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Citation: Chin. Phys. B, 2024, 33 (**5**): 053102. DOI: 10.1088/1674-1056/ad20de
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Theoretical investigation of excited dipole bound states of alkali-containing diatomic anions

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(Received 2 January 2024; revised manuscript received 9 January 2024; accepted manuscript online 22 January 2024)

Information about electronic excited states of molecular anions plays an important role in investigating electron attachment and detachment processes. Here we present a high-level theoretical study of the electronic structures of 12 alkali-metal-containing diatomic anions MX^- (MX = LiH, LiF, LiCl, NaF, NaCl, NaBr, RbCl, KCl, KBr, RbI, KI and CsI). The equation-of-motion electron-attachment coupled-cluster singles and doubles (EOM-EA-CCSD) method is used to calculate the electron binding energies (EBEs) of 10 electronic excited states of each of the 12 molecule anions. With addition of different s-/p-/d-type diffusion functions in the basis set, we have identified possible excited dipole bound states (DBSs) of each anion. With the investigation of EBEs on the 12 MXs with dipole moment (DM) up to 12.1 D, we evaluate the dependence of the number of anionic excited DBSs on molecular DM. The results indicate that there are at least two or three DBSs of anions with a molecular DM larger than 7 D and a molecule with DM $>$ 10 D can sustain a π-DBS of the anion. Our study has some implications for the excited DBS electronic states of alkali-metal-containing diatomic molecules.

Keywords: anions, dipole bound states, alkali-metal-containing diatomic molecules

PACS: 31.15.vn, 33.15.–e, 33.15.Ry **DOI:** 10.1088/1674-1056/ad20de

When an excess electron binds to a neutral molecule by short-range potential, a molecular anion is formed which has an important role in biological[1] and astrophysical science[2] as well as in the interstellar medium.[3] Generally, stable anions are formed in the valence ground electronic state for molecules with negative electron affinities (EAs), while it is difficult for a molecule to support a stable bound excited anion. However, polar molecules with large enough dipole moments (DMs) could bind an electron via the electron–dipole interaction, forming so-called excited dipole bound state (DBS) anions.[4–9] The DBS is a stable bound state formed by the temporary capture of an electron; it can serve as the 'doorway' to electron attachment[10–12] and plays an important role in various physical and chemical processes,[7,8,13–16] DNA damage by low-energy electrons[17] and verification of the unexplained interstellar absorption spectra.[18]

The search for the excited DBSs of anions and investigation of their structure and spectroscopy have attracted increasing research interest both experimentally and theoretically.[16,19–23] As first suggested by Fermi and Teller in 1947, the minimum DM for the formation of dipole-bound anions is about 1.625 D.[24,25] Refined theoretical studies later predicted an empirical critical DM of 2.5 D to support a σ-type DBS[4,8,9,13,14,26–28] and a second critical DM $>$ 9.6 D to support a π-type DBS.[8] On the other hand, the number of excited DBSs of an anion and the dependence on the DM of the corresponding neutral molecule are still under debate. It is difficult to experimentally determine the excited DBSs of anions, since the binding energy is very close to the neutral ground states, thus ultra-high resolution is required in the spectroscopic measurements. Theoretically, while the first excited DBSs have been computed for some diatomic molecular anions,[29–32] verification of the high excited DBSs is still required with calculations using large diffusive basis sets.

Here we perform a high-level theoretical study of the excited DBSs of anions for a total of 12 alkali-metal-containing diatomic molecules (MX = LiH, LiF, LiCl, NaF, NaCl, NaBr, RbCl, KCl, KBr, RbI, KI and CsI) with DMs covering a wide range from 5.8 D to 12.1 D. In theoretical work, Gutsev *et al*. used the equation-of-motion coupled-cluster method for electron attachment with single and double substitutions (EOM-EA-CCSD) on some polar diatomic molecules and predicted two or more excited DBSs for metal halides and metal oxides.[30] The only experimental study to verify the existence of two excited DBSs was reported very recently by Lu *et al*., in which both σ-type and π-type DBSs were demonstrated in potassium iodide (KI) anions (neutral DM $>$ 10 D) using the high-resolution slow-electron velocity-map imaging technique.[33] In the present study, with systematic investigation on electron binding energies (EBEs) of the 12 MXs with DM up to 12.1 D with the addition of diffusion functions in the basis sets, we evaluate the existence of excited DBSs, which could pave the way to reveal the spectrum and behavior of the molecular anions.

In our study, the calculations for electronic properties of the ground state of the neutral MX molecules were

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performed using the multireference configuration interaction with Davidson correction (MRCI + Q) method and restricted open-shell Hartree–Fock singles and doubles and non-iterative inclusion of all triple excitation (RCCSD(T)) levels[34] with the MOLPRO 2012 program package.[35] For H, Li, Na, F and Cl atoms, correlation-consistent polarized weighted core valence basis sets, (cc-pwcv$X$Z; X = T, Q, 5)[36,37] and correlation-consistent polarized valence basis sets with augmenting functions (aug-cc-pVXZ; X = T, Q, 5)[37–39] were employed. For K, Rb, Cs, Br and I, we use the small-core scalar relativistic effective core potentials (ECPs) ECP10MDF,[40] ECP28MDF,[41] ECP46MDF,[40] ECP10MDF,[40] and ECP28MDF,[41] together with the corresponding pseudopotential-based correlation-consistent polarized weighted core valence basis sets (cc-pwCVXZ-PP; X = T, Q, 5)[42,43] and polarized valence basis set augmenting functions (aug-cc-pVXZ-PP; X = T, Q, 5),[42,44] respectively. All calculations were done in the C_{2v} subpoint symmetry group. EBE values of all the MX^- anions were evaluated using the EOM-EA-CCSD[45–48] method in the Q-CHEM program package.[49] For the EOM-EA-CCSD method, we first performed CCSD calculations on the neutral ground state and then the resulting amplitudes were used to build an effective Hamiltonian $e^{-T}He^{T}$ for an anionic state using configuration interaction calculations.[50] Through the sharp decrease of EBE from the aug-cc-pVXZ basis set to aug-cc-pVXZ (+nsnpnd) basis sets, DBXs can be clearly identified. Because the valence excited state is mainly converged at the aug-cc-pVXZ level, the higher diffusion function basis sets have almost no effect on this. A pseudopotential-based correlation-consistent polarized valence triple-ζ basis set with augmenting functions (aug-cc-pVTZ-PP) basis set was used with the addition of the s, p, d-type diffusion functions to verify the excited DBSs of anions. The molecular orbitals (MOs) of the DBSs were plotted using Multiwfn software.[51]

In Table 1 we present the equilibrium bond length R_e, the DM and the adiabatic electron affinity EA_{ad} of the 12 MX neutral molecules; these were calculated with the MRCI + Q/cc-pwcv5Z and RCCSD(T)/aug-cc-pV5Z method. The effect of the basis set on the calculation was investigated and the results are presented in Table S1 in the supporting information. These show systematic improvement of the accuracy with increasing the basis sets from TZ to 5Z. Our calculated results are in relatively good agreement with previous theoretical[30,52,53] and experimental[54–57] results, where available. The DMs of the molecules are between 5.8 D and 12.1 D, which are sufficient to support one or more DBSs,[58] as we will discuss in detail in the following.

Table 1. The equilibrium bond length R_e, the dipole moment (DM) and the adiabatic electron affinity EA_{ad} of LiH, LiF, LiCl, NaF, NaCl, NaBr, RbCl, KI, KCl, KBr, CsI and RbI neutral molecules. R_e is in Å, EA_{ad} is in eV and DM is in Debye.

		LiH	LiF	LiCl	NaF	NaCl	NaBr
R_e (Å)	this work	1.5952	1.5617	2.0179	1.9231	2.3597	2.5005
	Cal.[a]	1.5976	1.5696	2.02	1.9354	2.361	2.502
	Exp.[b]	1.5957	1.5939	2.0207	1.9259	2.3608	2.5020[c]
EA_{ad} (eV)	this work	0.313	0.359	0.584	0.508	0.694	0.755
	Cal.[a]	0.311/0.303	0.357/0.356/0.347	0.578/0.577/0.568	0.511/0.510/0.501	0.710/0.697/0.701	–
	Exp.[d]	0.342 ± 0.012[e]	–	0.593	0.52	0.727	0.788
DM (D)	this work	5.81	6.32	7.2	8.18	9.14	9.29
	Cal.[f]	5.388/5.85[a]	5.993/6.31[a]	7.084/7.06[a]	7.949/8.17[a]	9.146/8.97[a]	9.175
	Exp.[g]	5.882/5.88[h]	6.284/6.33[h]	7.085/7.13[i]	8.123/8.16[h]	8.972/9.00[i]	9.092
		KCl	RbCl	KBr	KI	RbI	CsI
R_e (Å)	this work	2.6697	2.7937	2.8248	3.054	3.1884	3.3364
	Cal.[f]	2.667	2.787	2.821	3.052[j]/3.155[k]	3.334[k]	3.315
	Exp.[c]	2.6666	2.7868	2.8207	3.0478	3.1769	3.315
EA_{ad} (eV)	this work	0.46	0.444	0.558	0.666	0.578	0.498
	Exp.[d]	0.582	0.543	0.642	0.782	–	0.63
DM (D)	this work	10.4	10.68	10.86	11.4	11.21	12.1
	Cal.[f]	10.4	10.751	10.693	11.184	11.741	12.126
	Exp.[g]	10.238	10.483	10.603	11.05	–	12.1

[a]Ref. [30]; [b]Ref. [54]; [c]Ref. [55]; [d]Ref. [56]; [e]Ref. [57]; [f]Ref. [59]; [g]Ref. [60]; [h]Ref. [61]; [i]Ref. [29]; [j]Ref. [52]; [k]Ref. [53].

Because the EOM-EA-CCSD method is based on the equilibrium structure of neutral molecules for the EBEs of various excited states of the anions being calculated, it is necessary to calculate the more accurate equilibrium structure of neutral molecules through the aug-cc-pV5Z basis set. To calculate the excited state of anions, whether it is the T/Q/5 basis set or not, the influence of the diffusion function is more obvious. The calculation of the diffusion function under the large basis set of heavy atoms is difficult, so we use the aug-cc-pVTZ basis set. Therefore, in our study we utilize the EOM-

EA-CCSD calculations on the EBEs of a total of 10 states of each molecular anion MX^- at the aug-cc-pVTZ basis set with the addition of different diffusion functions (+nsnpnd). Most of the electronic states converge to energies higher than that of the neutral ground state $X^1\Sigma^+$, indicating that they are above the detachment threshold and embedded in the continuum region; this will not be discussed in this study. On the other hand, we find that besides the anionic ground state $X^2\Sigma^+$ there is at least one electronic state with a negative EBE for each MX^-, indicating the presence of electronic excited states of the molecular anions. Since a DBS of an anion is analogous to a high Rydberg state, the electronic wavefunction of which is much more diffusive than that of a valence state, we identify whether an anionic excited state is a DBS by adding different diffusion functions in our EBE calculations. Not only the s-type but also the p- and d-type diffusion functions are considered in the aug-cc-PVTZ basis set for the EOM-EA-CCSD calculations in order to identify both σ-type and π-type DBSs of an anion. The results of the EBEs calculated using different basis functions for excited states of all 12 MX anions are summarized in Tables S2–S13 in the supporting information.

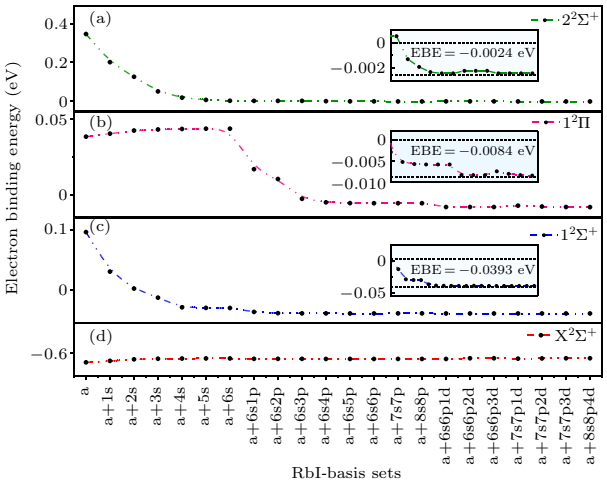


Fig. 1. The electron binding energy (EBE) values of the ground state and three excited states of RbI^- calculated by the EOM-EA-CCSD method at the aug-cc-pVTZ-PP basis sets with the addition of different diffusion functions (+nsnpnd). On the abscissa coordinate, 'a' represents the basis set aug-cc-pVTZ-PP.

As an example, we show in Fig. 1 the dependence of the EBEs on the basis functions for the excited states $1^2\Sigma^+$, $2^2\Sigma^+$ and $1^2\Pi$, as well as the ground state $X^2\Sigma^+$ of the RbI^- anion [the symmetry of each excited state is defined at the equilibrium geometry of the neutral RbI ($X^1\Sigma^+$)]. For the ground state $X^2\Sigma^+$ of the anion, the calculated EBE shows little dependence on the addition of diffusion functions since it is a valence state. On the contrary, a significant decrease in the EBE is observed for the anionic excited states with the addition of the diffusion functions to the aug-cc-pVTZ-PP basis set in EOM-EA-CCSD calculations. As shown in Fig. 1, for RbI^-, the EBE of $1^2\Sigma^+$ drops from +0.0959 eV with the aug-cc-pVTZ-PP basis set to −0.0302 eV with the aug-cc-pVTZ-PP + 8s basis set, and finally converges to −0.0393 eV with the aug-cc-pVTZ-PP+8s8p4d basis set. The addition of p-type or d-type diffusion functions has less effect on the EBE of $1^2\Sigma^+$ than the s-type functions, indicating the state is a σ-type DBS. A similar tendency can be observed in the results for the $2^2\Sigma^+$ state. On the other hand, the p-type and d-type diffusion functions have a more significant effect on the EBE of the $1^2\Pi$ state than the s-type functions, indicating that the $1^2\Pi$ state is a π-type DBS. Then, we identify three DBSs for the RbI^- anion, i.e., two σ-DBSs and one π-DBS. The corresponding bond lengths are 3.1640 Å, 3.1513 Å and 3.1628 Å, respectively, which are very close to the ground state of the neutral RbI molecule (R_{RbI} = 3.1884 Å).

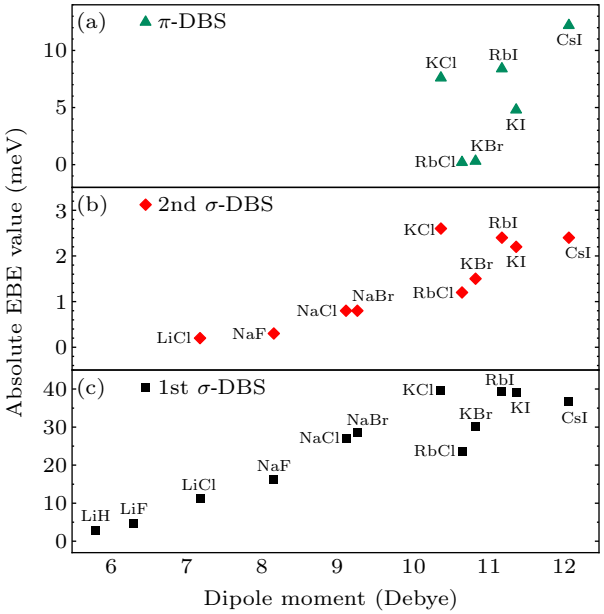


Fig. 2. The absolute electron binding energy (|EBE|) values of the excited dipole-bound states (DBSs) of MX^- = LiH, LiF, LiCl, NaF, NaCl, NaBr, RbCl, KCl, KBr, RbI, KI and CsI molecular anions.

Based on our calculations, we theoretically predict all the possible excited DBSs formed by an additional electron attached to a molecule MX via the electron–dipole interaction. These DBSs lie at energies corresponding to the absolute EBE value (|EBE|) beneath the threshold of the electron detachment level. In Fig. 2, we present the calculated |EBE| value of each DBS of the MX^- anion (for reference, the data for calculated EBE values are given in Table S14 in the supporting information). The x-axis in Fig. 2 lists the MX molecules in increasing order of DM. For LiH and LiF with the smallest DMs among the molecules investigated in the study of 5.81 D and 6.32 D, respectively, only one σ-DBS exists for the corresponding anion, with |EBE| of 2.9 meV and 4.7 meV, respectively. An additional σ-DBS is predicted for anions with a neutral molecular DM larger than 7 D (for LiCl DM = 7.20 D), and a π-type DBS can be supported by a MX with a DM larger than 10 D (for RbCl DM = 10.68 D). One can see that, in general, the

|EBE| of DBS increases with increasing molecular DM, indicating a stronger electron–dipole interaction.

Our study demonstrates the prediction of the finite dipole model,[8] that polar molecules with a large DM could support more than one anionic excited DBS. Investigating a total of 12 alkali halides with DMs in the range 5.81 D–12.1 D, we evaluated the effect of DM on the excited DBSs of anions. In Fig. 3, we summarize the number of anionic excited DBSs of each molecule obtained with the present EOM-EA-CCSD calculations, showing its dependence on the molecular DM. While the ground electronic state is a valence state and the first excited state is always a σ-DBS for each MX^-, the second excited anionic state could be a π-type DBS (for KCl^-, RbI^-, KI^- and CsI^-, DM $>$ 10 D) or a σ-type DBS (for $LiCl^-$, NaF^-, $NaCl^-$ and $NaBr^-$, 7 D $<$ DM $<$ 10 D). The π-DBS and the second σ-DBS of $RbCl^-$ and KBr^- (DM $>$ 10 D) are almost degenerate with an EBE difference of only 1 meV (8.07 cm^{-1}) and 1.2 meV (9.68 cm^{-1}), respectively. While the critical DM for a molecule to form an excited anion in DBSs is still under debate using different models,[25,62–66] our quantum calculations on various molecules with different DMs indicate that there are at least two or three excited DBSs of anions with a molecular DM larger than 7 D or 10 D, respectively. An additional σ-DBS can be formed with DM $>$ 7 D and a molecule with DM $>$ 10 D can sustain a π-DBS of the anion. We should mention that at present only those excited states of an anion with a final |EBE| converging to a value larger than 0.1 meV ($\sim$ 0.8 cm^{-1}) are considered, which would be practical for further high-resolution spectroscopic measurements.

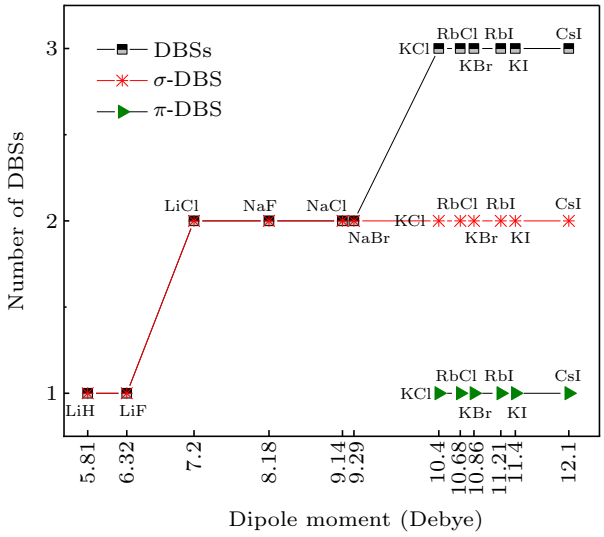


Fig. 3. Number of excited dipole-bound states (DBSs) of 12 alkali-metal-containing diatomic anions as a function of molecular dipole moment.

To date only the KI^- anion has been demonstrated experimentally to have two excited DBSs, i.e., a σ-type DBS at 39.7(10) meV and a π-type DBS at 5.0(12) meV beneath the neutral ground state.[33] Our calculated EBEs are in good agreement with the experimental measurements. The present study provides new information about the energy of excited DBSs, and could pave the way for further experimental investigations of the MX^- anions. Our results indicate that the excited DBSs of MX^- lie very close to below the neutral ground state, especially for the second σ-DBS and the π-DBS of the anions. The |EBE|s of the π-DBS are less than 10 meV and that of the second σ-DBS is less than 3 meV for all 12 MX^- anions investigated in the study (Fig. 2). Further studies with improvement in spectroscopic resolution are necessary to experimentally identify all the excited DBSs of the anions.

In Fig. 4, we further present the MOs of three excited DBSs for RbI^- along with the highest occupied molecular orbital (HOMO) of the ground $X^2\Sigma^+$ state (the results for other anions are similar and are not shown here). While the HOMO of the ground anionic state shows an obvious character of a σ-type valence orbital, the MOs of excited DBSs are very diffusive, with the electron density located far from the neutral MX and at the positive end of the dipole (i.e., the alkali metal atom). The distances between the MO and the nucleus are about 27 Bohr, 76 Bohr and 30 Bohr for the first σ-DBS, the second σ-DBS and the π-DBS of RbI^-, respectively. Thus the second σ-DBS and the π-DBS are more diffusive and lie closer to the neutral ground state than the first σ-DBS, consistent with the calculated EBEs mentioned above.

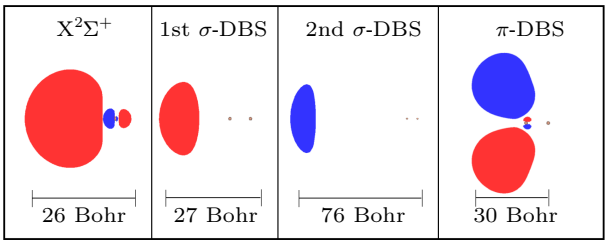


Fig. 4. The HOMO of the ground state and the MOs of the first σ-DBS, the second σ-DBS and the π-DBS of the RbI^- anion. All MOs were plotted with an iso-value of 0.005 except that of the second σ-DBS (0.0008). The Rb atom is on the left.

In summary, we have carried out high-level *ab initio* calculations for 12 alkali-containing diatomic molecular anions. Using the EOM-EA-CCSD method, we have identified possible excited DBSs for each anion by the addition of different diffusion functions in the basis set. Our calculations show that at least two σ-DBSs are present in LiCl, NaF, NaCl and NaBr molecular anions with 7 D $<$ DM $<$ 10 D and for KCl, RbCl, KBr, RbI, KI and CsI molecules with DM $>$ 10 D there exists an additional π-DBS. Our theoretical calculations could provide valuable information for future studies on electronic excited states of alkali halide anions.

Acknowledgments

Project supported by the National Natural Science Foundation of China (Grant Nos. 12274178 and 12174148). Support of High Performance Computing Center of Jilin Uni-

versity and the high-performance computing cluster Tiger@ IAMP is acknowledged.

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