Ab initio study of the alkali-dimer cation Li₂⁺

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Abstract

The potential energy curves and the spectroscopic constants of the electronic states of $^2\Sigma_{g,u}^+$, $^2\Pi_{g,u}$ and $^2\Delta_{g,u}$ symmetries of Li₂⁺ ionic system dissociating into Li (2s, 2p, 3s, 3p, 3d, 4s and 4p) + Li⁺, have been calculated using an *ab initio* approach. A non-empirical pseudo potential for the Li (1s²) core has been involved and a core–core and core–valence correlation have been added. A good agreement has been obtained for the ground and the first excited states with the available theoretical and experimental works. However, a clear disagreement between this study and the model potential work of [S. Magnier, S. Rousseau, A.R. Allouche, G. Hadinger, M. Aubert-Frécon, Chem. Phys. 246 (1999) 57] has been observed for several excited states. They found that the 6–7 $^2\Sigma_g^+$, 3–4, 6 $^2\Sigma_u^+$, 2 $^2\Pi_g$, 4 $^2\Pi_u$ and 1 $^2\Delta_u$ states are repulsive, although they are attractive with potential well depths of 10, 100 and 1000 cm⁻¹ in our study.
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Keywords: *Ab initio*; Li₂⁺; Spectroscopic constants

1. Introduction

The alkali dimers have been the subject of numerous theoretical and experimental investigations [1–19]. This is due to the simplicity of such systems with no more than two valence electrons. Experimentally, they are relatively easy to be handled. Their spectroscopy has been extensively studied using high resolution methods. Theoretically, their reduced number of valence electrons allowed high quality of *ab initio* calculations. The alkali dimers form prototype systems for investigation of non adiabatic coupling, collision process radiative association and dissociation, diabatisation and predissociation. In theory, several techniques have been used to study alkali dimers. Most of them have proposed to reduce the number of electrons to only valence electrons, by using pseudo potential or model potential replacing the effect of core electrons on the valence electron. Both methods non-empirical pseudo potential technique and model potential, have been used in the past. In

the model potential calculation, which has been developed first by Bottcher and Dalgarno [20], the alkali cations XY⁺ are treated as a system with one electron under a potential to fit experimental atomic energy levels. The use of pseudo potentials for X and Y cores reduce the number of active electrons to only one valence electron, where the SCF calculation produces the exact energy in the basis and the main source of errors corresponds to the basis-set limitations. Furthermore, we correct the energy by taking into account the core–core and core–electron correlation following the formalism of Foucrault et al. [21]. This formalism was used first for Rb₂ and RbCs molecules and later for several systems (LiH, LiH⁺, Li₂⁺, LiNa⁺) and its use was demonstrated efficiency. The non empirical pseudo potentials permit the use of very large basis sets for the valence and Rydberg states and allow accurate descriptions for the highest excited states.

Despite the relative simplicity of the Li₂⁺ system, few theoretical and experimental works have been done. For our best knowledge, only the ground state is experimentally explored [18,19]. Recently, Magnier et al. [1] have performed a model potential calculation for the ground and various excited states for Li₂⁺. The produced data have

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been exploited by Magnier et al. [2] to perform a simulation of one and two-color experiment on above threshold dissociation by monitoring an avoided crossing with femtosecond spectroscopy (ATD). The same work has been done recently for Na_2^+ [4,5] and $LiNa^+$ [9] using their potential energy curves [3,10]. This molecular process involves both bound–free and free–free transition and requires accurate potentials. In this study, Li_2^+, having only one active electron, will be a one of the simplest systems and the computing time is reduced. The present work succeeds our study on many diatomic systems, such as LiH [11], LiH^+ [12], $LiNa^+$ [13], LiK^+ [14] NaK^+ [15,16] and KRb^+ [17]. For all of them, we got a remarkable accuracy which shows the validity of this approach. The present results for Li_2^+, can be expected to reach a similar accuracy since the main restriction in the accuracy of the calculation is the basis set limitation. We present a complete set of results including all Rydberg states.

In the next section, we briefly present the computational method. In Section 3, we present the potential energy curves and their spectroscopic constants for the ground and numerous excited states of $^2\Sigma_{g,u}^+$, $^2\Pi_{g,u}$ and $^2\Delta_{g,u}$ symmetries dissociating into Li (2s, 2p, 3s, 3p, 3d, 4s and 4p) + Li^+. Finally we summarize our conclusion in Section 4.

2. Method of calculation

In this work, the Li atom is treated trough a one electron pseudopotential proposed by Barthelat et al. [22] in its semilocal form and used in many previous works [11–17]. For the simulation of the interaction between the polarizable Li^+ core and the valence electrons, a core polarization potential V_{CPP} is used according to the operatorial formulation of Müller et al. [23].

$$V_{CPP} = -\frac{1}{2} \sum_\lambda \alpha_\lambda f_\lambda . f_\lambda,$$

where α_λ is the dipole polarizability of the core λ and f_λ is the electric field produced by valence electrons and all other cores on the core λ.

$$f_\lambda = \sum_i \frac{\vec{r}_{i\lambda}}{r_{i\lambda}^3} F(r_{i\lambda}, \rho_\lambda) - \sum_{\lambda' \neq \lambda} \frac{\vec{R}_{\lambda'\lambda}}{R_{\lambda'\lambda}^3} Z_\lambda$$

where $r_{i\lambda}$ is a core–electron vector and $R_{\lambda'\lambda}$ is a core–core vector.

According to the formulation of Foucrault et al. [21], the cutt-off function $F(r_{i\lambda}, \rho_\lambda)$ is taken to be a function of l to consider differently the interaction of valence electrons of different spatial symmetry with core electrons.

$$F(r_{i\lambda}, \rho_\lambda) = \sum_{l=0}^\infty \sum_{m=-l}^{+l} F_l(r_{i\lambda}, \rho_\lambda^l) |lm\lambda\rangle\langle lm\lambda|,$$

where $|lm\lambda\rangle$ is the spherical harmonic centered on λ. $F(r_{i\lambda}, \rho_\lambda^l)$ is the cut-off operator expressed following the Foucrault et al. [21] formalism by a step function defined by

$$F(r_{i\lambda}, \rho_\lambda^l) = \begin{cases} 0, & r_{i\lambda} < \rho_\lambda \\ 1, & r_{i\lambda} > \rho_\lambda \end{cases}$$

It has a physical meaning of excluding the valence electrons from the core region for calculating the electric field. In Müller et al. [23] formalism, the cut-off function is unique for a given atom, generally adjusted to reproduce the atomic energy levels for the lowest states of each symmetry. The cut-off radii for the lowest valence s, p, d and f one-electron states are, respectively, 1.434, 0.982, 0.600 and 0.400 a.u. For lithuim, we used the same basis set of gaussian-type orbital (GTO) as in our previous works [11–14]. The core dipole polarizability of Li is 0.1915 a_0^3. Table 1 presents a comparison between our *ab initio*, the model potential [1] and the experimental [24] dissociation limit for all the electronic states dissociating into $Li^+ + Li$ (2s, 2p, 3s, 3p, 3d, 4s and 4p). There is a very good agreement between our dissociation energies and the experimental [24] ones. The difference between our work and the experimental values does not exceed 27×10^{-6} a.u ($6 \, cm^{-1}$). Such accuracy will be transmitted to the molecular energy. The potential energy calculations have been performed using the standard chain of programs of the Laboratoire de Physique Quantique de Toulouse.

3. Results and discussion

The potential energy curves of the molecular states dissociating into $Li^+ + Li$ (2s, 2p, 3s, 3p, 3d, 4s and 4p) have been computed for a large and dense grid of intermolecular distance from 3 to 200 a.u. They are displayed in Figs. 1–3,

Table 1
Dissociation energies (in a.u): comparison between our calculated energy, Magnier et al. [1] model potential calculated energy and the corresponding experimental dissociation

| Dissociation limit	Our work	Magnier et al. [1]	Experiment [24]	ΔE	ΔE [1]
$Li^+ + Li(2s)$	−0.198141	−0.198107	−0.198142	1×10^{-6}	3×10^{-5}
$Li^+ + Li(2p)$	−0.130227	−0.130200	−0.130235	8×10^{-6}	3×10^{-5}
$Li^+ + Li(3s)$	−0.074155	−0.074299	−0.074182	27×10^{-6}	1×10^{-4}
$Li^+ + Li(3p)$	−0.057232	−0.057303	−0.057236	4×10^{-6}	7×10^{-5}
$Li^+ + Li(3d)$	−0.055591	−0.055570	−0.055606	15×10^{-6}	4×10^{-5}
$Li^+ + Li(4s)$	−0.038602	−0.038672	−0.038615	13×10^{-6}	6×10^{-5}
$Li^+ + Li(4p)$	−0.031954	−0.032013	−0.031974	20×10^{-6}	4×10^{-5}
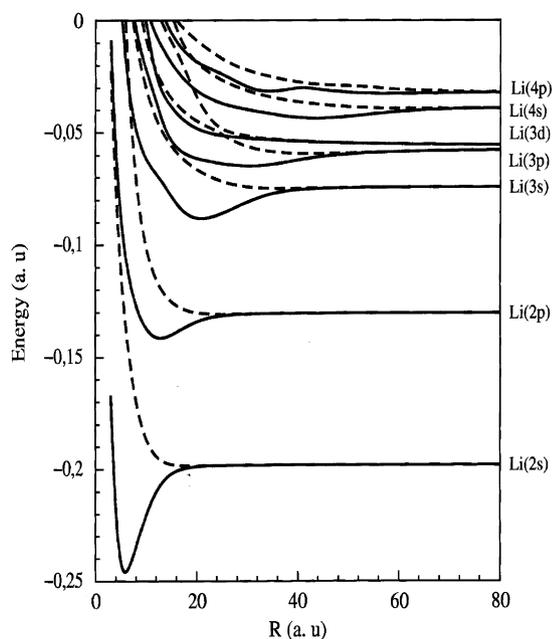
Fig. 1. Potential energy curves of the $^2\Sigma_g^+$ (solid line) and $^2\Sigma_u^+$ (dashed line) electronic states of Li_2^+ ionic molecule.
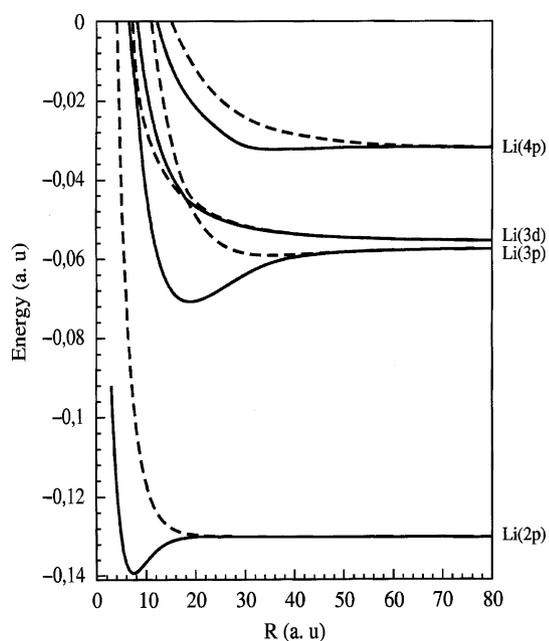

Fig. 2. Potential energy curves of the $^2\Pi_g$ (solid line) and $^2\Pi_u$ (dashed line) electronic states of Li_2^+ ionic molecule.

Fig. 3. Potential energy curves of the $^2\Delta_g$ (solid line) and $^2\Delta_u$ (dashed line) electronic states of Li_2^+ ionic molecule.

respectively, for the $^2\Sigma_{g,u}^+$, $^2\Pi_{g,u}$ and $^2\Delta_{g,u}$ symmetries. Several electronic states are found to be repulsive such as the 5 $^2\Sigma_g^+$, 5, 7 $^2\Sigma_u^+$, 1, 3–4 $^2\Pi_g$, 3 $^2\Pi_u$ and 1 $^2\Delta_g$. Numerous avoided crossings exist between neighbour states of same symmetry. Their existences are related to the charge transfer process between the two ionic systems Li^+Li and $LiLi^+$.

The spectroscopic constants (R_e, D_e, T_e, ω_e, $\omega_e\chi_e$ and B_e) of the ground and the low lying states are presented in Tables 2 and 3 and compared with the other theoretical
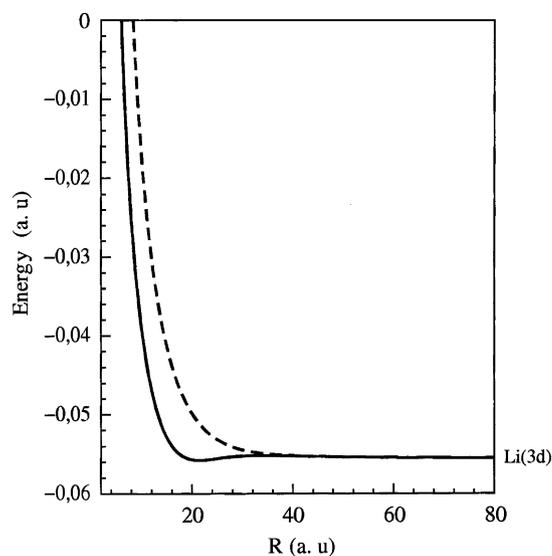
[1,25–27] and experimental [18,19] works. For our best knowledge, the only theoretical *ab initio* study done for Li_2^+ are the works of Müller and Meyer [25], Schmidt-Mink et al. [26] and Konowalow and Rosenkrantz [27]. They have reported the spectroscopic constants for the ground state and the first excited states. Our work can be considered as the first *ab initio* calculation on the higher excited states. Magnier et al. [1] have also explored many excited states by a model potential calculation. Therefore, the comparison for these excited states will be done, only between our work and that of Magnier et al. Our ground state equilibrium distance R_e is in good agreement, as well as the well depth D_e, with the work of Müller and Meyer [25]. We find for R_e and D_e, respectively 3.095 Å and 10475 cm^{-1} and they found 3.096 Å and 10444 cm^{-1}. The difference between our and their values is 0.001 Å for R_e and 31 cm^{-1} for D_e. This very good agreement between our results and those of Müller et al. for the ground state is also observed for ω_e, $\omega_e\chi_e$ and B_e spectroscopic constants. Our values for ω_e, $\omega_e\chi_e$ and B_e are, respectively, 264, 1.94 and 0.506 cm^{-1} and their values are 265.5, 1.89 and 0.501 cm^{-1}. This excellent agreement for all spectroscopic constants for the ground state is not surprising since we used similar method. Our ground state well depth is also in good agreement with the experimental [18,19] value of 10464 cm^{-1}. The 1 $^2\Sigma_u^+$ state is found to be weakly bound with a potential well depth of 88 cm^{-1} located at a rather large equilibrium distance of 9.911 Å. Magnier et al. [1], Schmidt-Mink et al. [26] and Konowalow and Rosenkrantz [27] have seen the same observation. They found a potential well depth of, respectively, 90, 90 and 86 cm^{-1} located at 10.001, 9.95 and 10.30 Å. A very good agreement between our and the other works [1,26] is observed for the transition energy T_e of the 1 $^2\Sigma_u^+$ state. Our T_e is equal to 10387 cm^{-1} to be compared with the value of Magnier et al. [1] and Schmidt-Mink et al. [26] of, respectively,

Table 2
Spectroscopic constants of the ground and excited $^2\Sigma_{g,u}^+$, electronic states of Li_2^+

State	R_e (Å)	D_e (cm^{-1})	T_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e\chi_e$ (cm^{-1})	B_e (cm^{-1})	Reference
$1\,^2\Sigma_g^+$	3.095	10475		264	1.94	0.506	This work
	3.122	10466		263.08	1.477	0.4945	[1]
	3.110	10464		262	1.7	0.496	[18,19]
	3.096	10444		265.5	1.89	0.501	[25]
	3.099	10441		263.76	1.646	0.5006	[26]
	3.127	10324					[27]
$1\,^2\Sigma_u^+$	9.911	88	10387	15.81	0.74	0.048998	This work
	10.001	90	10376	16.01	0.790	0.0493	[1]
	9.950	90	10350	20.10	0.130	0.0490	[26]
	10.300	86					[27]
$2\,^2\Sigma_g^+$	6.741	2424	22955	79.23	0.49	0.106	This work
	6.879	2525	22844	84.16	0.684	0.1154	[1]
	6.654	2390	22987	82.94	0.623	0.1085	[26]
$2\,^2\Sigma_u^+$	13.276	125	25255	12.44	0.34	0.027565	This work
	13.229	131	25239	13.07	0.401	0.0278	[1]
$3\,^2\Sigma_g^+$	11.08	3093	34593	54.56	0.16	0.039	This work
	11.113	3143	34496	56.62	0.212	0.0405	[1]
$3\,^2\Sigma_u^+$	19.478	169	37518	11.05	0.17	0.012805	This work
	Repulsive						[1]
$4\,^2\Sigma_g^+$	16.499	1674	39714	25.27	0.10	0.017	This work
	16.404	1724	39644	22.14	0.095	0.0178	[1]
$4\,^2\Sigma_u^+$	23.03	421	40967	14.21	0.15	0.004227	This work
	Repulsive						[1]
$5\,^2\Sigma_g^+$	Repulsive						This work
	Repulsive						[1]
$5\,^2\Sigma_u^+$	Repulsive						This work
	Repulsive						[1]
$6\,^2\Sigma_g^+$	23.05	1051	44432	18.57	0.04	0.0091	This work
	Repulsive						[1]
$6\,^2\Sigma_u^+$	33.31	130	45353	6.98	0.07	0.004227	This work
	Repulsive						[1]
$7\,^2\Sigma_g^+$	18.25	−188	47130	33.61	0.23	0.01457	This work
	28.22	133	46808	9.01	0.23	0.01457	This work
	Repulsive						[1]
$7\,^2\Sigma_u^+$	Repulsive						This work
	Repulsive						[1]

10376 and 10350 cm^{-1}. The $2\,^2\Sigma_g^+$ state is found to be attractive with a potential well of 2424 cm^{-1} located at $R_e = 6.741$ Å in good agreement with Magnier et al. [1] and Schmidt-Mink et al. [26]. They found for D_e and R_e, respectively, 2525 cm^{-1} and 6.879 Å, and 2390 cm^{-1} and 6.654 Å. The $1\,^2\Pi_g$ state is repulsive in good agreement with the model potential calculation, while the $1\,^2\Pi_u$ state is found to be attractive ($D_e = 1995$ cm^{-1}) with a rather closed equilibrium distance ($R_e = 3.952$ Å) to that of the ground state ($R_e = 3.095$ Å). This is in accord with the available *ab initio* [26,27] and model potential [1] studies.

For our best knowledge, there are neither experimental nor *ab initio* theoretical results for the other excited states. Equilibrium distance of all these states is found at intermediate and long range internuclear distances. Magnier et al. [1] have reported in their work the potential energy curves of 58 electronic states of Li_2^+ correlated to $Li^+ + Li$ (2s) up to $Li^+ + Li$ (6g), over internuclear distances from 4 to 40 a.u (1.59–21.16 Å). They found that only 1–4 $^2\Sigma_g^+$, 1–2 $^2\Sigma_u^+$, 1–2 $^2\Pi_u$ and $1\,^2\Delta_g$ are bound states. The other studied states are repulsive. We remark that the $5\,^2\Sigma_g^+$ and 5, $7\,^2\Sigma_u^+$ electronic states, which are dissociating into $Li^+ + Li(3d)$ and $Li^+ + Li(4p)$, are repulsive in good agreement with the model potential calculation [1]. In contrast to the 1–4 $^2\Sigma_g^+$ and 1–2 $^2\Sigma_u^+$ states, where the agreement between our work and the model potential calculations is good, there is a disagreement for the 6–7 $^2\Sigma_g^+$ and 3, 4 and 6 $^2\Sigma_u^+$ states. In the model potential calculation, the five states are repulsive, while they are found in our work to be attractive with potential wells of, respectively, 1051, 133, 169, 421 and 130 cm^{-1} located at, 23.05, 28.22, 19.478, 23.03 and 33.31 Å. Their vibrational frequencies (ω_e) are, respectively,

Table 3
Spectroscopic Constants of the excited $^2\Pi_{g,u}^+$, and $^2\Delta_{g,u}$ electronic states of Li_2^+

State	R_e (Å)	D_e (cm^{-1})	T_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e\chi_e$ (cm^{-1})	B_e (cm^{-1})	Reference
$1^2\Pi_g$	Repulsive						This work
	Repulsive						[1]
$1^4\Pi_u$	3.952	1995	23388	110.5	1.19	0.310921	This work
	4.022	2100	23270	108.26	1.246	0.3108	[1]
	3.976	2103	23277	105.58	0.922	0.3040	[26]
	4.014	1852					[27]
$2^2\Pi_g$	18.653	411	41009	18.15	4.69	0.014183	This work
	Repulsive						[1]
$2^2\Pi_u$	9.99	2979	38565	45.74	0.08	0.048655	This work
	9.631	3330	38039	50.79	0.86	0.0527	[1]
$3^2\Pi_g$	Repulsive						This work
	Repulsive						[1]
$3^2\Pi_u$	Repulsive						This work
	Repulsive						[1]
$4^2\Pi_g$	Repulsive						This work
	Repulsive						[1]
$4^2\Pi_u$	19.272	72	46879	12.30	2.87	0.013031	This work
	Repulsive						[1]
$1^2\Delta_g$	Repulsive						This work
	9.578	324	45626	28.14	0.431	0.0556	[1]
$1^2\Delta_u$	21.52	52	41877	20.52	0.38	0.037447	This work
	Repulsive						[1]

18.57, 9.01, 11.05, 14.21 and 6.98 cm^{-1}. The equilibrium distances of these states are located at intermediate and large distance and their dissociation energies (D_e) are of the order of 100 and 1000 cm^{-1}. The model potential proprieties have been extracted from potential energy curves calculated between $R_{min} = 1.59$ Å and $R_{max} = 21.16$ Å and our equilibrium distance for the 6, 7 $^2\Sigma_g^+$ and 3, 6 $^2\Sigma_u^+$ states ($R_e = 23.05, 28.22, 23.04$ and 33.31 Å) are larger than R_{max}. This can explain the raison why they do not find the potential wells associated to these states. Although, our equilibrium distance for the 3 $^2\Sigma_u^+$ state ($R_e = 19.478$ Å) is shorter than R_{max}, this state is purely repulsive in the model potential calculation.

For the $^2\Pi_{g,u}$ and the $^2\Delta_{g,u}$ electronic states, the potential energy curves are shown, respectively, in Figs. 2 and 3. Their spectroscopic constants are reported in Table 3 and compared with the model potential data. For our best knowledge, there is no experimental information for the $^2\Pi_{g,u}$ and the $^2\Delta_{g,u}$ electronic states. We remark that the 1, 3–4$^2\Pi_g$ and 3$^2\Pi_u$ states are repulsive in accord with Magnier et al. [1] calculations. A rather good agreement between our spectroscopic constants and those of the model potential calculations is observed for the $1^2\Pi_u$ and $2^2\Pi_u$ states. Their dissociation energies (D_e) are, respectively, 1995 and 2979 cm^{-1} to be compared with the model potential values of 2100 and 3330 cm^{-1}. We remark that our dissociation energy, for the two states, is lower than theirs values. The 1 and 2 $^2\Pi_u$ equilibrium distances are, respectively, 3.952 and 9.99 Å to be compared with 4.022 and 9.631 Å [1]. The same agreement is observed for the

vibrational frequencies (ω_e). We find for the latter, respectively, 110.5 and 45.74 cm^{-1} and they found 108.26 and 50.79 cm^{-1}. The $2^2\Pi_g$, $4^2\Pi_u$ and $1^2\Delta_u$ states are in our work attractive and they have potential wells located, respectively, at 18.653, 19.272 and 21.53 Å of, respectively, $D_e = 411, 72$ and 52 cm^{-1}. In the model potential calculations [1], these states were repulsive. The $1^2\Delta_g$ state is, in our work, repulsive in disagreement with the model potential calculation, where it is attractive and presents a relative deep well of 324 cm^{-1} at an equilibrium distance $R_e = 9.578$ Å.

From the comparison of our results with the model potential calculation, we remark first, a good agreement between the two works for the 1–5 $^2\Sigma_g^+$, 1–2, 5, 7 $^2\Sigma_u^+$, 1, 3–4$^2\Pi_g$ and 1–3$^2\Pi_u$ states. Second a disagreement for 6–7 $^2\Sigma_g^+$, 3–4, 6 $^2\Sigma_u^+$, 2 $^2\Pi_g$, 4 $^2\Pi_u$, $1^2\Delta_g$ and $^2\Delta_u$ states, is observed. The latter states are found to be attractive with potential wells of 10, 100 and 1000 cm^{-1}, while they are repulsive in the model potential calculation [1].

4. Conclusion

In this paper, we have reported an *ab initio* calculations for the ground and many excited states of the Li_2^+ ionic molecule dissociating up to $Li^+ + Li(4p)$ using the pseudo potential method. We have determined the potential energy curves and their spectroscopic constants for 24 electronic states of $^2\Sigma_{g,u}^+$, $^2\Pi_{g,u}$ and $^2\Delta_{g,u}$ symmetries. The spectroscopic constants of the ground and the first excited states have been compared with the available theoretical

[1,25–27] and experimental [18,19] results. A good agreement has been observed between our spectroscopic constants and the available theoretical and experimental values for the ground, $1^2\Sigma_g^+$, and the first excited states, $1\,^2\Sigma_u^+$ and $2\,^2\Sigma_g^+$. The comparison between our *ab initio* study and the model potential calculation done by Magnier et al. [1] has shown: first, a good agreement between the two works for the 1–5 $^2\Sigma_g^+$, 1–2, 5, 7 $^2\Sigma_u^+$, 1, 3–4 $^2\Pi_g$ and 1–3 $^2\Pi_u$ states. These states are in our work attractive, while they are repulsive in the model potential study. Second, a discrepancy for 6–7 $^2\Sigma_g^+$, 3–4, 6 $^2\Sigma_u^+$, 2 $^2\Pi_g$, 4 $^2\Pi_u$, $1\Delta_g$ and 1 $^2\Delta_u$ states is observed. The disagreement between our pseudopotential *ab initio* and the model potential calculations was also mentioned in the past for the LiNa$^+$ [13] ionic molecule. Furthermore, this discrepancy between the two works can not be due to the core–core and core–valence correlation effects, which strongly influence the lithium asymptotic spectrum and the shape of the potential curves, because this is present in the two methods of calculation. In fact, this discrepancy can be understood by the optimization, in the model potential calculation of the cut-off radius to produce only the spectroscopic constants of the ground state. Further, full electron theoretical calculations and experimental investigations on the homonuclear X$_2^+$ and the heteronuclear XY$^+$ ionic molecules have to be done for the higher excited states to understand clearly the discrepancy between the model potential and the pseudopotential *ab initio* calculations.

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