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Electron-impact ionization of L-shell atomic species

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Electron impact ionization cross sections (EIICS) of 30 *L*-shell targets, with open- and closed-shell configurations in the isoelectronic sequences ranging from Li to Ne, are evaluated using the generalized parameters of our recent modification of BELL formula (MBELL) [Haque *et al.*, Phys. Rev. A **73**, 012708 (2006)]. Three sets of parameters, one each for the 1*s*, 2*s*, and 2*p* orbits, provide an excellent account of the experimental EIICS data of atomic targets, neutral and ionic, up to the atomic number $Z=92$ and incident energies up to about 250 MeV. In comparison with the quantum mechanical predictions, it is found that the present MBELL cross sections are in better agreement with the experimental results.

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I. INTRODUCTION

Electron impact ionization (EII) is of fundamental importance in understanding the physics of the collision process, many-electron transitions, electron correlations, structure of matter, etc. Besides this, EII cross sections (EIICS), among other atomic data, are needed in modeling and diagnostics of laboratory and astrophysical plasmas. As such, EIICS find important applications in such diverse fields as mass spectrometry, radiation science, semiconductor physics, atmospheric physics, astrophysics, x-ray laser, and fusion research.

The EIICS data are generated from experiments and theoretical methods. A detailed quantum mechanical calculation of accurate EIICS is, in principle, possible. But in practice, it involves a many-body reaction mechanism and leads to many approximations. Recently, a fully quantun mechanical convergent closed coupling [1,2] method was applied to the calculation of atomic EIICS. However, this method was computationally intensive and had only been applied to a few electrons in the valence shell. Experiments and quantum theories produce data for selected targets and values of the incident energies. On the other hand, the applications, as mentioned earlier, which require EIICS data for a wide range of energies and targets including the exotic ones, demand rapid calculations of cross sections. Analytical or semianalytical models of sufficient accuracy are commonly used rather than quantum mechanical methods. Good reviews of the simple-to-use models for the EIICS data are given in [3,4].

The semirigorous model of Deutsch and Märk (DM) [5] has been widely applied to neutral atoms and molecules [6–12] The binary-encounter-dipole (BED) model of Kim and Rudd [13] has enjoyed many more applications in molecular targets [14–18] than their atomic counterparts. The DM and BED models have not been applied to ionic atomic targets except for one- or two-electron ions. Recently, Bernshtam *et al.* [19] analyzed published data and proposed an empirical formula, henceforth referred to as the BRY model, valid for atomic targets with charge $q>1$. The empirical formula of Bell *et al.* (BELL) [20,21] has been used extensibly to fit data for light atomic targets, neutral or ionic. The parameters of the model in these applications have been species dependent, varying even among the members of the same isoelectronic series. Moreover, the BELL formula has no relativistic ingredient in its structure, essential for the treatment of ionization at high energies as observed by Uddin *et al.* [22]. Recently, Haque *et al.* [23] modified the BELL formula (MBELL) and applied it with success to the *K*-shell ionization for wide ranges of atoms and ions, and incident energies using a single set of parameters.

As mentioned earlier, the DM and BED models have restricted applications on atomic ions. The BRY model has no relativistic component in its structure. The parameters of the DM and BRY models are dependent upon the angular momentum l of the contributing sub shell. The work of Uddin *et al.* [22] used l-dependent parameters in their modified improved BED model with relativistic and ionic corrections (MRIBED model). The success of the MBELL model [23] encouraged us to generalize the parameters of the MBELL model in the line of the DM, BRY and MRIBED models, so that one can easily obtain the cross sections of the direct single ionization for wide ranges of atomic species and incident energies. We seek to generalize the parameters to

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TABLE I. The BELL parameters A and B's, and the ionic parameters m and λ for the $1s$, $2s$, and $2p$ orbits. The parameters are in the unit of 10^{-13} eV^2 cm^2.

	Parameter values							
Orbit	A	B_1	B_2	B_3	B_4	B_5	m^b	λ^b
$1s^a$	+0.525	−0.510	+0.200	+0.050	−0.025	−0.100	+3.000	+1.270
$2s$	+0.530	−0.410	+0.150	+0.150	−0.200	−0.150	+3.000	+1.270
$2p$	+0.600	−0.400	−0.710	+0.655	+0.425	−0.750	+3.000	+0.542

[a]Parameters of [23] for the K-shell ionization.
[b]m and λ parameters are same for $1s$ and $2s$ orbits.

encompass wide ranges of targets, as far as possible.

This work reports the results of MBELL calculations using the generalized parameters for L-shell atoms and ions. The parameters of the MBELL model are obtained from a fitting procedure on reliably measured EIICS data for atomic species selected from the members of the Li, Be, B, C, N, O, and Ne isoeletronic series. Our MBELL calculations produce good to excellent agreement with the available experimental data for these targets.

The paper is organized as follows. The derivation of the MBELL model is outlined in Sec. II. In Sec. III, we discuss the procedure for extracting the parameters of the MBELL model, examine the deduced parameters in describing the the total EIICS data of 30 species in the range from Li to Ne

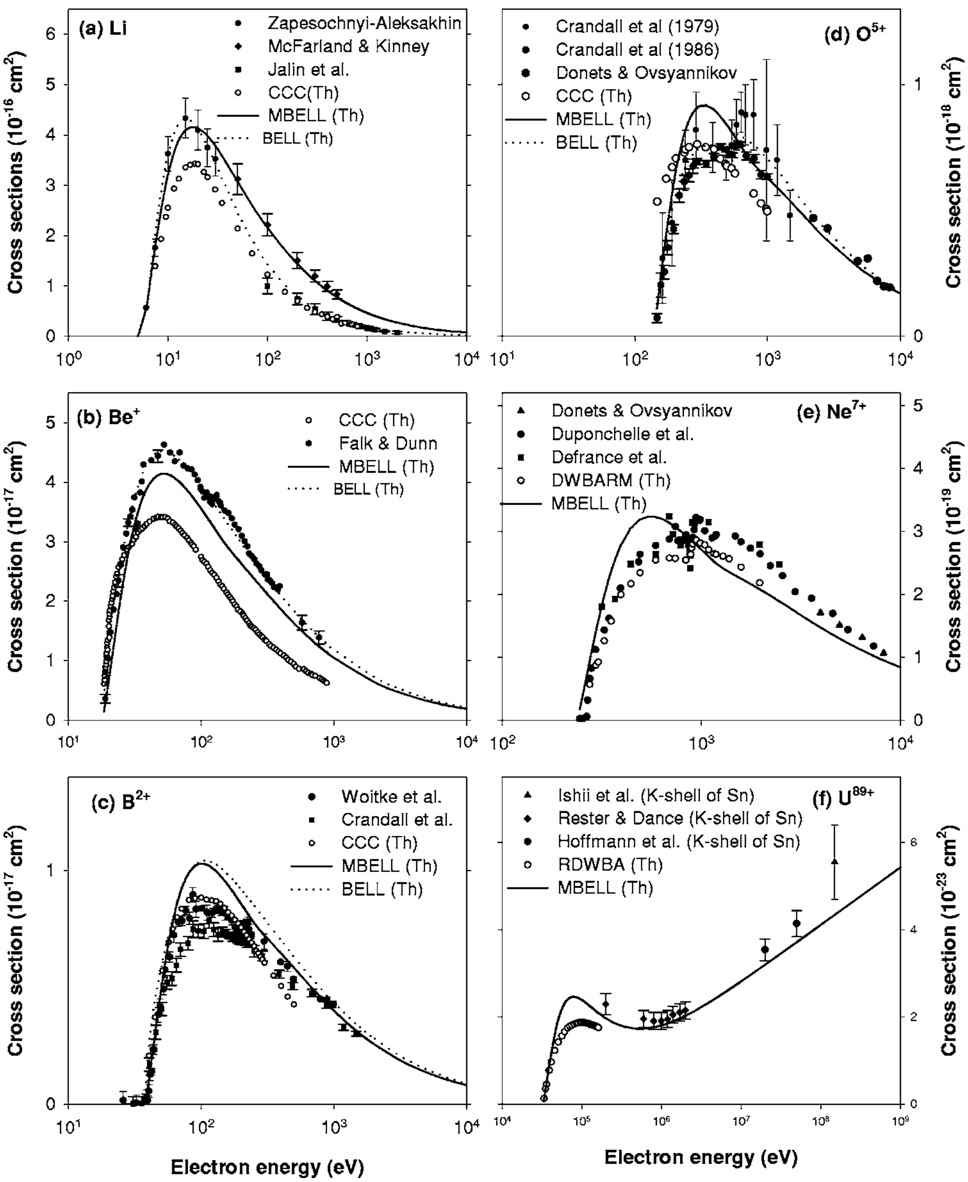

FIG. 1. EIICS of Li-like targets: (a) Li, (b) Be$^+$, (c) B^{2+}, (d) O^{5+}, (e) Ne^{7+}, and (f) U^{89+}. The data in (f) are evaluated from the K-shell ionization cross sections of Sn.

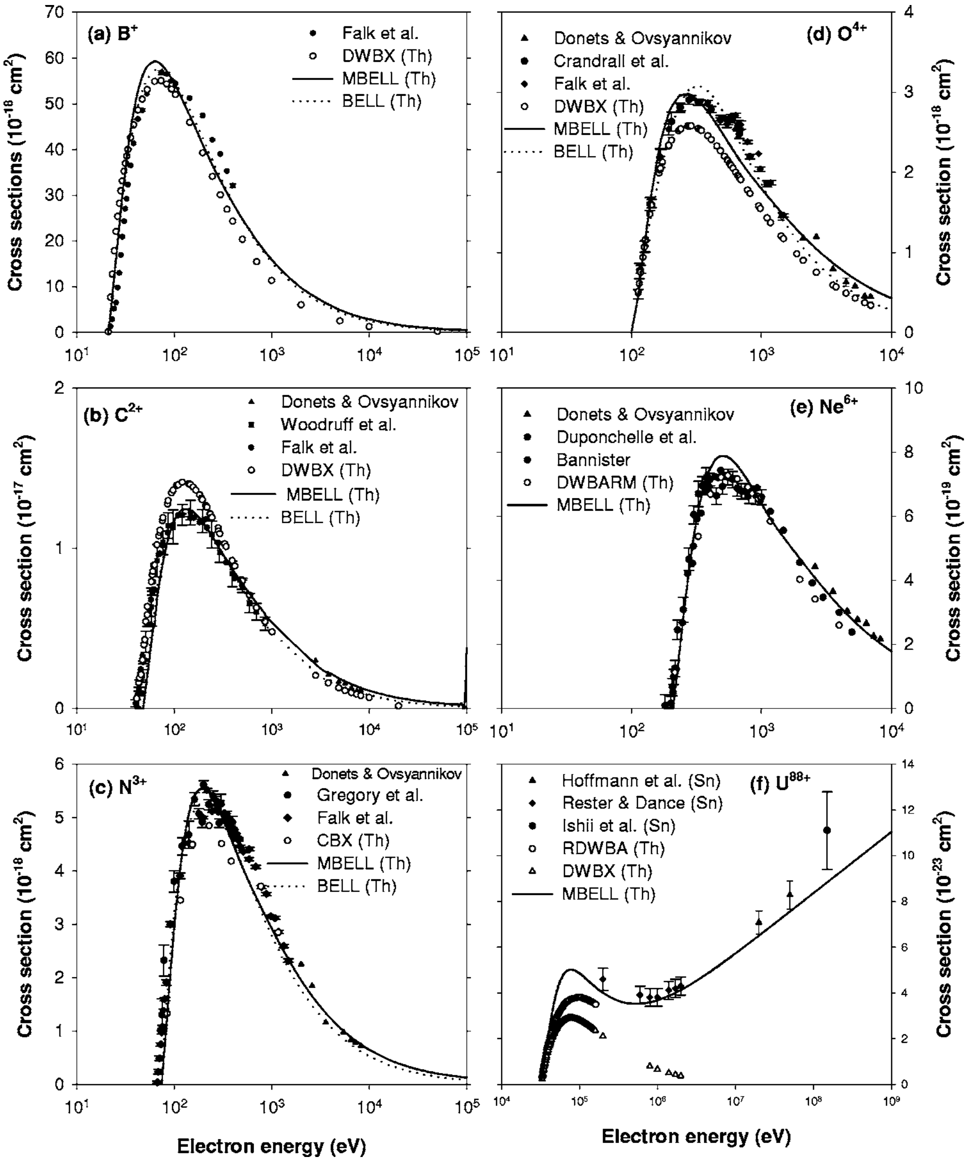

FIG. 2. Same as in Fig. 1 for Be-like targets: (a) B^+, (b) C^{2+}, (c) N^{3+}, (d) O^{4+}, (e) Ne^{6+}, and (f) U^{88+}.

isoelectronic sequences, and then compare the performance of the model with other theoretical methods. Section IV deals with a brief summary of the conclusions.

II. THEORETICAL BACKGROUND

The total cross section of electron impact single ionization, according to Haque *et al.* [23], contributed from different ionized *nl* orbits is given by

$$\sigma_{\mathrm{MBELL}}(E) = \sum_{nl} N_{nl} F_{\mathrm{ion}} G_R \sigma_{\mathrm{BELI}}(E), \tag{1}$$

where N_{nl} is the number of electrons in the ionized *nl* orbit. σ_{BELI} has the form [20,23]:

$$\sigma_{\mathrm{BELI}}(E) = \frac{1}{I_{nl}E}\left[A \ln\left(\frac{E}{I_{nl}}\right) + \sum_{K=1}^{5} B_K\left(1 - \frac{I_{nl}}{E}\right)^K\right]. \tag{2}$$

Here, E is the energy of the incident electron and I_{nl} is the ionization potential of the *nl* orbit. A and B_K's are the fitting (BELL) parameters. G_R is the Gryzinski's relativistic factor [24] defined in terms of the reduced energy $U=E/I_{nl}$ as

$$G_R = \left(\frac{1+2J}{U+2J}\right)\left(\frac{U+J}{1+J}\right)^2 \times\left(\frac{(1+U)(U+2J)(1+J)^2}{J^2(1+2J)+U(U+2J)(1+J)^2}\right)^{1.5}, \tag{3}$$

where $J=m_e c^2/I_{nl}$ with m_e as the electron rest mass. F_{ion} is the ionic correction factor involving the ionic parameters m and λ having the form:

$$F_{\mathrm{ion}} = 1 + m\left(\frac{q}{UZ}\right)^{\lambda}. \tag{4}$$

Here $q=Z-N_U$, with N_U representing the total number of electrons from the interior 1*s* orbit up to the relevant *nl* orbit, is the effective charge of the target as seen by the incident electron.

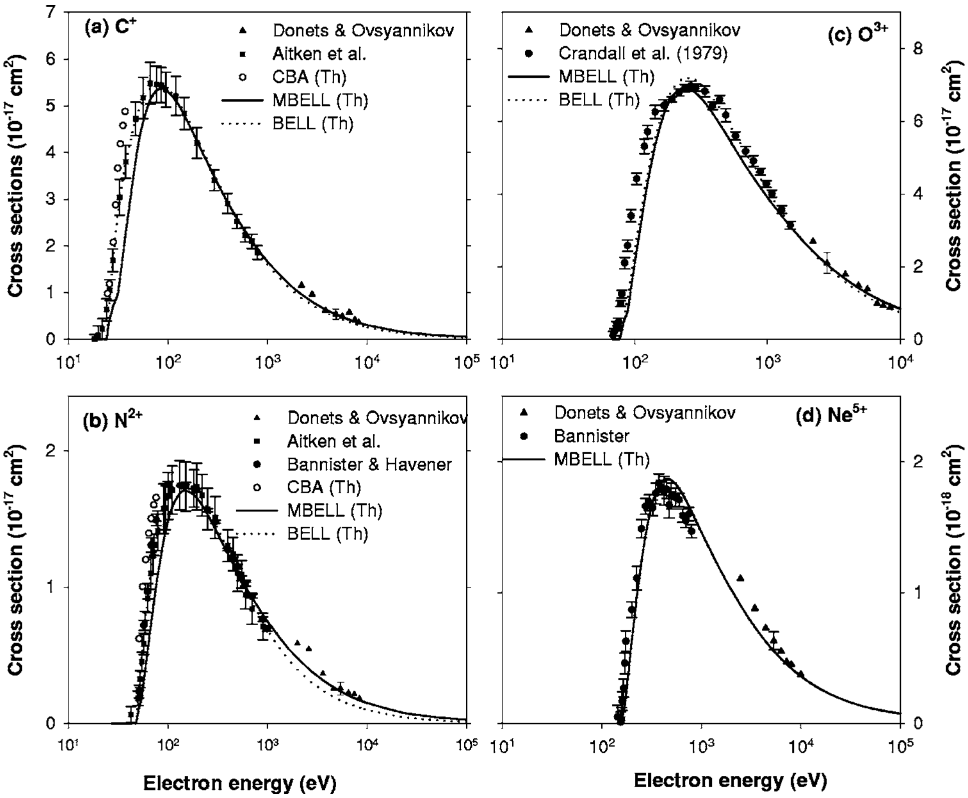

FIG. 3. EIICS B-like targets: (a) C^{+}, (b) N^{2+}, (c) O^{3+}, and (d) Ne^{5+}.

III. RESULTS AND DISCUSSIONS

The ionization potentials I_{nl} of the ionic targets are calculated from the Dirac-Hartree-Fock code [25] and those for the neutrals are taken from Desclaux [26]. A nonlinear least-squares fitting program is used to optimize the values of the BELL parameters A and B_i with $i=1-5$ in Eq. (2), and the ionic parameters m and λ in Eq. (4). The results of our systematic analyses of the experimental EIICS data for targets in the H, He, Li, Be, B, C, N, O, F, and Ne isoelectronic sequences suggest that the BELL parameters A and B_i's are dependent on the nl quantum numbers of the ionized orbits, while ionic parameters m and λ can be made to depend solely on the orbital quantum number l and are independent of the principal quantum number n.

In the analyses, we obtained the BELL parameters for an ionized orbital nl from fitting the EIICS data of the neutral atoms having their outer orbit with the configuration nl. The ionic parameters were then extracted from the experimental data of the ionic targets. Having obtained the values of m and λ for a particular l, these parameters are then employed for all orbits with the same l and different n. In the present work, the Bell parameters for the $1s$ orbit are taken form the work of [23], where the parameters have been deduced from fitting the EIICS data on the K-shell ionization of 14 atomic targets with the atomic number in the range $1 \le Z \le 92$ over a wide range of incident energies. The ionic parameters for s orbits, obtained from the analysis of the experimental EIICS data for the ionic targets in the H and He isoelectronic sequences, are collected from [27]. For the L-shell targets, these BELL parameters for the $1s$ orbit and the ionic parameters for s-orbits, which are noted in Table I, are held fixed.

The BELL parameters for the $2s$ orbit have been deduced from the best fit to the data of the neutral Li atom. The data are from Zapesochnyl and Aleksakhin [28], McFarland and Kinney [29], and Jalin *et al.* [30]. The fit is shown in Fig. 1(a) and the parameters are listed in Table I. These extracted BELL parameters coupled with the ionic parameters for the s orbits, previously obtained [27] from fitting the data of the ionic H and He-like targets, are examined for the Li-like ionic targets, namely Be^{+}, B^{2+}, O^{5+}, Ne^{7+}, and U^{89+} [Figs. 1(b)–1(f)]; as well as the ionic Be-like targets, namely B^{+}, C^{2+}, N^{3+}, O^{4+}, Ne^{6+}, and U^{88+} [Figs. 2(a)–2(f)]. The sources of the EIICS data are Falk and Dunn [31] for Be^{+}; Woitke *et al.* [32], and Crandall *et al.* [33] for B^{2+}; Crandall *et al.* [33,34], and Donets and Ovsyannikov [35] for O^{5+}; [35], Duponchelle *et al.* [36], and Defrance *et al.* [37] for Ne^{7+}; Falk *et al.* [38] for B^{+}; [35,38], and Woodruff *et al.* [39] for C^{2+}; [35,38], and Gregory *et al.* [40] for N^{3+}; [33,35,38] for O^{4+}; and [35,36], and Bannister [41] for Ne^{6+}. For the U^{89+} and U^{88+} targets, the evaluated cross sections have been used for the experimental EIICS data. The method of evaluation has been given in [22] for U^{89+}, and in [42] for U^{88+}, where the K-shell ionization cross sections for Sn, from Ishii *et al.* [43], Hoffmann *et al.* [44], and Rester and Dance [45], have been employed in both cases. The basis for evaluation is that the ionization potential $I_{1s} \approx 28.3$ keV and the kinetic energy of a bound electron $T_{1s} \approx 33.3$ for the K-shell of Sn being fairly close to $I_{2s} \approx 27.7$ keV and $T_{2s} \approx 27.8$ keV for the $2s$ orbit of U ions, the cross sections for U^{89+} and U^{88+} are, respectively, given by $\sigma_{2s}[U^{89+}] \approx 0.5\sigma_{1s}[Sn]$ and $\sigma_{2s}[U^{88+}] \approx \sigma_{1s}[Sn]$.

The BELL parameters A and B_i's for the $1s$ and $2s$ orbits, in conjunction with the single set of the ionic m and λ pa-

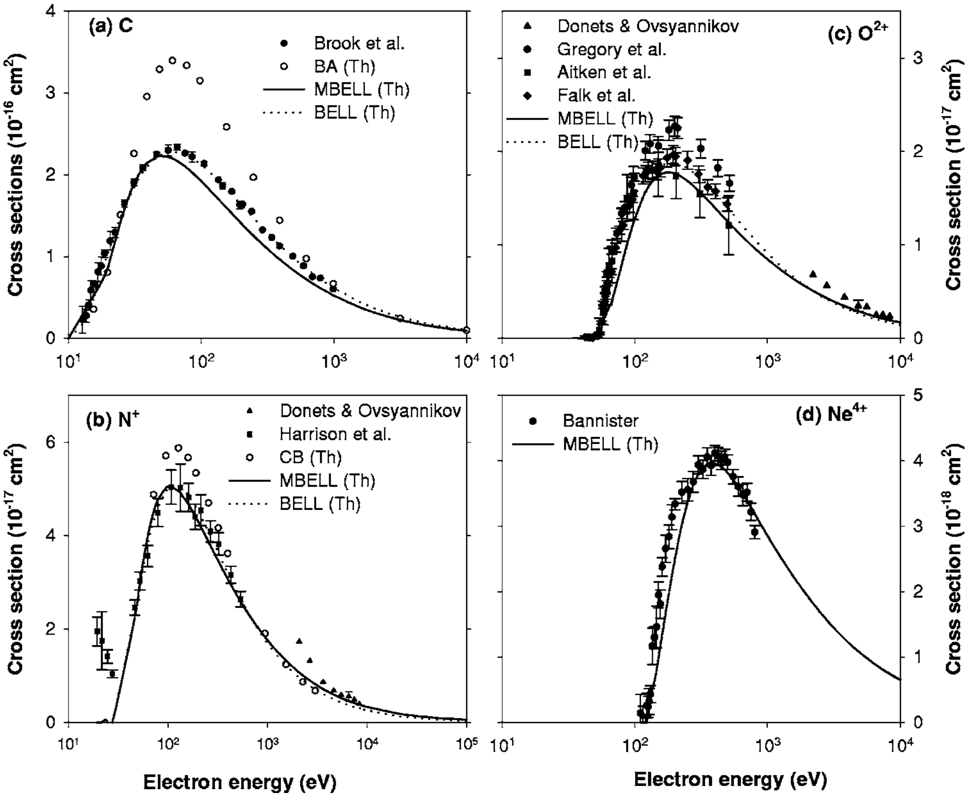

FIG. 4. Same as in Fig. 3 for C-like targets: (a) C, (b) N^+, (c) O^{2+}, and (d) Ne^{4+}.

rameters for the *s* orbits, are subsequently applied to 2*p*-subshell targets. The BELL parameters for the 2*p* orbit have been deduced from the best overall fits to the EIICS data for the atomic C with two electrons in the 2*p* orbit [Fig. 4(a)], and N with three electrons [Fig. 5(a)]. The data for C are taken from Brook *et al.*, and those for N, from the former work [46].

The ionic parameters m and λ for the 2*p* orbit, which are assumed to be same for other p orbits, are obtained from the overall fits to B-like ionic targets, namely C^+, N^{2+}, O^{3+}, and

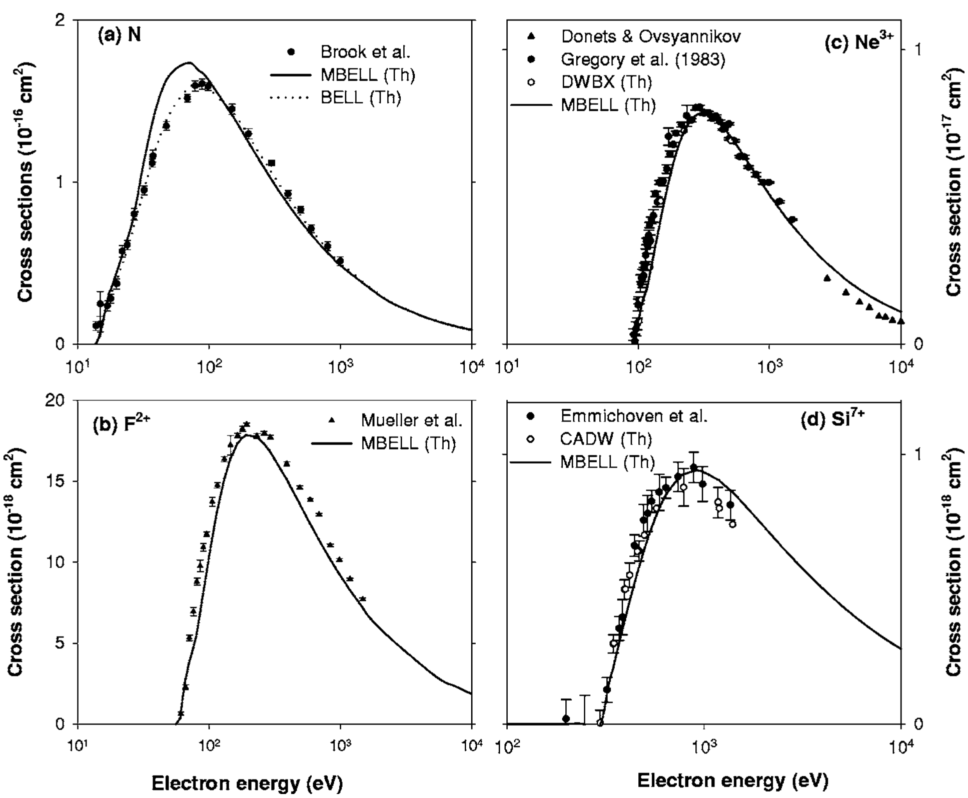

FIG. 5. Same as in Fig. 3 for N-like targets: (a) N, (b) F^{2+}, (c) Ne^{3+}, and (d) Si^{7+}.

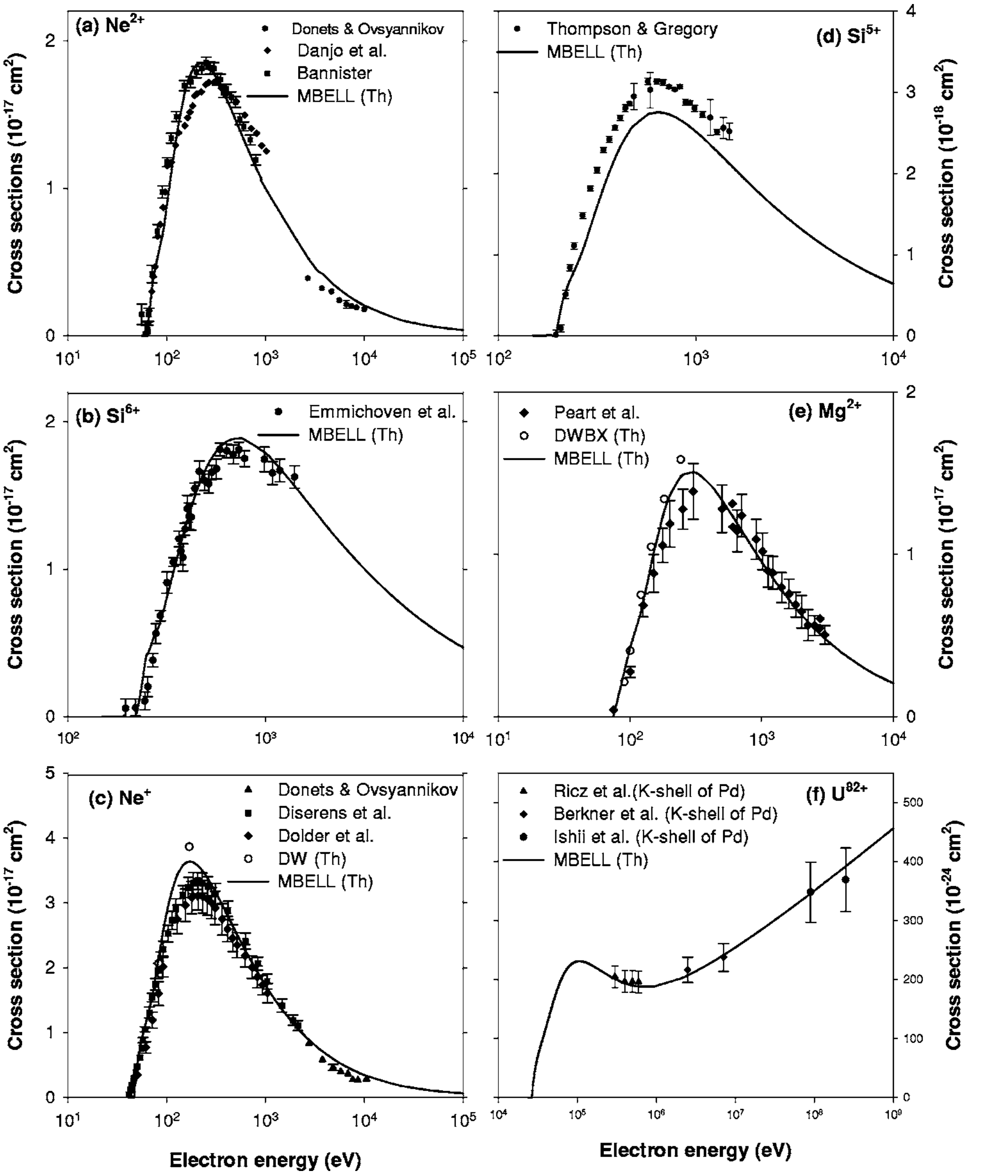

FIG. 6. EIICS of O-like targets: (a) Ne^{2+} and (b) Si^{6+}; F-like targets: (c) Ne^{+} and (d) Si^{5+}; and Ne-like targets: (e) Mg^{2+} and (f) U^{82+}. The data in (f) are evaluated from the *K*-shell ionization cross sections of Pd.

Ne^{5+} [Figs. 3(a)–3(d)]; C-like N^{+}, O^{2+}, and Ne^{4+} [Figs. 4(b)–4(d)]; N-like F^{2+}, Ne^{3+}, Si^{7+} [Figs. 5(b)–5(d)]; O-like Ne^{2+}, and Si^{6+} [Figs. 6(a) and 6(b)]; F-like Ne^{+}, and Si^{5+} [Figs. 6(c) and 6(d)]; and Ne-like Mg^{2+}, and U^{82+}. The data are from [35] for C^{+}, $N^{1+,2+}$, $O^{2+,3+}$, and $Ne^{1+,2+,3+,4+,5+}$; Aitken *et al.* [47] for C^{+}, N^{2+}, and O^{2+}; Bannister and Havener [48] for N^{2+}; [34] for O^{3+}; [41] for $Ne^{2+,4+,5+}$; Harrison *et al.* [49] for N^{+}; [38,40] for O^{2+}; Mueller *et al.* [50] for F^{2+}; Gregory *et al.* [51] for Ne^{3+}; Zeijmans van Emmichoven *et al.* [52] for $Si^{6+,7+}$; Danjo *et al.* [53] for Ne^{2+}; Diserens *et al.* [54], and Dolder *et al.* [55] for Ne^{+}; Thompson and Gergory [56] for Si^{5+}; and Peart *et al.* [57] for Mg^{2+}. The evaluated cross-section data, substitutes for the experimental data, for U^{82+} have been obtained from the *K*-shell EIICS data of Pd from the works of [43], Ricz *et al.* [58] and Berkner *et al.* [59]. The ionization potential $I_{2p} \approx 26.6$ keV and the kinetic energy of a bound electron $T_{2p} \approx 26.4$ keV for the $2p$ subshell of U^{82+} being fairly close, respectively, to $I_{1s} \approx 24.5$ keV and $T_{1s} \approx 28.2$ keV for the *K*-shell ionization of Pd, we have used the evaluated cross sections for the $2p$ ionization of U^{82+} as $\sigma_{2p}[U^{82+}] \approx 3\sigma_{1s}[Pd]$ for the same incident energies.

To assess the level of performance of the MBELL model, its predictions are compared with the results from the available parameters of the parent BELL model [20], where the parameters are species dependent, and there is no allowance for the ionic and relativistic corrections. The MBELL model, with a single set of parameters for each of the $2s$ and $2p$ orbits coupled with one set of parameters for the $1s$ orbit taken from [23] (Table I), produces from satisfactory to excellent fits to the EIICS data for 30 targets (Figs. 1–6) in the Li, Be, B, C, N, F, and Ne isoelectronic sequences. The fits are comparable to those obtained with the BELL model, where the target-dependent parameters are available only up to $Z = 8$.

To augment the comparative study on the performance of MBELL, we also show the results of the available *ab initio* theoretical methods, namely the Born approximation (BA) [60], Coulomb-Born approximation (CB) [61], distortedwave approximation (DW) [62], DW Born-exchange approximation (DWBX) [63–65], DWCB approximation with exchange (CBX) [66], CB approximation with autoionization (CBA) [67], convergent-close-coupling approximation (CCC) [68], configuration-average DW approximation (CADW) [69], relativistic DWBA (RDWBA) [70], and DWBA with *R*-matrix (DWBARM) [71]. The MBELL model seems to perform better than the CCC calculations [68] in Fig. 1 for Li, B^{2+}, and O^{5+}, except the case of Be^{+} where the latter is better near the peak region. MBELL does better than the DWBX results [63] for B^{+}, C^{2+}, O^{4+}, and U^{88+} (Fig. 2); and agrees with the DWBX predictions [64] for Ne^{3+} [Fig. 2(c)], and [65] for Mg^{2+} [Fig. 6(e)]. MBELL compares closely to the DWBARM calculations [71] for Ne^{7+} [Fig. 1(e)] and Ne^{6+} [Fig. 2(e)], except for the former case near the peak region where DWBARM performs better. MBELL tends to perform better than the RDWBA calculations [70] for U^{89+} [Fig. 1(f)] and U^{88+} [Fig. 2(f)], which are available only up to about 400 keV. MBELL works better that the CBX calculations [66] for N^{3+} [Fig. 2(c)] near the peak region. The CBA calculations of [67] including the autoionization effects overestimate the EIICS data for N^{2+} [Fig. 3(b)] below the peak region, where MBELL slightly underestimates but works excellently near and beyond the peak region. MBELL certainly works much better than the BA findings of [60] for C [Fig. 4(a)], where the latter overestimate greatly near the peak region. The CB calculations [61] for N^{+} overestimate the EIICS data near the peak region [Fig. 4(b)], where the MBELL predictions agree very well with the data. MBELL results agree well with the CADW findings of [69] for Si^{7+} [Fig. 5(d)], both fit the EIICS well. The MBELL model fits the EIICS data for Ne^{+} well over the entire energy region, while the DW results of [62] overestimate at the peak region.

IV. CONCLUSIONS

The present study reports an intriguing aspect of the simple MBELL model emanating from a detailed application over a wide number of targets and range of incident energies. The BELL parameters A and B_i's of the model in Eq. (2) are generalized in terms of the orbitals nl and the ionic parameters m and λ of Eq. (4) in only the l quantum number. Two sets of parameters for the 2*s* and 2*p* orbits in Table I, in conjunction with the parameters of the 1*s* orbit, can satisfactorily describe the EIICS data for the 30 neutral and ionic targets in eight isoelectronic sequences, ranging from Li to Ne.

In the MBELL model, a single set of parameters for the 2*p* orbit is found to account well for the experimental EIICS data of 18 atomic targets, neutral and ionic with open- and closed-shell configurations, in the B, C, N, O, F, and Ne isoelectronic sequences over a wide range of energies. The model, with built-in ionic and relativistic corrections, seems to perform better in most cases than the quantum mechanical calculations. In particular, it excellently describes the EIICS data of the heavy ionic targets, such as $U^{82+,88+,89+}$ [Figs. 1(f), 2(f), and 6(f)] up to the incident energies of about 250 MeV, while the quantum method, such as RDWBA [70], fails to reproduce the trend of the data of $U^{88+,89+}$ beyond 170 keV [Figs. 1(f) and 2(f)]. As far as we know, the ranges of atomic number Z, the number of isoelectronic sequences, and the incident energies in the present work go beyond the available empirical and quantum mechanical calculations. MBELL thus seems to be a very useful model for applications.

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