom has 4 electrons in the p orbital, and it can form a closed shell if it obtains two electrons from the Cd atom. At the same time, Cd has 2 valence electrons, and it still has a closed shell when it loses the two electrons. In this case, the CdSe will be in the  $^1\Sigma$  state, and its dissociation energy will be larger than that of the  $^3\Pi$  state because of the electron transfer. It is also a candidate of the ground state, so, several molecular states ( $^1\Sigma$ ,  $^3\Sigma$ ,  $^1\Pi$  and  $^3\Pi$ ) are calculated in the present work. The CASSCF/MRCI calculations of the four states start with an internuclear distance of  $1.7\text{\AA}$ , and totally 107 energy points are calculated for each state with an interval of  $0.05\text{\AA}$ . The four PECs for  $^1\Sigma$ ,  $^3\Sigma$ ,  $^1\Pi$  and  $^3\Pi$  with the basis sets ECP28MWB for both atoms Cd and Se are shown in Fig.1. For a comparison among the four states, Fig.1 shows the primitive potential energies of our MRCI calculations (the unit is Hartree). From the figure we can see clearly that  $^3\Pi$

is a ground state of the dimer, and the  $^3\Sigma$  state is obviously higher than the other three states. As expected,  $^1\Sigma$  state is only  $1132.49\text{ cm}^{-1}$  above the ground state, and the dissociation energy is  $13032.89\text{ cm}^{-1}$ , which is about 4 times that of the ground state. It is confirmed that the  $^3\Pi$  state is the ground state, and the other three states are all excited states.

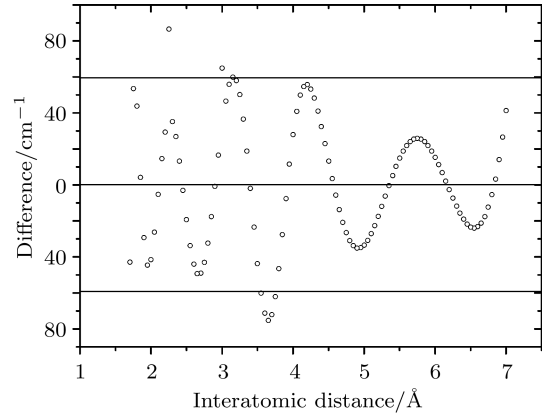


**Fig.1.** PECs of the ground and three low-lying excited states of CdSe (MRCI). (1 Hartree =  $110.5 \times 10^{-21}$  J).

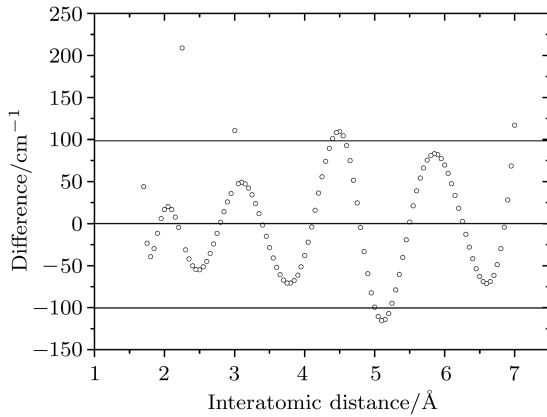
Figures 2–5 display intuitively the difference in energy between the fitting PECs and corresponding *ab initio* ones. The parameters of APEFs for all the four states including the root means square (RMS) errors, which are obtained using the MS potential function and least square fitting method, are collected in Table 1. The RMS error can be used to assess quantitatively the quality of the fitting process. As shown in Table 1, the values of the  $^1\Sigma$ ,  $^3\Sigma$ ,  $^1\Pi$ , and  $^3\Pi$  states are 21.12, 64.31, 36.14 and  $24.87\text{ cm}^{-1}$ , respectively, which are much smaller than the permitted chemical accuracy ( $1.0\text{ kcal/mol}$  or  $349.755\text{ cm}^{-1}$ ). Although some differences are large (see Figs.2–5, especially Fig.3), the percent errors are actually small. Take Fig.3 for example, at the point where  $R$  equals  $4.45\text{\AA}$ , the absolute difference will be as large as  $108.34615\text{ cm}^{-1}$ , however, its percent error is only 1.48%. So, it is safe to conclude that our fitting process is of high quality, and the MS potential function is reliable for reproducing the PECs of the transition-metal atom containing dimer CdSe. From Figs.2–5 we can see that the differences in energy between the fitting PECs and *ab initio* values display a trend of periodic change, which indicates that it is possible to find some modification terms to improve the fitting quality. This kind of work will be presented in future.



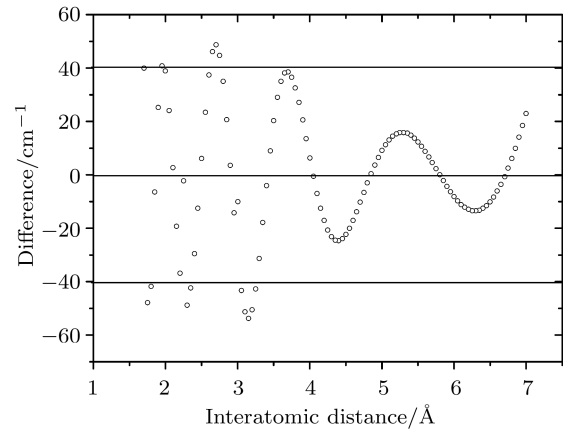
**Fig.2.** Fitting error of the PEC for  $^1\Sigma$  state.



**Fig.4.** Fitting error of the PEC for  $^1\Pi$  state.



**Fig.3.** Fitting error of the PEC for  $^3\Sigma$  state.



**Fig.5.** Fitting error of the PEC for  $^3\Pi$  state.

**Table 1.** Parameters of MS analytical potential energy function for the ground and three low-lying states of CdSe.

	$^1\Sigma$	$^3\Sigma$	$^1\Pi$	$^3\Pi$
$R_e/\text{\AA}$	2.43	2.58	2.59	2.64
$D_e/\text{cm}^{-1}$	13032.89	25541.07	11351.53	3148.23
$a_1/\text{\AA}^{-1}$	2.01	1.21	1.70	1.88
$a_2/\text{\AA}^{-2}$	-1.03	-0.29	-1.22	-3.99
$a_3/\text{\AA}^{-3}$	-0.24	0.34	-0.47	1.24
$a_4/\text{\AA}^{-4}$	-0.29	-0.21	-0.32	1.35
$a_5/\text{\AA}^{-5}$	0.40	0.12	0.62	-0.13
$a_6/\text{\AA}^{-6}$	0.08	-0.09	0.02	-0.57
$a_7/\text{\AA}^{-7}$	-0.15	0.03	-0.18	0.23
$a_8/\text{\AA}^{-8}$	0.04	-0.003	0.06	-0.03
$a_9/\text{\AA}^{-9}$	-0.04	—	-0.005	—
RMS/ $\text{cm}^{-1}$	21.12	64.31	36.14	24.87

Based on the APEFs and Eqs.(5)–(9), we calculate the spectroscopic parameters of the four states, including the dissociation energies and equilibrium po-

sitions. We did not make any comparison between theoretical or experimental results, because there have existed no such kinds of reports for the CdSe dimer up

to date. The inspection of Table 2 shows that for the ground state  $^3\Pi$ , its equilibrium position  $R_e$  (2.64Å) is larger than those of the other three states, while its dissociation energy  $D_e$  (3148.23 cm<sup>-1</sup>) is the smallest in the four considered states. It is known that the ground state of the group IIB transition-metal atom containing excimer usually presents a shallow minimum arising from van der Waals interactions (and is computationally very challenging), so it is not difficult for us to understand that the dissociation energy of the  $^3\Pi$  state is much smaller than those of the other excited states, which results in a relatively larger equilibrium position. The potential energies of  $^1\Sigma$  and  $^1\Pi$  states are very close to each other, and even intercross with each other at an internuclear distance larger than 2.7Å. This fact results in inconvenience for the experimental observation of these two states. However, according to our calculation, the equilibrium position of the  $^1\Sigma$  state is 0.15Å smaller than that of  $^1\Pi$  state, and on the other hand, its dissoci-

ation energy is 1618.36 cm<sup>-1</sup> larger than that of the  $^1\Pi$  state. These differences between the two singlet states can help us distinguish them experimentally. As for the  $^3\Sigma$  state, its potential energy curve is apparently higher than those of the other states in the full considered region of  $R_e$ . And from Table 2 we can see that the dissociation energy of the  $^3\Sigma$  state is as large as 25541.07 cm<sup>-1</sup>, which is singular for diatomic molecules. The above properties of the  $^3\Sigma$  state imply that CdSe has a prospective role as a vehicle excimer laser media and can become a likely candidate for high-efficiency laser systems. There exist also other very important spectroscopic parameters that have not been reported theoretically or experimentally for the four states of CdSe, such as harmonic vibrational frequency  $\omega_e$ , rotational constant  $D_{\text{rot}}$  and so on. These parameters are also collected in Table 2, and can give a beneficial inducement to experimental research of the dimer's spectroscopy.

**Table 2.** Spectroscopic parameters of the ground and three low-lying excited states of CdSe (in cm<sup>-1</sup>).

states	$^1\Sigma$	$^3\Sigma$	$^1\Pi$	$^3\Pi$
$\omega_e$	240.31	209.40	209.74	162.32
$\omega_e X_e$	0.80	0.49	0.53	1.56
$B_e$	0.06	0.05	0.05	0.05
$\alpha_e$	$2.47 \times 10^{-4}$	$1.92 \times 10^{-4}$	$1.81 \times 10^{-4}$	$4.04 \times 10^{-4}$
$-D_{\text{rot}}$	$1.61 \times 10^{-8}$	$1.48 \times 10^{-8}$	$1.46 \times 10^{-8}$	$2.14 \times 10^{-8}$
$D_e$	13032.89	25541.07	11351.53	3148.23
$R_e/\text{\AA}$	2.43	2.58	2.59	2.64

**Table 3.** Vibrational levels for the four states with  $J = 0$  (the levels for  $v = 0$  are set to be zero, unit is cm<sup>-1</sup>).

$v$	$^1\Sigma$	$^3\Sigma$	$^1\Pi$	$^3\Pi$
0	0	0	0	0
1	239.00	194.03	208.84	159.32
2	476.38	387.09	416.59	315.42
3	712.12	579.20	623.25	468.24
4	946.20	770.35	828.79	617.69
5	1178.63	960.56	1033.21	763.70
6	1409.39	1149.81	1236.49	906.18
7	1638.47	1338.13	1438.62	1045.05
8	1865.87	1525.52	1639.58	1180.20
9	2091.56	1711.97	1839.36	1311.54
10	2315.53	1897.50	2037.95	1438.93

Based on the APECs, the vibrational energy levels for each state are determined by solving the one-dimensional Schrödinger equation of nuclear motion. These calculations are carried out with the Fortran Package Level7.5. The obtained vibrational levels

(with  $J=0$ ) of the four states are shown in Table 3. For the sake of convenient comparison, the value of the ground vibrational level for each state is set to be zero. It is found that the vibrational levels for each state are very serried, and there are too many levels

(more than one hundred levels) for some states that have relatively larger dissociation energies, such as the  $^1\Sigma$  and  $^3\Sigma$  states. As a result, we just present the ten lowest vibrational energy levels for each state in Table 3. If we take a simple comparison among the levels, we can obtain the conclusion that the vibrational levels of the ground state ( $^3\Pi$ ) is obviously lower than those of all the other excited states, which indicates that the vibration of the ground state is the feeblest. On the other hand, the level of the  $^3\Sigma$  state is very close to that of the  $^1\Pi$  state and lower than the vibrational level of the  $^1\Sigma$ , which is the highest in the four calculated states. As there are no observed data for comparison, our present values can give a reference to further studies.

## 5. Conclusions

The potential energy curves of the ground and three low-lying excited states of the transition metal containing molecule CdSe have been reported on the basis of the CASSCF/MRCI calculations for the first time, by employing the quasi-relativistic effective core potential ECP28MWB for both atoms Cd and Se. According to our calculations, the  $^3\Pi$  state is identified as the ground state, and the  $^3\Sigma$  state is the highest in

the four calculated states, while the first excited state is only  $1132.49\text{ cm}^{-1}$  above the ground state. So, it is difficult to distinguish the first excited state from the ground state by energy difference. Fortunately, the Cd-Se bond in the first excited state is at least  $0.20\text{ \AA}$  shorter than the ground state bond and their vibrational frequencies are obviously different, which may be used to pick out the ground state. The ground state of CdSe is very weakly bound, because its dissociation energy is computed to be  $0.39\text{ eV}$ .

The  $^3\Sigma$  and  $^3\Pi$  states lie between the ground state ( $^3\Pi$ ) and the highest state ( $^3\Sigma$ ), and their energies are in good agreement with each other in a region of internuclear distances larger than  $2.7\text{ \AA}$ . The APEFs of the four states have been fitted, from which the spectroscopic parameters and the vibrational levels are obtained for the first time. The vibrational levels of all the four considered states are found to be very separated, and the vibration of the ground state is strengthless. Our reports on the molecular properties such as the spectroscopic parameters and vibrational levels can give a beneficial reference to the experimental observation of dimmers. The fitted analytical potential energy functions can be used in further molecular dynamical calculation. The obtained information forms the basis of study on large CdSe cluster or even its solid material.

## References

- [1] Nelves R J and McMohan M I 1998 *Semicond. Semimater* **54** 145
- [2] Chen A B and Sher A 1982 *J. Vac. Sci. Technol.* **21** 138
- [3] Rowe J M, Nicklow R M, Price D L and Zanio K 1974 *Phys. Rev. B* **10** 671
- [4] Kayanuama Y 1988 *Phys. Rev. B* **38** 9797
- [5] Kim Y D, Klein M V, Ren S F, Chen Y C, Lou H, Samarth N and Furdyna J K 1994 *Phys. Rev. B* **49** 7262
- [6] Tomasulo A and Ramakrishna M V 1996 *J. Chem. Phys.* **105** 3612
- [7] Wei S and Zhang S B 2000 *Phys. Rev. B* **62** 6944
- [8] Kitamura M, Muramatsu S and Harrison W A 1992 *Phys. Rev. B* **46** 1351
- [9] Kanoun M B, Sekkal W, Aourag H and Merad G 2000 *Phys. Lett. A* **272** 113
- [10] Wright R and Gale J 2004 *Phys. Rev. B* **70** 035211
- [11] Coté M, Zakharov O, Rubio A and Cohen M L 1997 *Phys. Rev. B* **55** 13025
- [12] Aorag F and Cartier H 2000 *Mater. Chem. Phys.* **66** 10
- [13] Agrawal B K and Agrawal S 1992 *Phys. Rev. B* **45** 8321
- [14] Corsa A D, Baroni S, Resta R and Gironcoli S 1993 *Phys. Rev. B* **47** 3588
- [15] Benkhetou N, Rached D, Soudini B and Driz M 2004 *Phys. Stat. Solid (b)* **241** 101
- [16] Rajput S D and Browne D A 1996 *Phys. Rev. B* **53** 9052
- [17] Zakharov O, Rubio A, Blasé X, Cohen M L and Loui S G 1994 *Phys. Rev. B* **50** 10780
- [18] Deligoz E, Colakoglu K and Ciftci Y 2006 *Physica B* **373** 124
- [19] Yang C L, Zhang Z H and Ren T Q 2002 *J. Chem. Phys.* **116** 6656
- [20] Werner H -J and Knowles P J 1988 *J. Chem. Phys.* **89** 5803
- [21] Knowles P J and Werner H -J 1988 *Chem. Phys. Lett.* **145** 514
- [22] Werner H -J and Knowles P J 1985 *J. Chem. Phys.* **82** 5053
- [23] Knowles P J and Werner H -J 1985 *Chem. Phys. Lett.* **115** 259
- [24] Yang C L, Gao F, Zhang X Y and K L Han 2005 *J. Chem. Phys.* **123** 4308
- [25] Dolg M 2000 *Modern Methods and Algorithms of Quantum Chemistry* **3** 507
- [26] Werner H J, Knowles P J, Amos R D *et al* 2002 *MOLPRO* (Universität Stuttgart, Stuttgart, Germany, University of Birmingham, Birmingham, United Kingdom)
- [27] Dawning4000A is a large parallel compute containing 134 CPUs (AMD Opteron 64-bit 1.8GHZ) in Yantai Normal University.

- [28] Le Roy R J, 'level7.5: A Computer Program for Solving the Radial Schrödinger Equation for Bound and Quasi-bound Levels,' University of Waterloo Chemical Physics Research Report No. CP-665, 2002.
- [29] Yang C L, Zhu Z H, Wang R and Liu X Y 2001 *J. Mol. Struct. (THEOCHEM)* **548** 47
- [30] Yang C L, Zhu Z H and Wang R 2001 *Chinese Journal of Atomic and Molecular Physics* **18** 355
- [31] Yang C L, Huang Y J and Han K L 2003 *J. Mol. Struct. (THEOCHEM)* **625** 289
- [32] Yang C L, Zhang X and Han K L 2004 *J. Mol. Struct. (THEOCHEM)* **678** 183
- [33] Yang C L, Zhang X and Han K L 2004 *J. Mol. Struct. (THEOCHEM)* **676** 209
- [34] Gao F, Yang C L and Ren T Q 2006 *J. Mol. Struct. (THEOCHEM)* **758** 81
- [35] Li Q and Zhu Z H 2006 *Acta Phys. Sin.* **55** 102 (in Chinese)
- [36] Xu G L, Zhu Z H, Ma M Z and Xie A D 2005 *Acta Phys. Sin.* **54** 3087 (in Chinese)
- [37] Li Q, Liu X Y, Wang R, Zhu Z H, Fu Y B and Wang X L 2000 *Chin. Phys.* **9** 501
- [38] Zhang X Y, Yang C L, Gao F and Ren T Q 2006 *Chin. Phys.* **15** 1981
- [39] Shi D H, Sun J F, Yang X D, Zhu Z L and Liu Y F 2005 *Chin. Phys.* **14** 1566
- [40] Wang F H, Yang C L, Zhu Z H and Jing F Q 2005 *Chin. Phys.* **14** 317
- [41] Luo D L, Meng D Q and Zhu Z H 2003 *Acta Phys. Sin.* **52** 2438 (in Chinese)
- [42] Li Q, Liu X Y, Wang H Y, Zhu Z H, Fu Y B, Wang X L and Sun Y 2000 *Acta Phys. Sin.* **49** 2347 (in Chinese)
- [43] Meng D Q, Jiang G, Liu X Y, Luo D L, Zhang W X and Zhu Z H 2001 *Acta Phys. Sin.* **50** 1268 (in Chinese)
- [44] Mao H P, Wang H Y, Tang Y J, Zhu Z H and Zheng S T 2001 *Acta Phys. Sin.* **53** 37 (in Chinese)
- [45] Lu G H, Sun W G and Feng H 2004 *Acta Phys. Sin.* **53** 1753 (in Chinese)
- [46] Murrell J N and Sorbe K S 1974 *J. Chem. Soc. Faraday Trans.* **2** 1552