PHYSICAL REVIEW A VOLUME 43, NUMBER 1 1 JANUARY 1991

Selective-state charge transfer in a collision between a Li^{3+} ion and a ground-state Li atom: A molecular-state approach

A. Kumar* and N. F. Lane
Department of Physics, Rice Quantum Institute, Rice University, Houston, Texas 77251

M. Kimura
Argonne National Laboratory, Argonne, Illinois 60439
and Department of Physics, Rice Quantum Institute, Rice University, Houston, Texas 77251

(Received 4 June 1990)

The semiclassical, impact-parameter method, based on a 15-state molecular-orbital expansion, is employed to calculate the cross sections for charge transfer in Li^{3+}-Li collisions. Electron-translation effects have been taken into account. In addition to total capture, cross sections for capture into individual states have also been calculated. The present results show qualitative agreement with the other available theory; details, however, are different. It is found that this reaction, through state-selective capture into the $n=4$ manifold of Li^{2+}, may provide a useful mechanism to achieve population inversion necessary for short-wavelength lasers.

I. INTRODUCTION

Electron capture by multiply charged ions is important from both fundamental and practical perspectives. Cross sections for such reactions provide useful input data for the study of astrophysical plasmas, the search for soft-x-ray lasers, and the diagnostics of controlled thermonuclear fusion (for example, see Kadota *et al.*[1] and references therein). Such processes also provide tests of various theoretical models. For example, studies of few-electron systems (i.e., few active electrons outside closed shell) at intermediate collision energies using atomic- and molecular-orbital methods[2-17] have provided good tests of the methods as well as the approximations therein. In these studies, the total electronic wave function of the colliding system is expanded in terms of either atomic states or adiabatic molecular states. In general, it has been found that the atomic-state expansion yields good results for higher energies[2], but at lower energies the molecular-state results appear to be better suited as they take account of molecular binding effects which are expected to be significant in low-energy collisions. Attempts have been made by Fritsch and Lin[2-5] who take care of this aspect by including some of the tightly bound orbitals of the united atom: AO+method. The resulting calculations seem to be in better agreement with the experimental observations at low impact energies.

As stated earlier, the molecular expansion method has been found to be suited to the low- to intermediate-energy region in particular. However, as shown by Bates and McCarroll,[18] use of a finite basis set may lead to inaccurate results if the motion of the electrons translating along with the nuclei is not taken into account. Noninclusion of the electron translation factor (ETF) in such calculations causes spurious long-range couplings among various states, and thus presents an overall wrong picture of the interaction. Kimura and co-workers[6-14] have successfully used the ETF corrected molecular-orbital (MO) method to calculate charge-transfer cross sections in case of various reactions.

In the present study, the charge-transfer cross sections for the reaction

$$Li^{3+}+Li(2s)\rightarrow Li^{2+}(nl)+Li^{+} \tag{1}$$

are calculated by making use of the MO expansion method in which electron-translation effects have been taken into account using the atomic-ETF approach (see, for example, Ref. 18). To the best of our knowledge, there exist no experimental measurements of this reaction. Attempts were made by Stollberg and Lee[19] to estimate the cross sections for the above system as a means of achieving population inversion for short-wavelength lasers. They used the Stueckelberg-Landau-Zener (SLZ) model[20] to estimate $\sigma_{\max}$ (the peak of the cross section) in the velocity range 0.05–0.5 a.u. Because the SLZ model is known to fail in cases where the internuclear distance at the crossing is large (see Bates[21]), the authors considered only capture into the $n=3$ manifold of Li^{2+}. However, the dynamics of this reaction, as we will see later, suggest that capture into the $n=4$ manifold of Li^{2+} should be the dominant process. This early theoretical attempt has been considerably improved by Opradolce, Casaubon, and Piacentini,[17] who used a molecular-state description of the above reaction. By making use of a model potential, they obtain the electronic energies of the $Li_2{}^{3+}$ quasimolecule formed during the collision. They then estimate the coupling matrix elements, which are used to solve the close-coupled equations to determine electron-capture cross sections. They replace the pseudocrossings by real crossings and define diabatic states in terms of combinations of various adiabatic molecular states. This reduces the number of effective states involved in the collision and enables them to employ a three-state calculation to estimate the capture cross sections over a large range of impact energies. In addition to the omission of capture into the $n=3$ and 5 manifolds of Li^{2+}, which may be important under certain circumstances, this calculation does not provide a realistic picture of the l distribution of the probability of charge transfer into the $n=4$ manifold of Li^{2+}, since the Π states were ignored while solving the close-coupled equations.

In the present treatment, we attempt to provide a detailed molecular description of the colliding system in which all Σ and Π states that are important are taken into account. We present calculations not only of the total capture cross sections but also of the cross sections for individual states. We note that cross sections for capture into individual states can be important in the search for soft-x-ray lasers.[1] The capture cross sections for specific nl levels may change rapidly with energy, e.g., in case of highly charged ions, even though the total cross section exhibits slow energy variation.[10] Thus, through the present study we intend not only to provide a reliable theoretical estimate of the specific cross sections, but also to encourage the experimental determination of partial cross sections as well as the total.

The paper is organized as follows. Section II provides a short description of the theoretical formulation. In Sec. III we provide the details of the molecular structure calculations. Results for the total as well as the partial charge-transfer cross sections are presented and discussed in Sec. IV. Concluding remarks appear in Sec. V. Throughout the article we use atomic units ($m=e=a_0=\hbar=1$) unless stated otherwise.

II. THEORETICAL FORMULATION

Since the details of the theoretical formulation have been provided in a number of previous articles (for example, see Kimura, Sato, and Olson[9]), we present only the basic outline and specific information about the present calculation. In the semiclassical formulation, the total time-dependent, electronic wave function for the interacting system is expanded in terms of an ETF modified molecular basis set

$$\Psi=\sum_i a_i(t)\Phi_i(\mathbf{r},\mathbf{R})F_i(\mathbf{r},\mathbf{R}) , \tag{2}$$

where $\Phi_i(\mathbf{r},\mathbf{R})$ is the adiabatic wave function, $F_i(\mathbf{r},\mathbf{R})$ is the ETF, and R depends explicitly on time according to the classical trajectory chosen; we assume a straight-line path. The adiabatic wave functions are represented in terms of a linear combination of atomic orbitals constructed from Slater-type orbitals (STO). Substitution of Eq. (2) into the time-dependent Schrödinger equation yields the standard set of coupled equations

$$i\dot{a}_j=E_j a_j+\sum_i \mathbf{v}\cdot(\mathbf{P}+\mathbf{A})_{ji}a_i , \tag{3}$$

where E_j is the adiabatic potential energy. The vectors $\mathbf{P}$ and $\mathbf{A}$ are the nonadiabatic coupling matrix and its ETF correction term, respectively. The coupling $\mathbf{v}\cdot(\mathbf{P}+\mathbf{A})$ can be expressed as a sum of radial and angular terms

$$\mathbf{v}\cdot(\mathbf{P}+\mathbf{A})=\dot{R}(P+A)^R+\dot{\theta}(P+A)^\theta . \tag{4}$$

Forms of these coupling matrix elements have been given by Kimura, Sato, and Olson.[9] In Eq. (3) the effect of the ETF has been included to first order in v in the form of an atomic ETF.[18] The probabilities (i.e., squares of the coefficients a_j) for transitions from the initial state to various possible final states are provided by the solutions of the coupled Eqs. (3) and, on being integrated over all possible values of the impact parameters, yield the respective cross sections.

III. MOLECULAR STRUCTURE CALCULATION

Through the use of the pseudopotential method,[22] the short-range part of the pseudopotential due to the core is given by an l-dependent Gaussian type expression

$$V_p^{sr}=\sum_{l,m} A_l\exp(-\xi_l r^2)|Y_{lm}\rangle\langle Y_{lm}| , \tag{5}$$

where $|Y_{lm}\rangle$ represents the spherical harmonics. The long-range part due to dipole and quadrupole interactions is expressed with a cutoff parameter d as

$$V_p^{lr}(r)=-\alpha_d/[2(r^2+d^2)^2] -\alpha_q/[2(r^2+d^2)^3]-Z_{\mathrm{eff}}/r . \tag{6}$$

The l-dependent parameters A_l and ξ_l for the core Li^+, chosen to fit the spectroscopic data, have been given by Bardsley.[22] Z_{eff} is an effective charge and is 2 and 3 for Li^{2+} and Li^{3+}, respectively.

By making use of the pseudopotentials and a modified valence bond configuration-interaction (CI) method,[9], we find that the calculated atomic energy levels for the Li^{2+} ion agree very well with the spectroscopic values.[23] Actually, the maximum difference between the calculated and spectroscopic values never exceeds 0.3%; in most of the cases the difference is less than 0.1%. In case of Li(2s) as well, the calculated energy value is within 0.1% of its spectroscopic value.

The potential energies correlating to the initial channel as well as to the capture channels Li^{2+} ($n=4$) are presented in Fig. 1 (see also Fig. 2). For the sake of clarity only the Σ states are shown here. In Table I, we list molecular states considered for the present calculation. As observed by Opradolce, Casaubon, and Piacentini,[17] we also find that energy separations at avoided crossings among Li $2s\,\Sigma$, $4f\,\Sigma$, $4d\,\Sigma$, and $4p\,\Sigma$ are small ($\sim 10^{-5}$ a.u.). Consequently, the colliding pair can diabatically pass onto the $4p\,\Sigma$ state even if the collision energy lies in the low-keV region (see also Kumar, Lane, and Kimura[24]). This enables us to construct a diabatic state, as has also been done by Opradolce, Casaubon, and Piacentini, in the following way:

$$\begin{aligned}\Sigma_{\mathrm{diab}}&=4p\,\Sigma(R\le 24.0)+4d\,\Sigma(24.0\le R\le 25.75)\\&\quad+4f\,\Sigma(25.75\le R\le 27.0)\\&\quad+\mathrm{Li}\,2s\,\Sigma(R>27.0) .\end{aligned}$$

However, in contrast to Opradolce, Casaubon, and Piacentini,[17] we have explicitly retained all the Π states. We have used 25 and 12 configurations, respectively, for constructing the Σ and Π molecular states.[7] Finally we

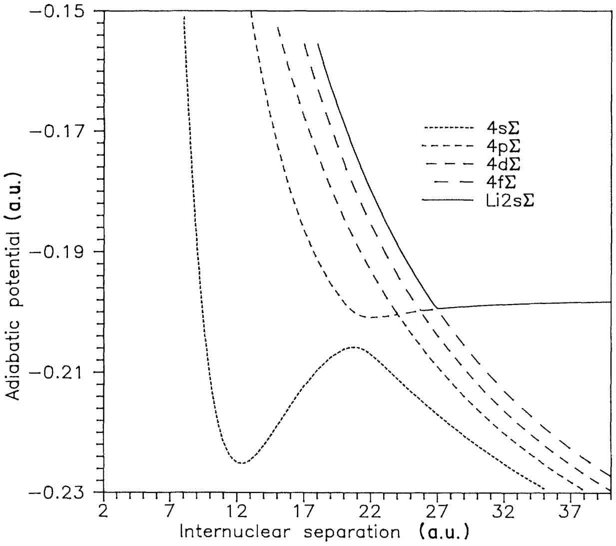

FIG. 1. Adiabatic potential energies of $(\mathrm{LiLi})^{3+}$ correlating to the initial channel and the $n=4$ manifold of Li^{2+}.

have carried out two sets of (15- and 5-state) semiclassical calculations for charge transfer in reaction (1). A number of test calculations with a smaller, as well as a larger, MO basis have also been performed to test convergence of the expansion of the wave function

Coupling matrices

The important radial coupling relevant to the present calculation is between Σ_{diab} and $4s\ \Sigma$ and has a peak around $R \sim 22a_0$, the region of avoided crossing between the corresponding molecular states. These states couple with different Σ states correlating to $\mathrm{Li}^{2+}(n=3)$ at small R values. They are also responsible for populating $\mathrm{Li}^{2+}(n=3)$ at higher energies. The initial state Σ_{diab} also couples the upper states around $R=14a_0$; these couplings, however, are not very strong.

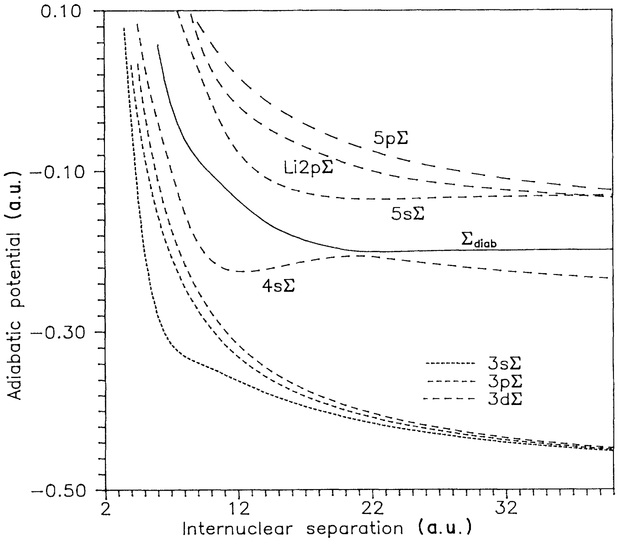

FIG. 2. Adiabatic potential energies including additional states.

TABLE I. Molecular states used in the present calculation.

Approximate asymptotic state	Molecular state Σ	Π
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(3s)$	$3s\ \Sigma$	
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(3p)$	$3p\ \Sigma$	$3p\ \Pi$
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(3d)$	$3d\ \Sigma$	$3d\ \Pi$
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(4s)$	$4s\ \Sigma$	
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(4p)^{a}$	$4p\ \Sigma$	$4p\ \Pi$
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(4d)^{a}$	$4d\ \Sigma$	$4d\ \Pi$
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(4f)^{a}$	$4f\ \Sigma$	$4f\ \Pi$
$\mathrm{Li}^{3+}+\mathrm{Li}(2s)^{a}$	Li $2s\ \Sigma$	(Initial channel)
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(5s)$	$5s\ \Sigma$	
$\mathrm{Li}^{3+}+\mathrm{Li}(2p)$	Li $2p\ \Sigma$	Li $2p\ \Pi$
$\mathrm{Li}^{+}+\mathrm{Li}^{2+}(5p)$	$5p\ \Sigma$	$5p\Pi$

[a]combine to make Σ_{diab}.

Angular couplings among various molecular states correlating to the $n=4$ manifold of Li^{2+} also play an important role in the charge-transfer reaction (1). The initial channel Σ_{diab} couples significantly with the immediate neighboring state ($4f\ \Pi$) in two different regions. The first coupling is observed in the range of $14.5a_0 \le R \le 26a_0$, followed by another coupling in the small-R region around $R \sim 6a_0$. Flux captured into $4f\ \Pi$, however, does not stay there permanently as different Σ and Π states correlating to the $n=4$ manifold of Li^{2+} tend to couple with one another over the whole range of R values.

IV. RESULTS AND DISCUSSION

We have carried out a 15-state (eight Σ and seven Π) calculation to estimate the charge-transfer cross sections for reaction (1). In this calculation are incorporated all Σ and Π states correlating to the $n=3$ and 4 manifolds of Li^{2+} along with the ground and the first excited state of Li ($2p$). From the $n=5$ manifold of Li^{2+} we include only the Σ and Π states of the $5s$ and $5p$ states. This seems to be quite sufficient in light of the fact that capture into the $n=5$ manifold is not very important in the low-energy region (see also Table I). The capture cross sections so obtained are presented in Fig. 3.

Opradolce, Casaubon, and Piacentini[17] have reported low-energy oscillations in their calculated cross sections for the Li^{3+}-Li pair. To investigate the low-energy behavior up to 1 keV amu^{-1} of the present results we carried out another set of calculations involving a smaller number of states. Nearly 93% of the total charge transfer at an impact energy of 1 keV amu^{-1} comes from capture into $\mathrm{Li}^{2+}(n=4)$. The relative contribution of capture into other manifolds (like $n=3$ and 5) of Li^{2+} is significant only at higher energies; a point we will return to later. Consequently, a five-state calculation (Σ_{diab}, $4s\ \Sigma$, $4p\ \Pi$, $4d\ \Pi$, and $4f\ \Pi$) which accounts for total capture into the $n=4$ manifold of Li^{2+}, should be

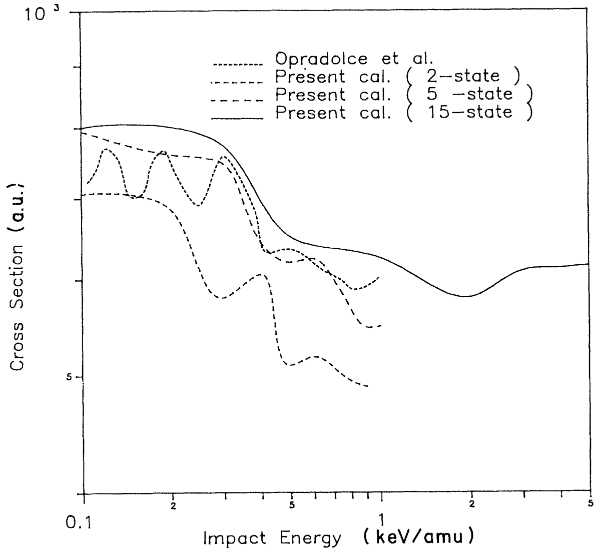

FIG. 3. Cross sections for electron capture by Li^{3+} from Li(2*s*).

sufficient to make a reliable estimate of the charge-transfer cross sections at low impact energies. These calculated cross sections, up to the impact energy 1 $keV\,amu^{-1}$, are graphically represented in Fig. 3.

Beyond 1 $keV\,amu^{-1}$, the selectivity of the charge-transfer process seems to be losing ground and the $n=3$ and 5 manifolds of Li^{2+} enter the picture. At 1 $keV\,amu^{-1}$, capture into the $n=3$ and 5 manifolds of Li^{2+} account for 4.1% and 2.9%, respectively, of the total capture cross sections. The contribution of capture into $Li^{2+}(n=3)$ rises rapidly with increase in the impact velocity, becoming more than 31% at an impact energy of 5 $keV\,amu^{-1}$. Thus in going from 1 $keV\,amu^{-1}$ to 5 $keV\,amu^{-1}$ we observe an increase of nearly 27% in the relative contribution of capture into $Li^{2+}(n=3)$, which is of nearly the same magnitude as the decrease in the relative contribution of capture into the $n=4$ manifold of Li^{2+}. The magnitude of the partial cross section for capture into $Li^{2+}(n=5)$ is found to increase slowly with increasing impact energies. Strong couplings in the small-*R* region, among various Σ and Π states correlating to Li^{2+} ($n=3$ and 4), are responsible for flux transfer to the $n=3$ manifold of Li^{2+} at higher impact energies. Within the $n=3$ manifold of Li^{2+}, capture into the 3*p* state has the maximum probability in the investigated energy region; and both Σ and Π states make approximately equal contributions. On the other hand, formation of the Π state dominates that of the Σ state in leading to capture into $Li^{2+}(3d)$.

Inclusion of Π states appears to be important for estimating the cross sections for total as well as partial charge transfer. Capture into $Li^{2+}(4p)$ due to formation of the 4*p* Π state is the dominant process at moderate and higher energies (above 0.7 $keV\,amu^{-1}$).

To assess the importance of including Π states in the present calculation we carried out another set of two-state test calculations. As we will see later, such calculations are also helpful in understanding the low-energy behavior of the capture cross sections. In this two-state calculation Σ_{diab} is taken as the initial state and 4*s* Σ represents the final capture channel. By comparing the two-state result with the previously obtained 5- and 15-state results, we find that inclusion of the Π states not only augments the magnitude of the total capture cross section but also alters the *l* distribution of the partial cross sections. For example, the five-state calculation suggests that capture into the 4*p* state of Li^{2+} would have an appreciable probability in the low-energy region. This result is significant from the point of view of laser application since $Li^{2+}(4p)$, through direct deexcitation to the ground state, can produce soft-x-ray lasers, whereas deexcitation of $Li^{2+}(4s)$ takes place only through cascade. Since Opradolce, Casaubon, and Placentini[17] do not include Π states in their calculation (see Fig. 3), their calculated cross sections may be somewhat smaller than the true capture cross sections. Moreover, their calculation does not yield the *l* distribution of the partial cross sections.

To test the convergence of our cross sections we compare the results of the 15-state calculations at a number of impact energies in the low-energy region. At an impact energy 0.1 $keV\,amu^{-1}$, the cross sections for total capture obtained through the 15-state calculation is only 1% larger than that obtained in the 5-state calculation. As the impact energy increases, the difference between the two sets of results is found to increase slowly. For example, the two sets of cross sections agree within 3% and 5% at impact energies 0.3 and 0.5 keV $eV\,amu^{-1}$, respectively. At an impact energy of 1 $keV\,amu^{-1}$, the two agree to within 7%. A discussion of convergence also should address the effect of neglecting higher $|m_l|$ molecular states (e.g., Δ and Φ), which are ignored in the present calculation as well. We assessed the effect of this approximation by carrying out a few test calculations at energies around the peak value of the cross sections. It is found that inclusion of Δ states has very little effect on the magnitudes of either the total or partial capture cross sections. In fact, at the peak the two sets of calculations (including and excluding Δ states) agree within 5%. It is also found that inclusion of $|m_l|=2$ states enhances the partial cross section for electron capture into $Li^{2+}(4d)$ alone; the rest of the cross sections remain unaffected. Noninclusion of Φ states is not expected to cause any significant change in the cross sections. We conclude that the maximum uncertainty in our cross sections, due to neglect of higher $|m_l|$ states, is about 5%. Similarly, neglect of molecular states correlating to other higher excited states of Li or Li^{2+} is not expected to cause any significant change in our cross sections.

Comparison with other results

Opradolce, Casaubon, and Piacentini[17] have carried out a three-state calculation using the MO expansion method to estimate capture cross sections for reaction (1) in the low-energy region (up to 1 keV amu^{-1}). Since they neglected the Π states correlating to various capture channels, their calculation cannot provide accurate cross sections for electron capture into specific states. However, it is still interesting to see how our calculated results compare with the magnitudes of their total capture cross sections (see Fig. 3). Since they have carried our their calculations at energies where capture into the $n=4$ manifold of Li^{2+} is expected to be the dominant process, we compare their cross sections with our five-state results.

As observed by Opradolce, Casaubon, and Piacentini,[17] we also find some oscillations in the magnitude of the total charge-transfer cross section in the low-energy region. Beyond 0.4 keV amu^{-1}, both sets exhibit similar oscillations in the cross sections but the oscillations are out of phase. Also, at lower energies, our cross sections are in general larger than theirs, and we obtain a somewhat different oscillation pattern. Instead of obtaining three peaks, as reported by Opradolce, Casaubon, and Piacentini,[17] the present calculation exhibits only one flat peak. This difference may be due to the neglect of Opradolce, Casaubon, and Piacentini,[17] of the Π states, which not only cause differences in the magnitude of the total capture cross section, but also give a significantly different l distribution of the partial cross sections. We also note that the model of Opradolce, Casaubon, and Piacentini,[17] is not appropriate at higher impact energies, where capture into the $n=3$ manifold becomes significant. Also, the error introduced due to their neglect of the electron-translation effect will become increasingly important at higher impact energies.

Now we focus our attention on oscillations observed in the cross sections at low impact energies. It is clear that our two-state and five-state calculations exhibit nearly the same low-energy dependence except for a slight shift in the positions of oscillations. Also the two-state calculation yields smaller cross sections than the five-state calculation. The low-energy behavior of the cross sections (both by two- and five-state calculations) should be viewed as Stuckelberg-Landau-Zener oscillations arising due to the presence of an extremum in the difference between the two most strongly coupled electronic states involved in the charge exchange process (for example, see Olson[25]). Opradolce, Casaubon, and Piacentini[17] refer to the peculiar molecular energy behavior at internuclear distance around $10a_0$ as the possible reason for the oscillation.

V. CONCLUDING REMARKS

We have carried our a semiclassical MO calculation of charge-transfer cross sections for the reaction $\mathrm{Li}^{3+}+\mathrm{Li}$. This collision process is found to proceed primarily via electron capture into the $n=4$ manifold at low impact energies. With increasing impact energy, the selectivity of charge transfer is weakened as capture into the $n=3$ manifold also becomes significant. Up to 1 keV amu^{-1}, nearly 93% of the total charge transfer arises from selective population of $\mathrm{Li}^{2+}(n=4)$. This reaction therefore provides a possible mechanism for a soft-x-ray laser system. The cross sections have been compared with the other available theoretical results.[17] We hope that the calculations will encourage the experimental studies of both the total and partial cross sections for charge transfer in the reaction reported here, especially in the low-energy region where high state selectivity and oscillatory behavior of the calculated cross sections are of particular interest.

ACKNOWLEDGMENTS

This work was supported in part by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, and the Robert A. Welch Foundation (A.K. and N.F.L.), and by the U.S. Department of Energy, Office of Health and Environment Research (M.K.)

---

*On leave from Department of Physics, D.A.V. College, Siwan 841 226, India.

[1] K. Kadota, D. Dijkkamp, R. K.van der Woude, A. de Boer, Pan Guan Yan, and F. J. de Heer, J. Phys. B **15**, 3275 (1982).

[2] W. Fritsch and C. D. Lin, J. Phys. B **15**, 1255 (1982).

[3] W. Fritsch and C. D. Lin, J. Phys. B **15**, L281 (1982).

[4] W. Fritsch and C. D. Lin, J. Phys. B **16**, 1595 (1983).

[5] W. Fritsch and C. D. Lin, J. Phys. B **17**, 3271 (1984).

[6] M. Kimura and W. R. Thorson, Phys. Rev. A **24** 1780 (1981)

[7] M. Kimura, R. E. Olson, and J. Pascale, Phys. Rev. A **26**, 3113 (1982).

[8] M. Kimura and W. R. Thorson, J. Phys. B **16**, 1471 (1983).

[9] M. Kimura, H. Sato, and R. E. Olson, Phys. Rev. A **28**, 2085 (1983).

[10] M. Kimura and R. E. Olson, J. Phys. B **17**, L713 (1984).

[11] M. Kimura and R. E. Olson, J. Phys. B **18**, 2729 (1985).

[12] H. Sato, M. Kimura, A. E. Wetmore, and R. E. Olson, J. Phys. B **16**, 3037 (1983).

[13] N. Shimakura, H. Sato, M. Kimura, and T. Watanabe, J. Phys. B **20**, 1801 (1987).

[14] F. K. Men, M. Kimura, and R. E. Olson, Phys. Rev. A **33**, 3800 (1986).

[15] R. J. Allan, J. Phys. B **19**, 321 (1986).

[16] A. E. Wetmore, H. R. Cole, and R. E. Olson, J. Phys. B **19**, 1515 (1986).

[17] L. Opradolce, J. I. Casaubon, and R. D. Piacentini, J. Phys. B **22**, 1809 (1989).

[18] D. R. Bates and R. McCarroll, Proc. R. Soc. London Ser. A **245**, 175 (1958).

[19] M. T. Stollberg and W.-H. Lee, Phys. Rev. A **29**, 2448 (1984).

[20] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon, Oxford, 1960), Chap. XIII.

[21] D. R. Bates, Proc. R. Soc. London Ser. A **257**, 22 (1960).
[22] J. N. Bardsley, Case Stud. At. Phys. **4**, 299 (1974).
[23] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U.S.) Circ. No. 467 (U.S. Department of Commerce, Washington, D.C., 1949), Vol. 1.
[24] A. Kumar, N. F. Lane, and M. Kimura, Phys. Rev. A **42**, 3861 (1990).
[25] R. E. Olson, Phys. Rev. A **2**, 121 (1970).