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Diffusion Monte Carlo calculations on LaB molecule

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Potential energy curves for the lowest electronic states of LaB and LaB^- have been calculated by *ab initio* calculations. The diffusion Monte Carlo method has been employed in combination with three different trial functions. Spectroscopic constants have also been numerically derived for the neutral molecule and compared with the only available theoretical work;[19] however, predictions are provided for the corresponding constants for the anionic species which have not been reported yet. Our calculations suggest the high spin quintet state of LaB as the ground state with the triplet state higher in energy irrespective of the type of the functional used. This suggestion is in good accordance with the previous theoretical results calculated at B3LYP/LANL2DZ level of theory, whereas it contradicts with the prediction based upon B3LYP/SDD calculations in the same study. Moreover, variations of the permanent dipole moments as a function of the internuclear separations for the two electronic states of the neutral molecule have been studied and analyzed.

Keywords: potential energy curve, lanthanum boride, diffusion Monte Carlo, dipole moment

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1. Introduction

Over the years, systems containing rare earths have received much attention in many fields of physics and chemistry. As far as the *ab initio* calculations are concerned, several problems have probably obstructed accurate theoretical treatments for these systems. On one hand, relativistic and electron correlation effects become important in heavy elements and should not be neglected in accurate calculations. On the other hand, there are several open shells with different main and angular quantum numbers, i.e. 4f, 5d, and 6 s, whose orbitals are comparable in energies and therefore the bonding can take place with any of these orbitals, which adds additional complexity for quantum chemical calculations for systems involving these elements.

Understanding the electronic structures of lanthanide diatomics is of great importance for studying lanthanide compounds. Lanthanum diatomics, in particular, are good candidates for providing useful information on more complex systems involving lanthanides, owing to their simpler open d shell electronic configurations. Several research groups have performed *ab initio* calculations and experimental investigations on diatomic lanthanum molecules. Lanthanum monohydride, for instance, has been extensively studied in the past, both theoretically[1–8] and experimentally.[9–12] Spectroscopes of lanthanum halides[1,13–17] and lanthanum monoxide[1,3,4,18] have also been thoroughly investigated during the past few decades. However, studying diatomic lanthanum boride, which is the focus of this study, is scarce in literature. To our knowledge, there is no experimental study up to now on lanthanum boride. Only recently, a theoretical study has been reported on the 5d-transition metals monoborides by Kalamse *et al.*[19] In their paper, the authors have done the first theoretical study on lanthanum monoboride using density functional method based B3LYP functional with LANL2DZ and SDD basis sets. They have also calculated the lowest spin states, bond lengths, electron affinities, ionization potentials, and binding energies of diatomic lanthanum boride. However, no potential curves for LaB states have been reported. Unfortunately, Kalamse and co-workers have predicted in their work two different ground states for LaB based on the basis set used. They have predicted that LaB has triplet ground state at B3LYP/SDD level whereas it is quintet using B3LYP/LANL2DZ method.

The confusion provided by the previous study for assigning the LaB ground state as well as the lack of reliable information on lanthanide boride are the motivations of our present work, in which we apply the diffusion Monte Carlo (DMC) method to study the neutral and anionic LaB. Nowadays, DMC is considered as a promising method for treating the strongly correlated electron systems. Besides its favorable scaling with system size, it explicitly includes electron-electron correlation effects. A primary goal of this study is to provide the first calculations of potential energy curves (PECs) for neutral and anionic LaB molecules and to determine the nature of the ground states of them as well. The effects of different trial wavefunctions are also examined using single determinants constructed from HF orbital as well as from density functional theory (DFT) orbitals with the commonly used B3LYP and

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B3PW91 functionals. This work is also relevant to study the dipole moment dependence on internuclear distances for the two states of the neutral LaB molecule. An estimation of the electron affinity of LaB is also the subject of this work.

2. Computational methods

All computations for energies and dipole moments presented in this paper were carried out via the diffusion Monte Carlo method by making use of the QWalk package.[20] The diffusion Monte Carlo method has been extensively described in the literatures, so we only refer the reader interested in details to Refs. [21]–[23]. In our DMC calculations, the trial wavefunction was generated using the quantum chemistry program Gamess.[24] We propose to employ the DFT-type trial wavefunctions instead of using highly expensive correlated functions. Two density functionals were employed: (i) the Becke three parameters hybrid exchange (B3) + LYP correlation (B3LYP),[25–27] (ii) the Becke three parameter hybrid exchange (B3) + PW91 correlation (B3PW91).[25,28] In addition, HF trial wavefunction was also included for the sake of comparison. The basis set used in our calculations for lanthanum atom is CRENBS ECP,[29] where 54 core electrons are replaced by effective potentials. However, for the boron atom we utilized the pseudopotential of Burkatzki *et al.*[30] produced for use with quantum Monte Carlo. Through all the DMC calculations a time step of $\tau = 0.001$ H^{-1} and a mean population of 2000 walkers were used which proved to be successful for the calculations.

To construct the potential energy curves, we perform an accurate fit of the discrete DMC computed values of the total energy via the Morse potential function with the analytical form

$$V(R) = D_e[1 - \exp(-\beta(R - R_e))]^2,$$

where the parameter β defines the asymmetry of the Morse potential, R is the internuclear distance. R_e and D_e are the equilibrium bond length and the dissociation energy, respectively, which were numerically derived from the fitting process. Finally, accurate calculations on the ground state energies of neutral LaB and anion at the equilibrium bond lengths were carried out in order to obtain computational estimate of the electron affinity by difference.

3. Results and discussion

3.1. Potential energy curves and spectroscopic constants

The calculated DMC potential energy curves of LaB in triplet and quintet states using the three different functionals are presented in Fig. 1. The triplet states are represented by solid lines, while dashed lines are used for the quintet states. As can be seen from the figure, the PECs calculated using DMC/HF and DMC/B3LYP approaches have very similar behavior. However, the shape of potential curves changes somewhat at DMC/B3PW91 level of theory. Examining the figures employing HF and B3PW91 trial functions more closely, it can be seen that the intersection distances of PECs obtained by B3LYP function shifts to slightly larger internuclear distances compared with those obtained employing HF functional. The same remark was previously observed by Bytautas *et al.*[31] who confirmed in their study that the increase in the correlation recovery shifts the intersection distances to longer distances.

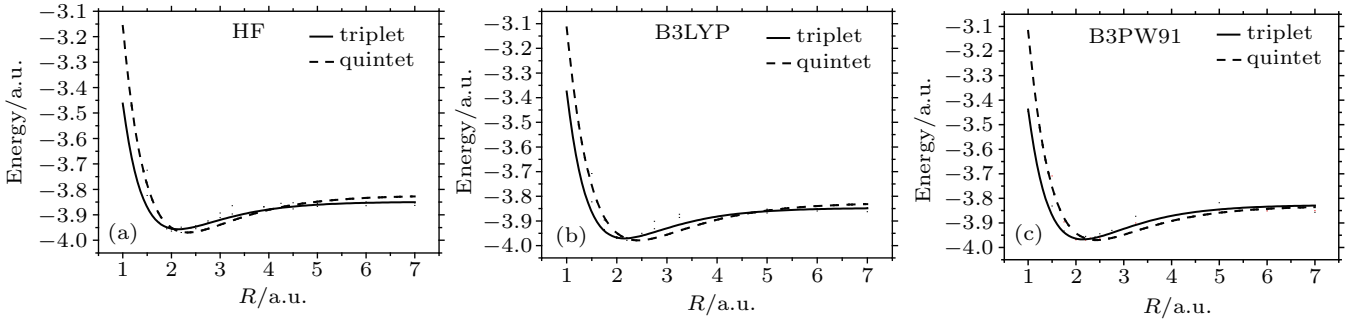


Fig. 1. DMC potential energy curves of the triplet and quintet states for neutral LaB molecule using different functionals. (a) HF, (b) B3LYP, and (c) B3PW91. The unit a.u. is short for atomic units.

The derived bond lengths, dissociation energies, and transition energies for the two electronic states are summarized in Table 1 together with theoretical data available in the literature. As no experimental data are available for LaB molecule, we discuss our results by comparison with the only theoretical work performed by Kalamse and co-workers.[19] It is very evident from Table 1 that our calculated dissociation energies for the two states provide a significant overestimation relative to the values reported by the former authors using the two approaches. We believe that this discrepancy is most probably be ascribed to the different methods and basis sets used in the calculations. In the previous theoretical study, the electron calculations were calculated at the limited B3LYP level. At this point it should be noted that single reference method such as DFT has more troubles in describing the electronic structure of strongly correlated sys-

tems. However, DMC is a great improvement over DFT because the former explicitly includes electron-electron correlation effect. Herein we only use the DFT as the starting point to the multireference DMC method. In fact, the underestimations of all DFT methods for D_e find confirmation in many studies.[32–39] Moreover, a more recent *ab initio* calculation performed by Sevy *et al.*[40] on MSi molecule pointed out that the bond dissociation energy of the latter molecule was systemically underestimated using the same strategy of, Kalamse and co-workers, B3LYP/LANL2DZ. Also, in agreement with our view, LANL2DZ basis gave very low dissociation energy for the chromium dimer using the multireference perturbation in Ref. [41]. In light of these considerations, we believe that our DMC results employing DFT functionals are more reliable and the value of D_e cited by Ref. [19] seems to be too low.

On the other hand, one can see that our estimated DMC bond lengths are in good accordance with that reported previously using LANL2DZ basis set. However, our estimated value of the same quantity for the triplet state is significantly shorter than the previous result calculated via SDD basis set. We believe that the multireference character of the triplet state is the main source of error in the previous B3LYP calculations for such state. In fact, the multireference triplet state is poorly dominated by single reference methods. This interpretation is confirmed in the study of Černušák and co-workers[42] on scandium boride. In their work, the quintet state was well described by a single reference method. However, the triplet state gave unacceptable results using the same strategy, confirming the multireference character for the latter state. The different basis sets utilized in the previous B3LYP calculations might be also partially responsible for the contradictory prediction of LaB ground state. On the other hand, the bond length and the corresponding dissociation energy are most likely underestimated at DMC/HF, which is an expected consequence of using HF trial function. As we stated before, HF orbitals have been utilized here for comparative purposes only.

Table 1. Bond lengths R_e, dissociation energies D_e, and transition energies T_e computed within DMC for the triplet and quintet states of LaB molecule together with the available reference data.

	Method	R_e/Å	D_e/eV	T_e/cm^{-1}
Triplet	DMC (HF)	2.133	2.94	6343
	DMC (B3LYP)	2.150	3.37	3424
	DMC (B3PW91)	2.145	3.81	2019
	B3LYP/SDD[a]	2.336	2.10	0.00
Quintet	DMC (HF)	2.333	3.97	0.00
	DMC (B3LYP)	2.428	4.16	0.00
	DMC (B3PW91)	2.427	3.78	0.00
	B3LYP/LANL2DZ[a]	2.435	2.49	0.00

[a]See Ref. [19].

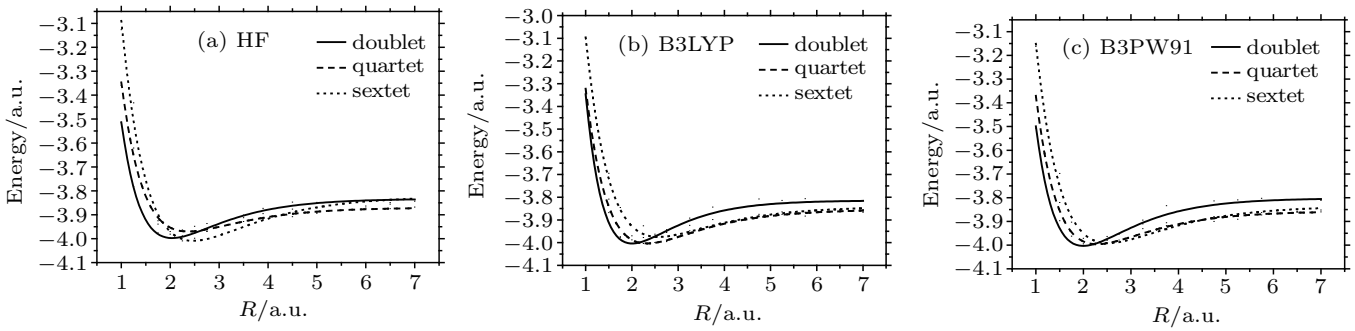


Fig. 2. DMC potential energy curves of the doublet, quartet, and sextet states for LaB^- molecule using different functionals. (a) HF, (b) B3LYP, and (c) B3PW91.

It may be seen from Table 1 that our DMC results using the three functionals reveal that the quintet state is lower in energy, predicting a high spin quintet ground state for LaB. This suggestion is in good accordance with the previous theoretical results calculated at B3LYP/LANL2DZ level of theory, whereas it contradicts with the prediction based upon B3LYP/SDD calculations in the same study. Our computed T_e value using DMC/HF is 6343 cm^{-1}. However, lower energy separations 3424 cm^{-1} and 2019 cm^{-1} are obtained using B3LYP and B3PW91 trial wavefunctions, respectively. Again, based on our results, we are certain that the high spin quintet state of LaB is the ground state with the triplet state higher in energy irrespective of the trial functions used. Similar high spin ground state has been found previously for other transition metals.[43–45] More specifically, based upon the fact that the electronic structure of atomic lanthanum resembles that of scandium, our result of the quintet ground state of LaB is consistent with the premise suggested by Černušák *et al.*[42] that the high spin quintet state of ScB is the ground state using the multireference configuration interaction method.

Now we turn the attention to the anionic LaB which is treated with the same ansatz like its neutral counterpart. The PECs are displayed in Fig. 2 and the corresponding spectroscopic constants are summarized in Table 2. To our knowledge, neither experimental nor theoretical spectroscopic constants are currently available for LaB^-. Therefore, our data for

the anionic molecule are predictive in nature and should be of similar precision as discussed for the neutral one. Inspection of Table 2 shows that the DMC results at the three levels predict that the ground state is most likely to be the doublet state. Within B3LYP and B3PW91 functionals, the next lowest state is the quartet followed by the sextet state placed 3160 cm^{-1} and 6628 cm^{-1} above the ground state respectively. However, the ordering of the excited states is reversed at DMC/HF level. At this point it should be noted that HF generally favors the high spin states results due to the absence in this method to electron correlation between unlike spins; whereas it provides poor performance to treat the low spin states attributed to their multireference character. We believe that this is the main source for reversing the order of excited states at DMC/HF level. In any case, at the three approaches considered we predict a stable negative ion of LaB with D_e value ranging from 4.46 eV to 5.47 eV which is much greater than the corresponding values (3.78 eV to 4.16 eV) for the neutral one.

Table 2. Bond lengths R_e, dissociation energies D_e, and transition energies T_e computed within DMC for the doublet, quartet, and sextet states of LaB^-.

	Method	R_e/Å	D_e/eV	T_e/cm^{-1}
Doublet	DMC (HF)	2.03	4.46	0.00
	DMC (B3LYP)	2.003	5.14	0.00
	DMC (B3PW91)	1.996	5.47	0.00
Quartet	DMC (HF)	2.368	2.69	15144
	DMC (B3LYP)	2.329	4.05	44
	DMC (B3PW91)	2.285	3.78	4675
Sextet	DMC (HF)	2.468	5.06	6079
	DMC (B3LYP)	2.577	3.62	3160
	DMC (B3PW91)	2.523	4.24	6628

Table 3. Electron affinity of LaB molecule computed with DMC method using different functionals together with the available reference data.

Method	EA/eV
DMC (HF)	1.20
DMC (B3LYP)	0.61
DMC (B3PW91)	0.97
B3LYP/LANL2DZ[a]	1.01
B3LYP/SDD[a]	0.41

[a]See Ref. [19].

Now it seems appropriate to compute the electron affinity (EA) of LaB molecule. Table 3 gives the electron affinities of LaB molecule calculated at the three levels together with the theoretical available values. Unfortunately, experimental value of LaB electron affinity has not been yet estimated. From Table 3, it is remarkable that our predicted DMC value of EA employing B3PW91 function (0.97 eV) compares well with that obtained previously (1.01 eV) by the B3LYP/LANL2DZ approach. Meanwhile, the EA estimated at DMC/HF (1.20 eV) is somewhat higher. Our predicted EA based upon DMC/B3LYP calculations (0.61 eV), on the other hand, is much closer to the value quoted previously by B3LYP/SDD (0.41 eV) than B3LYP/LANL2DZ (1.01 eV).

3.2. Dipole moments

It is well known that the dipole moment is a sensitive tool to test the accuracy of both the calculated wavefunction and energy. Theoretical predictions of the dipole moments of lanthanide diatomics, in particular, depend strongly on the level of treatment of the electron correlation. Our goal in this section is to investigate the permanent dipole moment for the lowest two states of LaB molecule as a function of internuclear distances using both DFT functionals as well as HF. This is presented graphically in Fig. 3. For the triplet states, one can easily see from Fig. 3(a) that the permanent dipoles obtained at DMC/B3LYP and DMC/B3PW91 approaches show similar behavior as a function of internuclear distance R. The magnitude of the dipole moment μ gradually increases as R increases, and reaches its maximum at R smaller than the equilibrium distance. The same trend was previously observed for LiBe,[46] LiCa,[47] and RbCa[48] molecules. Beyond the equilibrium region, abrupt change has been observed for μ at a distance around 2.5 a.u., consistent with regions of internuclear distances exhibiting crossing in the corresponding potential curves. As R further increases, μ starts to decrease and vanishes to zero, as expected for the neutral molecule. Alternatively, when the reference function for the DMC calculation was HF, one can find that μ becomes very small in magnitude and exhibits many fluctuations particularly around the equilibrium region, demonstrating the poor performance of

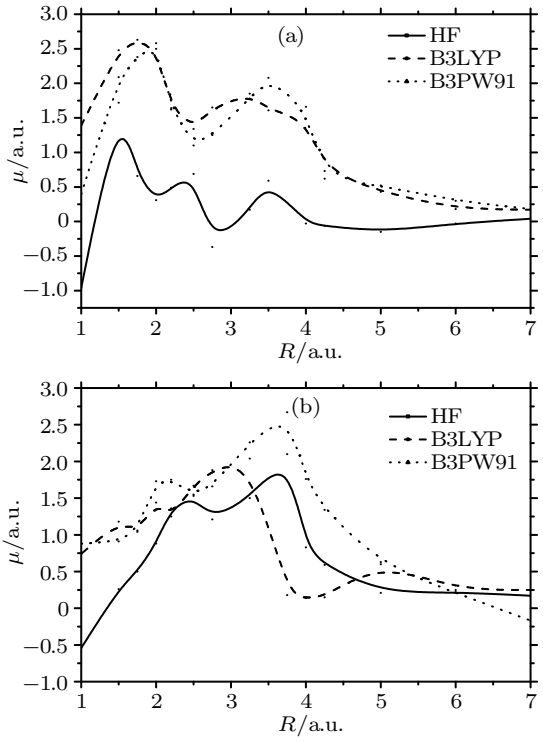


Fig. 3. The permanent dipole moments of (a) the triplet and (b) the quintet states of LaB molecule computed with the DMC method using different functionals.

Hartree–Fock for describing the low spin triplet state as indicated in the preceding subsection. Alternatively, a pronounced enhancement of the quintet state dipole moment is obtained using HF as indicated in Fig. 3(b). At DMC/B3PW91 level of theory, the distribution of the dipole exhibits the same trend of the triplet state mentioned earlier with significant differences in its magnitude. Meanwhile, the shape of DMC/B3LYP dipole function alters considerably in comparison to the low spin state with no clear trend observed.

It is still interesting to compare the dipole moment values obtained at equilibrium separations for the two states of LaB along with the data in Ref. [19]. It is apparent from Table 4 that our μ value estimated at DMC/HF level of calculation is no more than 0.17 times for the related values employing the hybrid functionals. This discrepancy was expected from our previous analysis. However, this complication was avoided by employing the DFT orbitals, highlighting the importance of dynamic correlation in the trial wavefunction. Another feature to note in Table 4 is that the μ value calculated by the previous study tends to be larger in magnitude than ours for the triplet state. A possible reason for the discrepancy in the magnitude of μ noted for the triplet state in the work of Kalamse and co-workers and ours is the too long bond length yielded by them for the latter state. For the quintet state, however, our DMC values for μ with the two hybrid functionals systemically overestimate the value quoted by the previous study.

Table 4. The permanent dipole moment μ of the triplet and quintet states for LaB molecule computed with DMC method using different functionals together with the available reference data.

	Method	μ/debye
Triplet	DMC (HF)	0.68
	DMC (B3LYP)	4.22
	DMC (B3PW91)	4.19
	B3LYP/SDD[a]	5.02
Quintet	DMC (HF)	3.63
	DMC (B3LYP)	5.16
	DMC (B3PW91)	4.58
	B3LYP/LANL2DZ[a]	4.29

[a]See Ref. [19].

4. Conclusion

In the present work, we have computed the potential energy curves for the lowest electronic states of LaB and LaB^- by means of the DMC method employing three different functionals. The PECs are accurately fitted to Morse potential and the spectroscopic constants are numerically derived. Our calculations conclude that the ground state of LaB is most likely to be the high spin quintet state in line with the previous theoretical results calculated at B3LYP/LANL2DZ level of theory, whereas it contradicts with the prediction based upon B3LYP/SDD calculations in the same study. Our estimated quintet states bond lengths, employing the three functionals, compare well to the value obtained by the previous study; meanwhile, our calculations yield triplet bond lengths which are considerably longer. In addition, our results of D_e for the two states provide a significant overestimation compared with the earlier values.

On the other hand, the ground state for LaB^- has been determined and the corresponding spectroscopic constants have been reported for the first time. This work further studies the dipole moment distribution for the two lying states of the neutral molecule as a function of the internuclear separations. Our results concerning the neutral LaB and anion are entirely new, and will certainly be helpful for guiding future experimental and theoretical spectroscopic works.

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