

Calculated electron impact *K*-shell ionization cross sections for atoms

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Abstract

A simple-to-use empirical model for the calculation of electron impact single *K*-shell ionization total cross sections for 60 atomic targets from H to U ($1 \leq Z \leq 92$) and the energies from threshold to ultra-relativistic range is described. Simplified BELL formula [K.L Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, F.J. Smith, J. Phys. Chem. Ref. Data 12 (1983) 891] is used in the proposed model by incorporating in it both the ionic and relativistic corrections. The predicted *K*-shell ionization cross sections are compared with recently measured experimental data. Better agreement is found for all atoms considered except Xe. Moreover, the calculated results are also compared with other theoretical methods and empirical formulae. The predicted results achieve a level of agreement with both experimental data those are better than the predictions from the existing theoretical methods and empirical models. With the inherent simplicity of its structure, this model may be a prudent selection for the users where fast generation of electron impact single *K*-shell ionization total cross sections are required.

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1. Introduction

Electron impact ionization (EII) of *K*-shell atoms plays a vital role not only in fundamental studies but also in technological developments. EII cross sections of *K*-shell are widely used in numerous fields of applications such as radiation physics, astrophysics, environmental physics, electron probe microanalysis (EPMA), Auger electron spectroscopy (AES), electron energy loss spectroscopy (EELS), and so on.

Over the past five decades, many experimental and theoretical studies have been carried out to estimate the electron impact *K*-shell ionization cross sections. Theoretical determination of EII cross sections of *K*-shell is based on the classical, semi-classical and quantum mechanical approaches. None of them has been successful completely to describe experimental cross-section data over a wide range of atomic number *Z* and incident electron energies. Gryzinski's classical formula [1] provides a

fairly good description over a wide energy range except near the threshold region ($U < 4$, where *U* is the reduced energy defined as the ratio of incident electron energy *E* to the *K*-shell ionization potential I_k).

Efforts [2–5] have been given through quantum mechanical calculation for the description of *K*-shell ionization based on first-order perturbation theory [2], plane-wave Born approximation (PWBA) [3], and distorted-wave Born approximation (DWBA) [4,5]. Luo and Joy [2] performed a series of extensive calculations for inner-shell EII cross sections using first-order perturbation theory and Hartree–Slater–Fock wave function. Scofield [4] proposed a model over a wide incident energies taking into account the relativistic effect in PWBA (RPWBA) through Dirac equation. Segui et al. [5] proposed a model considering the relativistic DWBA (RDWBA) theory for the EII of *K*-shell applicable to the limited incident energy only. The above-mentioned theories with approximations in them are applicable to restricted incident energies and to limited atoms. Both the quantal and classical approaches are much complex to use in practical applications.

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Several workers [6–10] have proposed different empirical and semi-empirical models. Quarles developed an empirical model [6] that works well within $1 \leq U \leq 10^5$ but is restricted to few targets only. Casnati et al. [7] proposed an empirical model that describes fairly good cross sections for $1 < U < 20$ and $6 < Z < 79$. The empirical model proposed by Hombourger [8] provides a fairly good fits to the *K*-shell data within $1 \leq U \leq 10^5$ and $6 \leq Z < 79$. Bell et al. [9], which is referred to as BELL, proposed an analytical formula involving species-dependent parameters for the determination of EII cross sections of light atoms and ions with $Z \leq 8$. Moreover, the BELL

formula lacks in relativistic component in its structure and does not make any allowance for ionic effect. Both the relativistic and ionic effects are essential for treating heavier species.

In this paper, we propose a simplified version of BELL formula taking into account relativistic and ionic effects, will be called as SBELL model, which predicts almost a similar quality of cross sections to the experimental data. This paper is organized as follows. Description of the proposed model is provided in Section 2. Results and discussion are provided in Section 3. A conclusion is drawn in Section 4.

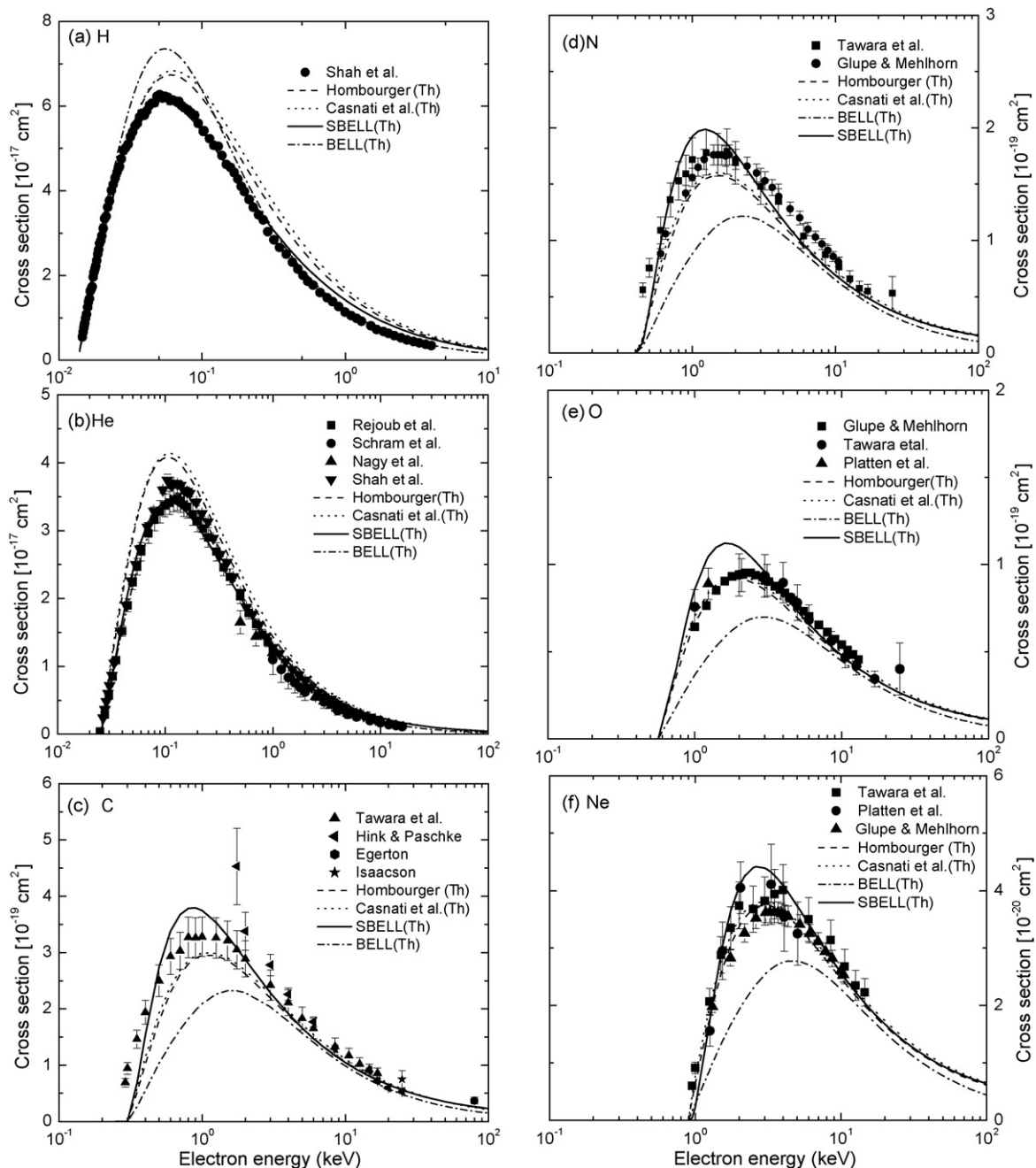


Fig. 1. Electron impact ionization cross sections of *K*-shell for: (a) H, (b) He, (c) C, (d) N, (e) O, and (f) Ne.

2. Outline of the model

In the BELL model [9], the EII cross section $\sigma_{\text{BELL}}(E)$ for K -shell is given by

$$\sigma_{\text{BELL}}(E) = \frac{1}{I_k E} \left\{ A \ln \left(\frac{E}{I_k} \right) + \sum_{k=1}^5 B_k \left(1 - \frac{I_k}{E} \right)^k \right\}, \quad (1)$$

where I_k and E are the ionization potential of K -shell of the respective targets and the energy of the incident electron, respectively, as mentioned earlier, A and B are the BELL parameters needed to fit the experimental data. To increase the performance, to reduce the number of fitting parameters and to extend the

energy of the incident electron up to ultra-relativistic region of the BELL model, σ_{BELL} is replaced by σ_{BR} in the proposed model and is given by

$$\sigma_{\text{BR}}(E) = \left\{ A \ln \left(\frac{E}{I_k} \right) + B \left(1 - \frac{I_k}{E} \right) \right\} a_0^2, \quad (2)$$

where $a_0 = 0.529 \times 10^{-8}$ cm is the Bohr radius. Here only two fitting parameters A and B are used instead of six in Eq. (1). Since Eq. (2) is much simpler than Eq. (1).

It is found adequate to introduce relativistic factor when the energy of the incident electron is comparable to or higher than the relativistic or ultra-relativistic range for the descrip-

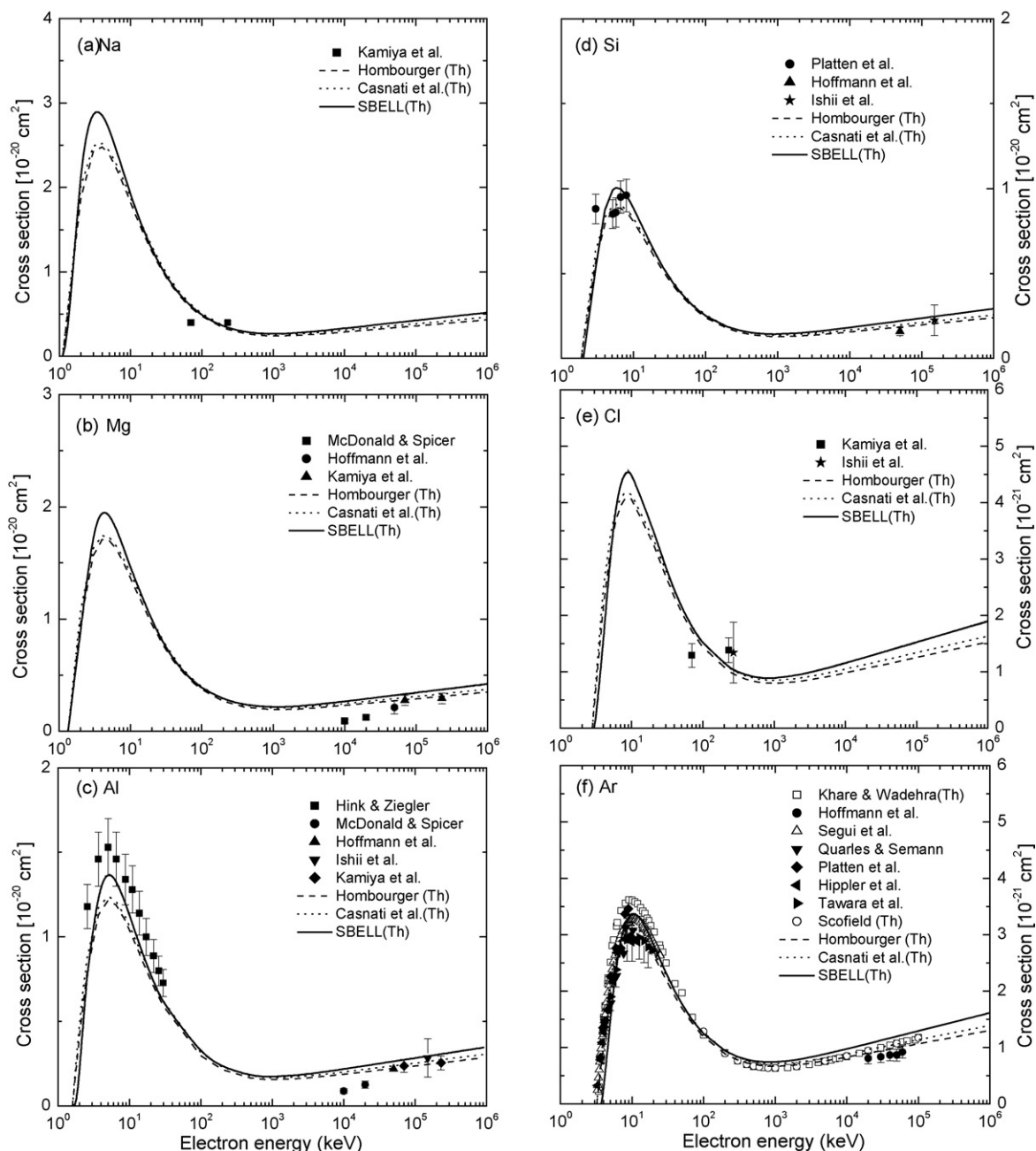


Fig. 2. Electron impact ionization cross sections of K -shell for: (a) Na, (b) Mg, (c) Al, (d) Si, (e) Cl, and (f) Ar.

tion of *K*-shell EII cross sections. Gryzinski’s relativistic term [1] is included as a multiplying factor with Eq. (2) to take into account the relativistic effect. Gryzinski’s relativistic factor F_G , as applied by Deutsch et al. [10], is given by

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

where $J = (mc^2)/I_k$, m is the mass of electron and c is the velocity of light in vacuum. The third term of Eq. (3) is found insignif-

icant as compared to the first and second terms at relativistic energies in the proposed model. However, F_G is replaced by the Gryzinski’s simpler factor [1] F_{SG} having the form:

$$F_{SG} = \frac{2(1 + J/U)^2}{J(1 + 2J/U)}. \quad (4)$$

When the incident electron is becoming closer to the *K*-shell electron(s), the atom behaves as an ion of charge $q = Z - N_k$, where N_k is the number of electrons in the *K*-shell. Consequently the charge cloud of electron feel attractive force towards the *K*-shell electron, thereby leading to a greater overlap of the charge clouds of the incident and target electrons and as a result EII cross section is enhanced. However, the ionic effect on cross

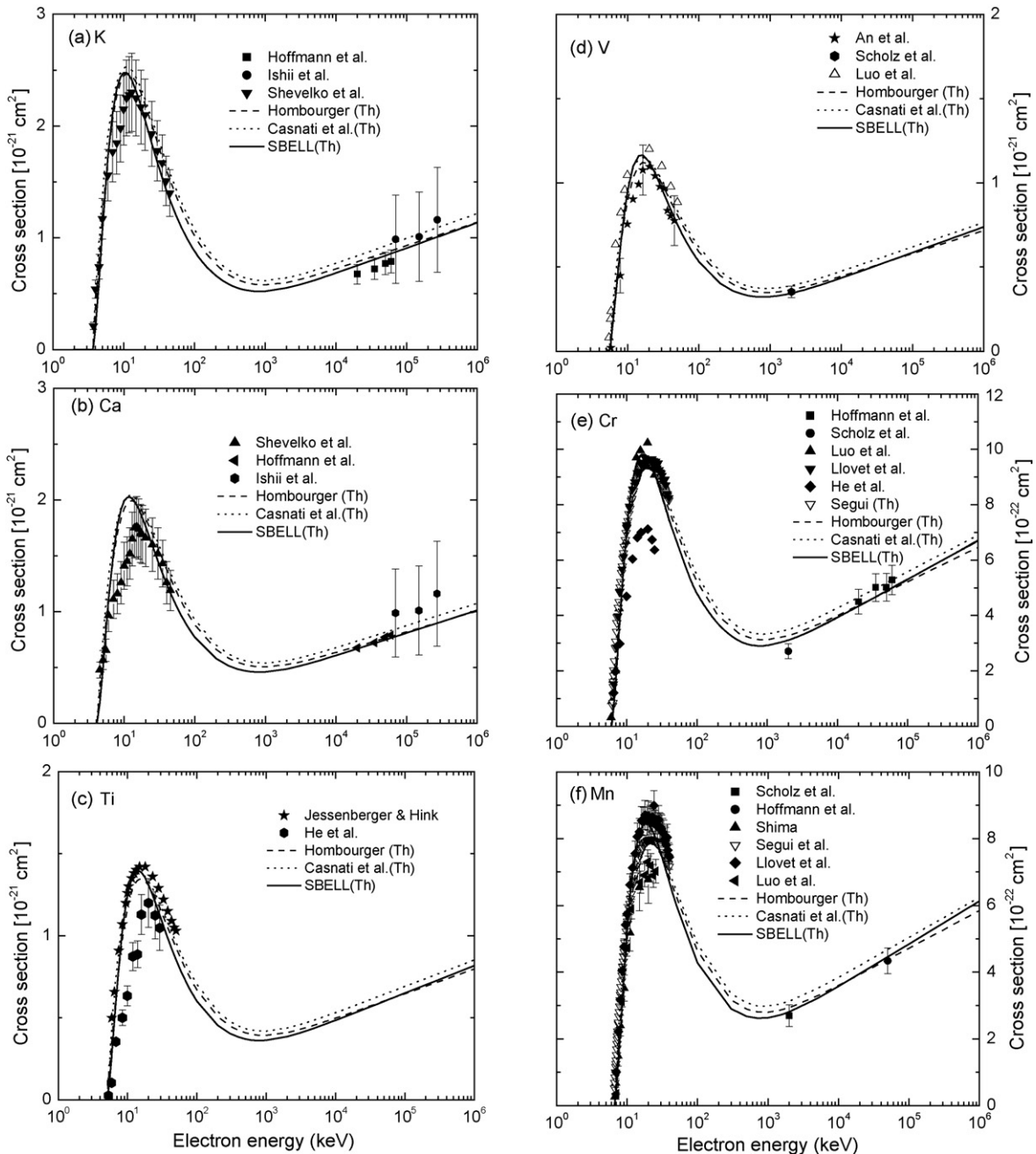


Fig. 3. Electron impact ionization cross sections of *K*-shell for: (a) K, (b) Ca, (c) Ti, (d) V, (e) Cr, and (f) Mn.

sections decreases with an increase of incident energy as the electron spends less time in the vicinity of atomic force field. The ionic correction factor [11] F_I is given by

$$F_I = 1 + n \left(\frac{q}{ZU} \right)^\lambda, \quad (5)$$

where n and λ are the fitting parameters. The ionic correction factor [11] F_I is modified, included as a multiplying factor also with Eq. (2), and is given by

$$F_{IM} = \left\{ 1 + n \left(\frac{q}{ZU} \right)^\lambda \right\}. \quad (6)$$

The optimum values obtained for n and λ , as will be discussed later, are $n = 3.65$ and $\lambda = 1.15$.

Finally, the proposed SBELL model for the electron impact single K -shell total ionization cross-section σ_{SBELL} is given by

$$\sigma_{SBELL} = N_k F_{IM} F_{SG} \sigma_{BR}(E). \quad (7)$$

In Eq. (7) the fitting parameters A and B are generalized by making them dependent on I_k . Ionization potential is normalized by $U_R = I_k/R$, where R is the Rydberg energy. The parameters A and B are expressed as

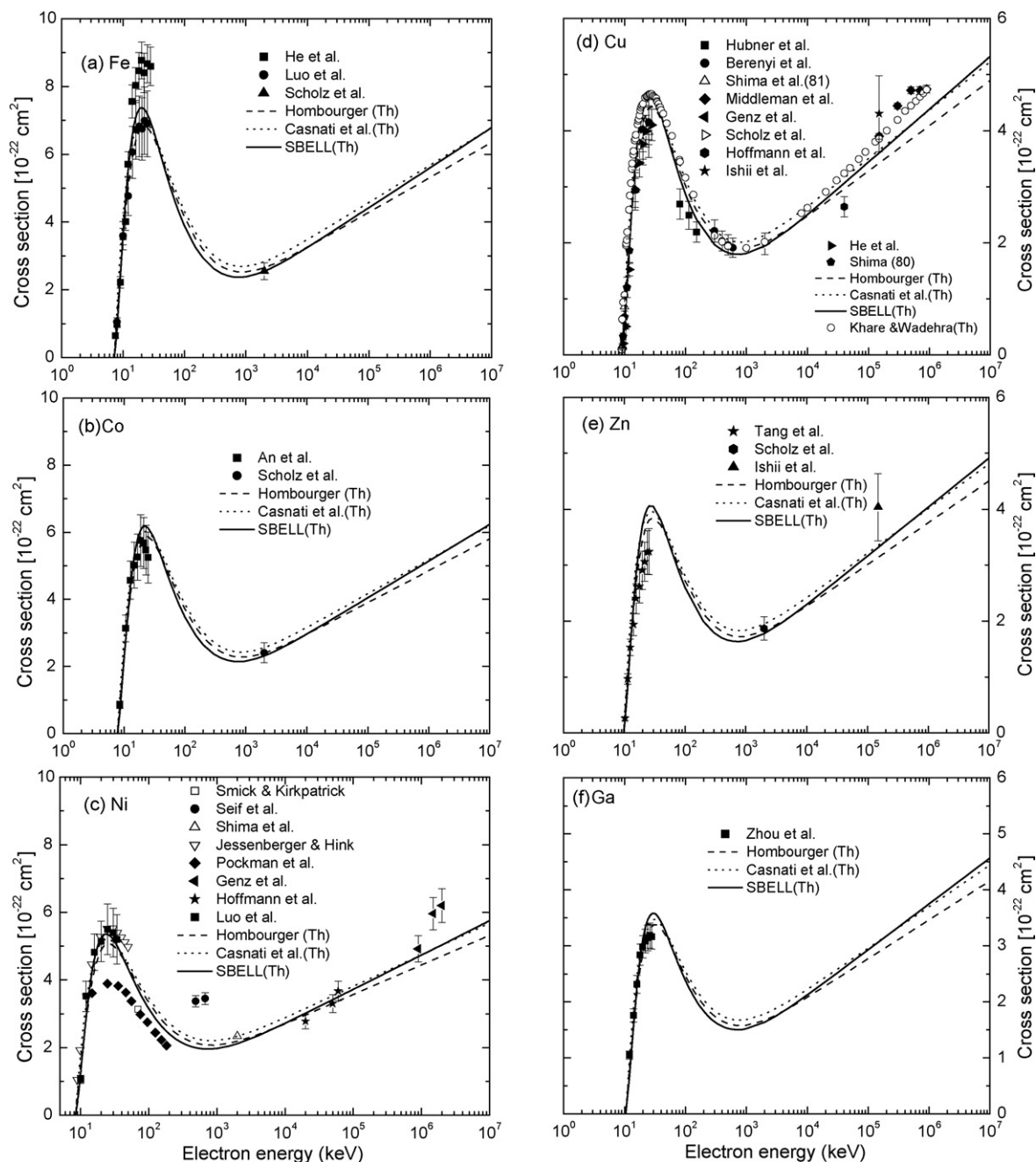


Fig. 4. Electron impact ionization cross sections of K -shell for: (a) Fe, (b) Co, (c) Ni, (d) Cu, (e) Zn, and (f) Ga.

(a) For $Z=1$ and 2

$$A = \left(\frac{2.560 \times 10^{-4} U_R}{1 + 1.012 U_R} \right)^3, \quad (8)$$

$$B = - \left(\frac{1.062 \times 10^{-4} U_R}{1 + 0.67 U_R} \right)^3, \quad (9)$$

(b) For $Z=3-18$

$$A = \left(\frac{2.680 \times 10^{-3} U_R}{1 + 3.4 U_R} \right)^3, \quad (10)$$

$$B = - \left(\frac{1.519 \times 10^{-5} U_R}{1 + 0.59 U_R} \right)^3, \quad (11)$$

(c) For $Z=19-92$

$$A = \left(\frac{4.545 \times 10^{-7} U_R}{1 + 0.2 U_R} \right)^3, \quad (12)$$

$$B = - \left(\frac{3.363 \times 10^{-3} U_R}{1 + 4.0 U_R} \right)^3. \quad (13)$$

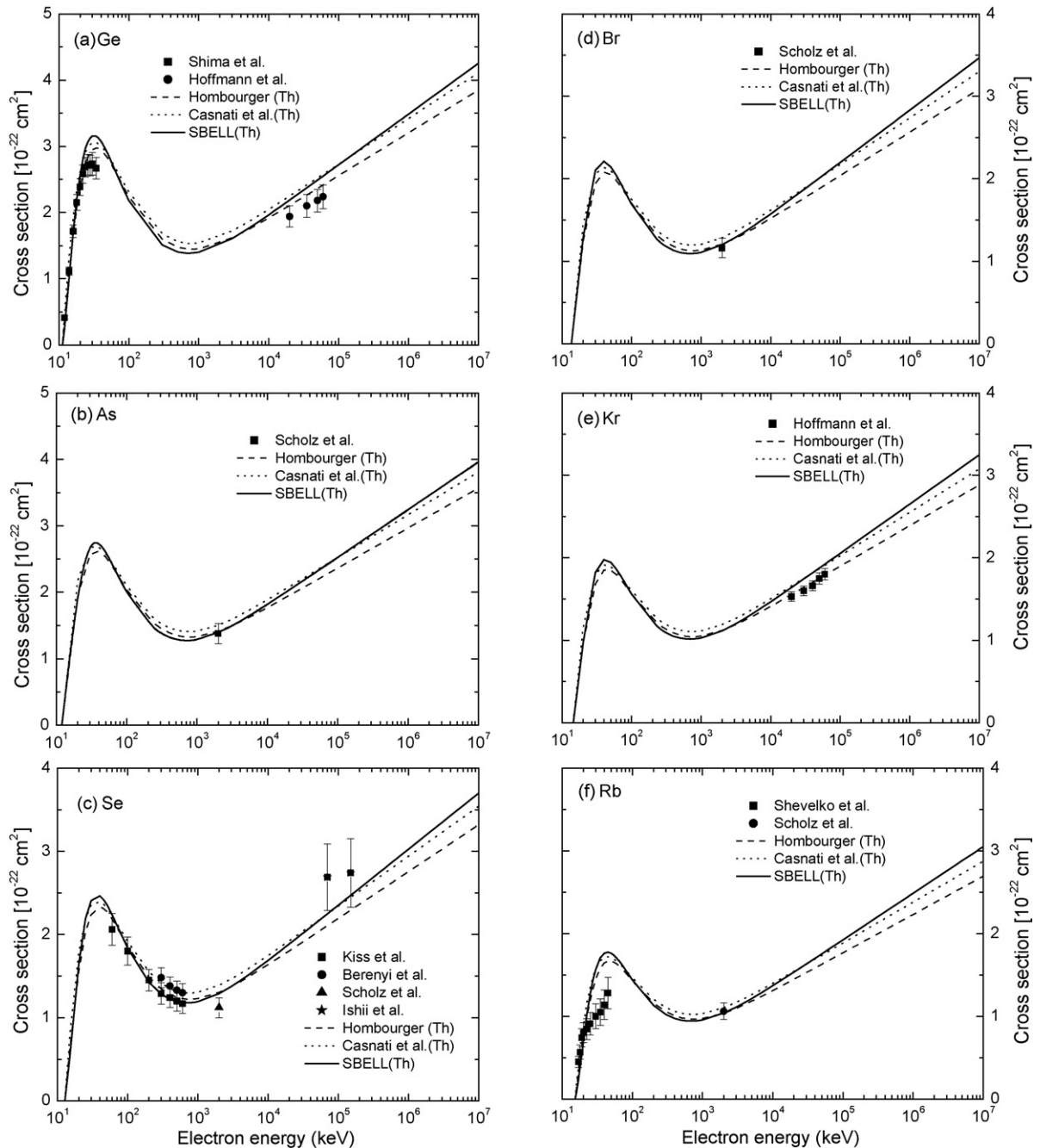


Fig. 5. Electron impact ionization cross sections of K -shell for: (a) Ge, (b) As, (c) Se, (d) Br, (e) Kr, and (f) Rb.

3. Results and discussions

In the analysis, 60 atomic targets H, He, C, N, O, Ne, Na, Mg, Al, Si, Cl, Ar, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Pd, Ag, Cd, In, Sn, Sb, Te, Xe, Ba, La, Pr, Sm, Eu, Gd, Ho, Er, Tm, Yb, Ta, W, Pt, Au, Pb, Bi, and U whose experimental data are available in the range of $Z=1-92$ have been considered.

The coefficients of the parameters A and B in Eqs. (8)–(13) are determined from the overall best fits of our predicted cross sections to the experimental data of the 60 targets, considered herein. A measure of the quality of best fit is obtained by mini-

mizing the χ^2 defined by

$$\chi^2 = \sum_i \left[\frac{\sigma_{\text{SBELL}}(E_i) - \sigma_{\text{exp}}(E_i)}{\sigma_{\text{exp}}(E_i)} \right]^2,$$

where $\sigma_{\text{SBELL}}(E_i)$ and $\sigma_{\text{exp}}(E_i)$ refer, respectively, to the theoretical and experimental cross sections at the energy point E_i . The optimum values of the coefficients, in terms of which the parameters A and B are defined, are obtained using a non-linear least-square fitting program.

The experimental and theoretical data are collected from: Shah et al. [12] for H; Rejoub et al. [13], Schram et al. [14],

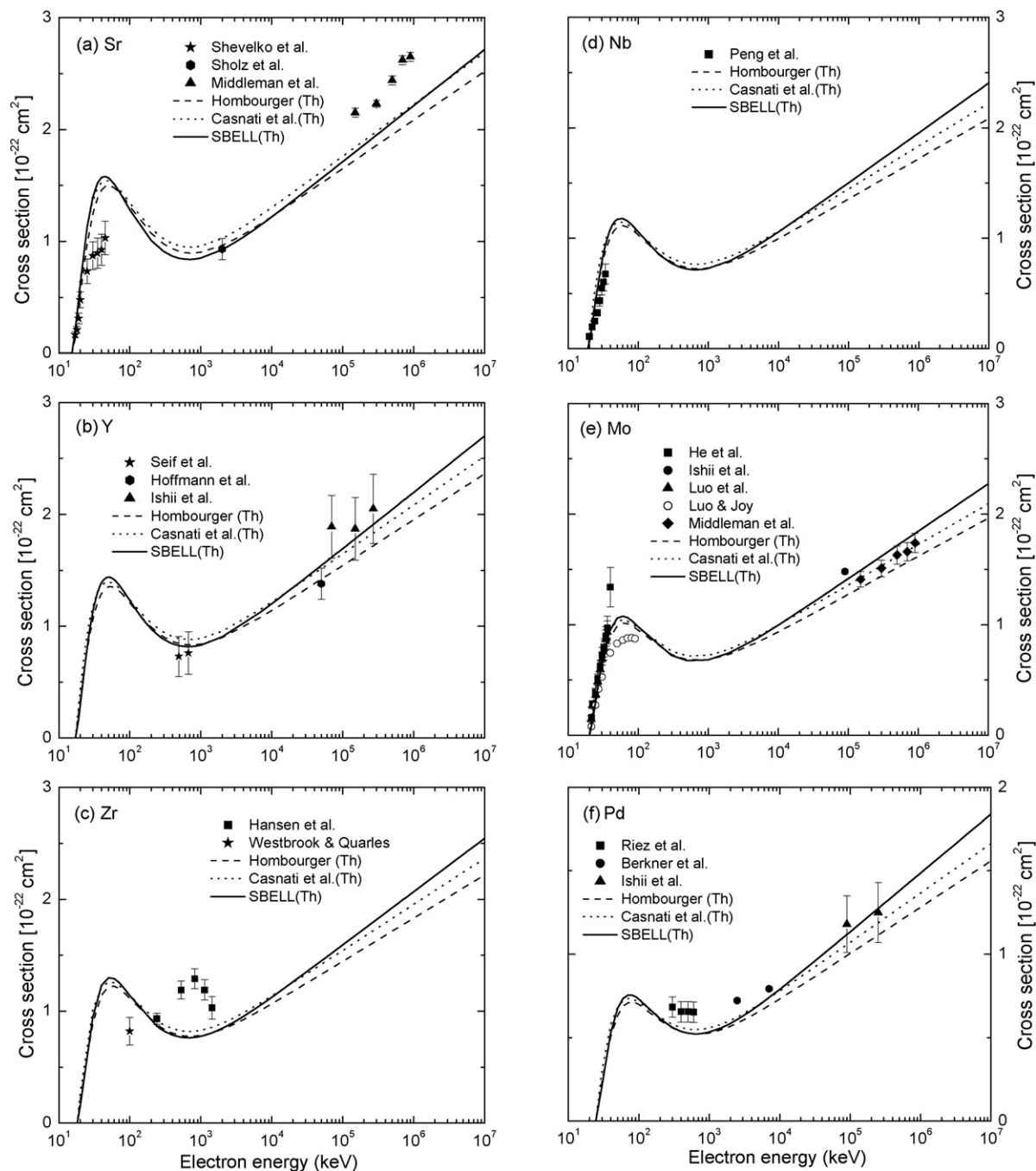


Fig. 6. Electron impact ionization cross sections of K -shell for: (a) Sr, (b) Y, (c) Zr, (d) Nb, (e) Mo, and (f) Pd.

Nagy et al. [15], and Shah et al. [12] for He; Tawara et al. [16], Hink and Paschke [17], Egerton [18], and Isaacson [19] for C; Tawara et al. [16], and Glupee and Mehlhorn [20] for N; Glupee and Mehlhorn [20], Tawara et al. [16], and Platten et al. [21] for O and Ne; Kamiya et al. [22] for Na; McDonald and Spicer [23], Hoffmann et al. [24], and Kamiya et al. [22] for Mg; Hink and Ziegler [25], McDonald and Spicer [23], Hoffmann et al. [24], Ishii et al. [26], and Kamiya et al. [22] for Al; Platten et al. [21], Hoffmann et al. [24], and Ishii et al. [26] for Si; Kamiya et al. [22], and Ishii et al. [26] for Cl; Khare and Wadehra [3], Hoffmann et al. [24], Segui et al. [5], Quarles and Semann [6], Platten et al. [21], Hippler et al. [27], Tawara et al. [16], and

Scofield [4] for Ar; Hoffmann et al. [24], Ishii et al. [26], and Shevelko et al. [28] for K and Ca; Jessenberger and Hink [29], and He et al. [30] for Ti; An et al. [31], Scholz et al. [32], and Luo et al. [33] for V; Hoffmann et al. [24], Scholz et al. [32], Luo et al. [33], Llovet et al. [34], He et al. [30], and Segui [5] for Cr; Tang et al. [35], Scholz et al. [32], Hoffmann et al. [24], Shima [36], Luo et al. [33], and Segui [5] for Mn; He et al. [30], Luo et al. [33], and Scholz et al. [32] for Fe; An et al. [31], and Scholz et al. [32] for Co; Smick and Kirkpatrick [37], Seif el Naser et al. [38], Shima et al. [36], Jessenberger and Hink [29], Pockman et al. [39], Genz et al. [40], Hoffman et al. [24], Luo et al. [30] for Ni; Hubner et al. [41], Berenyi et al. [42], Shima

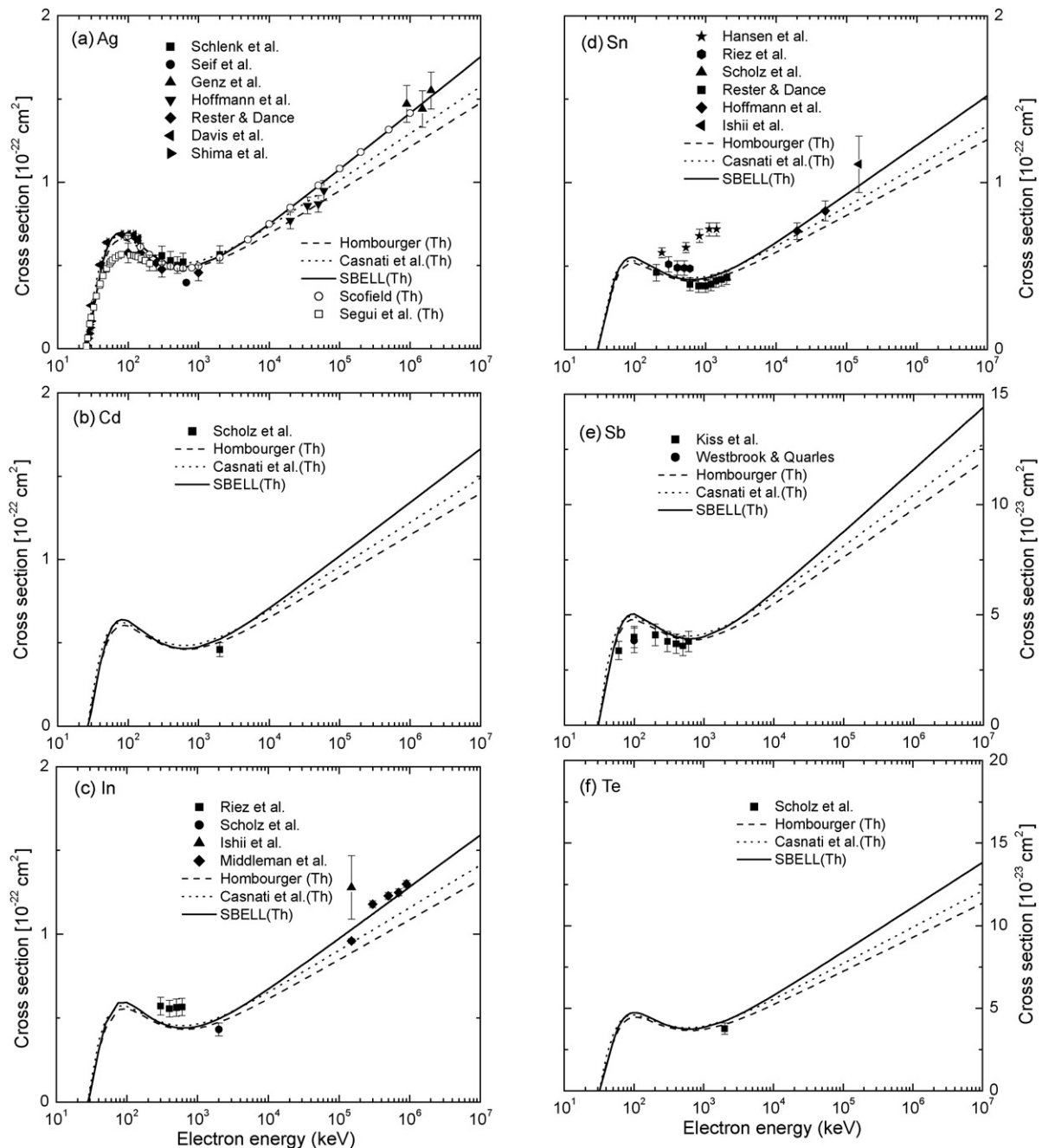


Fig. 7. Electron impact ionization cross sections of K-shell for: (a) Ag, (b) Cd, (c) In, (d) Sn, (e) Sb, and (f) Te.

et al. [36], Middleman et al. [43], Genz et al. [40], Scholz et al. [32], Hoffmann et al. [24], Ishii et al. [26], He et al. [30], and Shima [36] for Cu; Tang et al. [35], Scholz et al. [32], and Ishii et al. [26] for Zn; Zhou et al. [44] for Ga; Shima et al. [36], and Hoffmann et al. [24] for Ge; Scholz et al. [32] for As; Kiss et al. [45], Scholz et al. [32], and Ishii et al. [26] for Se; Scholz et al. [32] for Br; Hoffmann et al. [24] for Kr; Shevelko et al. [28], and Scholz et al. [32] for Rb; Shevelko et al. [28], Scholz et al. [32], and Middleman et al. [43] for Sr; Seif et al. [38], Hoffmann et al. [24], and Ishii et al. [26] for Y; Hansen et al. [46], and Westbrook and Quarles [47] for Zr; Hansen et al. [46], and Peng et al. [48] for Nb; He et al. [30], Ishii et al. [26], Luo et

al. [33], Luo and Joy [2], and Middleman et al. [43] for Mo; Riez et al. [49], Berkner et al. [50], and Ishii et al. [26] for Pd; Schlenk et al. [51], Seif el Naser et al. [38], Genz et al. [40], Hoffmann et al. [24], Rester and Dance [52], Davis et al. [53], Shima et al. [36], Scofield [4], and Segui et al. [5] for Ag; Scholz et al. [32] for Cd; Riez et al. [49], Scholz et al. [32], Ishii et al. [26], and Middleman et al. [43] for In; Hansen et al. [46], Riez et al. [49], Scholz et al. [32], Rester and Dance [52], Hoffmann et al. [24], and Ishii et al. [26] for Sn; Kiss et al. [45], and Westbrook and Quarles [47] for Sb; Scholz et al. [32] for Te; Hoffmann et al. [24] for Xe; Scofield [4], Scholz et al. [32], and Ishii et al. [26] for Ba; Scholz et al. [32], and Westbrook and Quarles

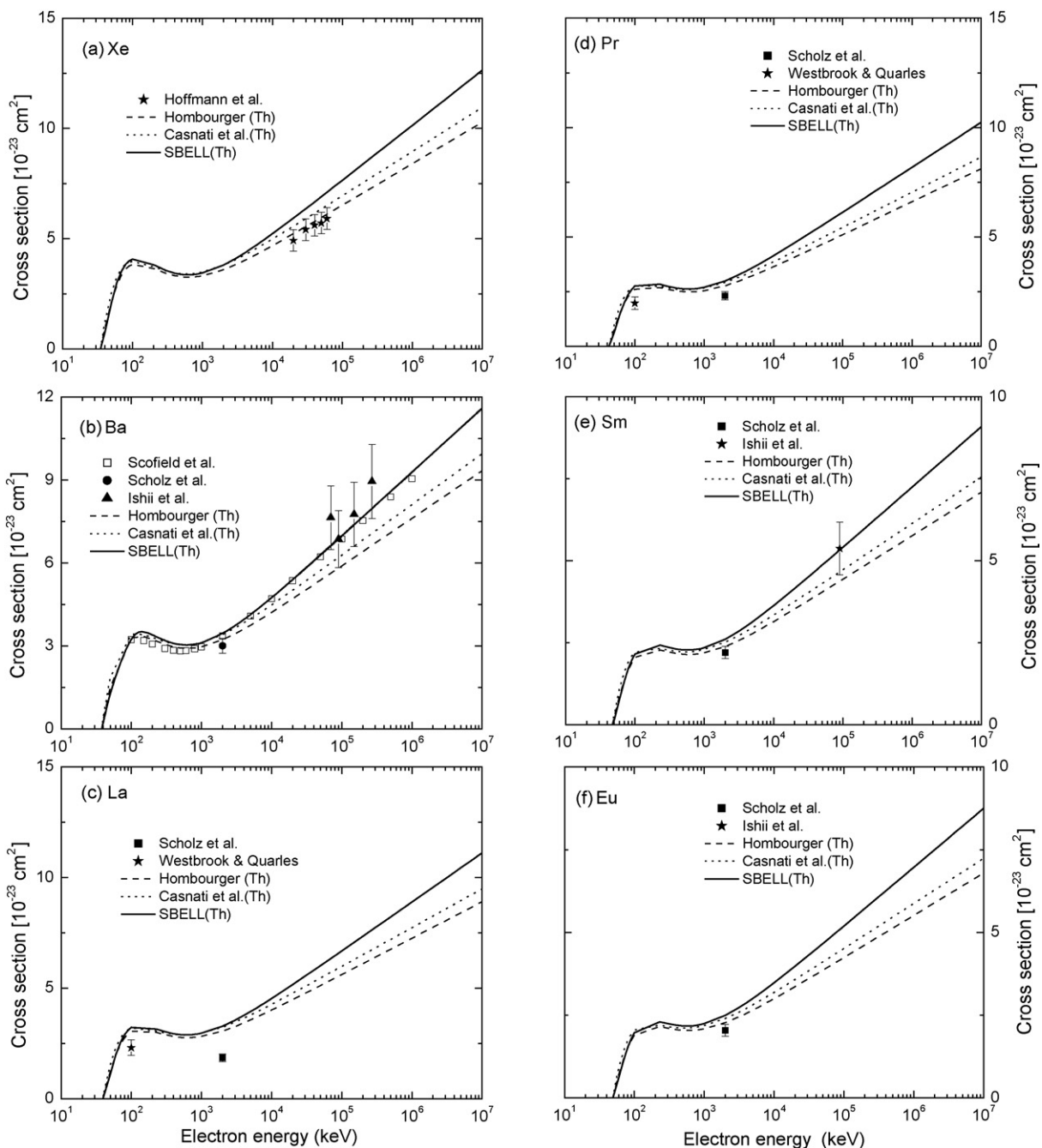


Fig. 8. Electron impact ionization cross sections of *K*-shell for: (a) Xe, (b) Ba, (c) La, (d) Pr, (e) Sm, and (f) Eu.

[47] for La; Scholz et al. [32], Westbrook and Quarles [47] for Pr; Scholz et al. [32], and Ishii et al. [26] for Sm, Eu and Gd; Hoffmann et al. [24], and Ishii et al. [26] for Ho; Scholz et al. [32] for Er; Middleman et al. [43] for Tm; Seif et al. [38], and Scholz et al. [32] for Yb; Seif et al. [38], and Middleman et al. [43] for Ta; Hansen et al. [46] for W; Scholz et al. [32] for Pt; Scofield [4], Seif el Naser et al. [38], Scholz et al. [32], Davis et al. [53], Berkner et al. [50], Middleman et al. [43], Rester and Dance [52], Hoffmann et al. [24], and Ishii et al. [26] for Au; Scholz et al. [32], Hoffmann et al. [24], Ishii et al. [26], Kare and Wadehra [3], and Seif el Naser et al. [38] for Pb; Scofield [4], Scholz et al. [32], Middleman et al. [43], Hoffmann et al.

[24], and Ishii et al. [26] for Bi; and Scofield [4], and Ishii et al. [26] for U.

Figs. 1–10 compare the experimental EII cross sections (bold symbols) with the predicted results obtained by quantum (open symbols) and model calculations. The dashed, dotted and dash-dotted lines are used, respectively, predicted by Hombourger [8], Casnati et al. [7] and Bell et al. [9] models. The bold continuous line represents SBELL calculations using Eq. (7). The ionization potentials I_k of K -shell electrons are taken from Desclaux [54]. The ionic factor F_{IM} in Eq. (6) with the parameter values $n = 3.65$ and $\lambda = 1.15$ are optimized in such a way for which Eq. (7) describes the best EII cross sections with respect to the

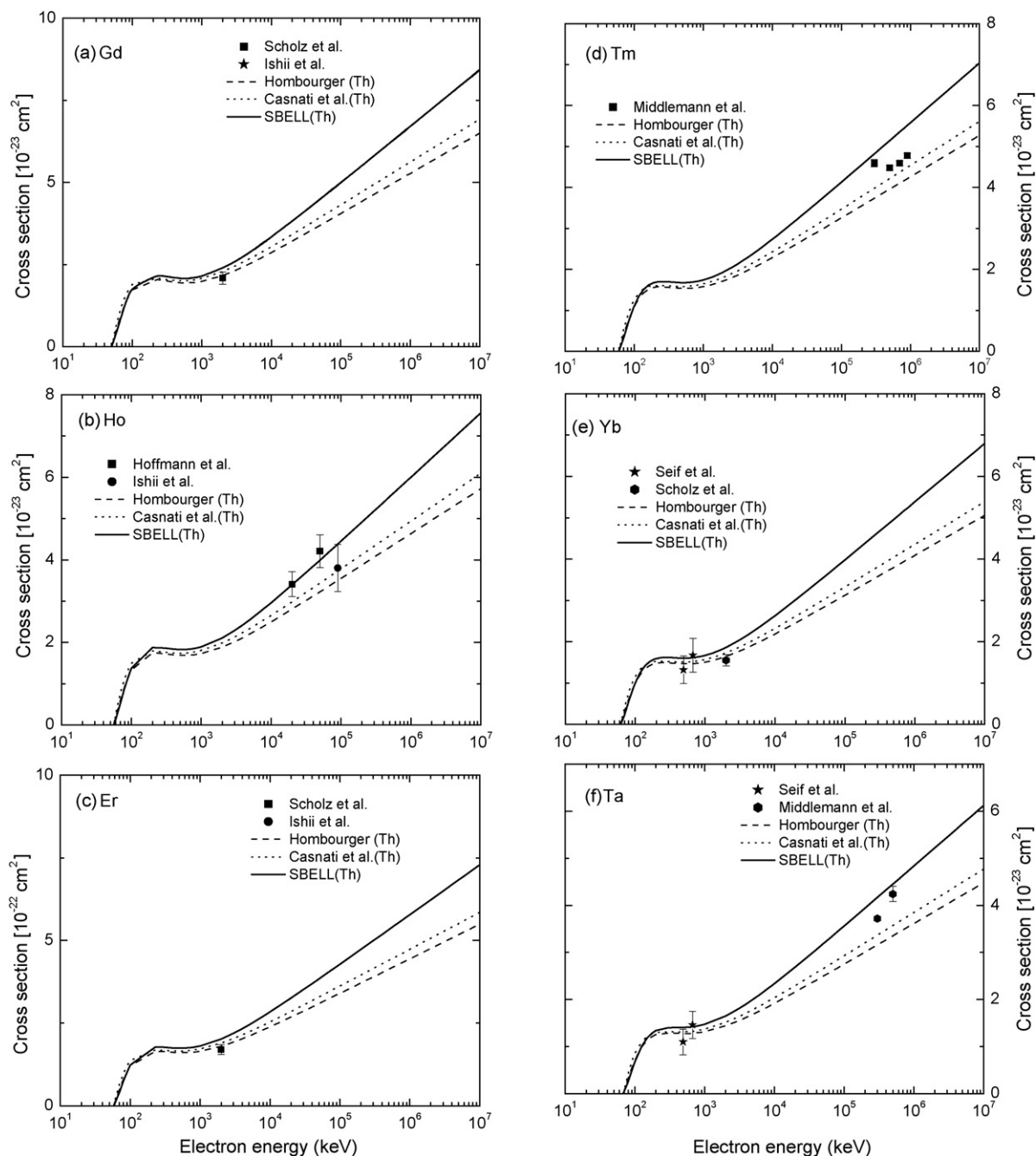


Fig. 9. Electron impact ionization cross sections of K -shell for: (a) Gd, (b) Ho, (c) Er, (d) Tm, (e) Yb, and (f) Ta.

experimental data for the range of energies and for the targets $Z=1-92$ considered. Fig. 1(a)–(f) show the EII cross sections for H–Ne, respectively. The parameter values of $A=0.1854$, $B_1=-0.00186$, $B_2=0.1231$, $B_3=-0.1901$, $B_4=0.9527$, and $B_5=0.0$ for H, and $A=0.5720$, $B_1=-0.3440$, $B_2=-0.5230$, $B_3=-3.4450$, $B_4=-6.8210$, and $B_5=5.5780$ for He, as mentioned in Bell et al. [9], are used in the calculations. The units used of these parameters are in $10^{-13} \text{ eV}^2 \text{ cm}^2$. We use the same parameters values for C–Ne as used for He because *K*-shell of the entire C–Ne atoms are also filled. As seen from Fig. 1 that the BELL formula overestimates EII cross sections in the peak

region for H while it underestimates for C–Ne in the low-energy region. But it calculates better for the whole energy region considered for He only. Since this model does not work well for heavier atoms and not included for the rest targets. On the other hand, EII cross-sections predicted by Hombourger [8] and Casnati et al. [7] largely overestimate in the low-energy region for H and He, and in the relativistic energy region for K, Cr, Mn, Fe, and Co; while underestimate at low incident energies for C, N, and Al, and at relativistic energies for Ni, Cu, Zn, Ge, Se, Y, Pd, Ag, In, Sn, Ba, Sm, Ho, Tm, Ta, Au, Pb, Bi, and U, as seen from Figs. 1–10. However, SBELL model predicts excellently,

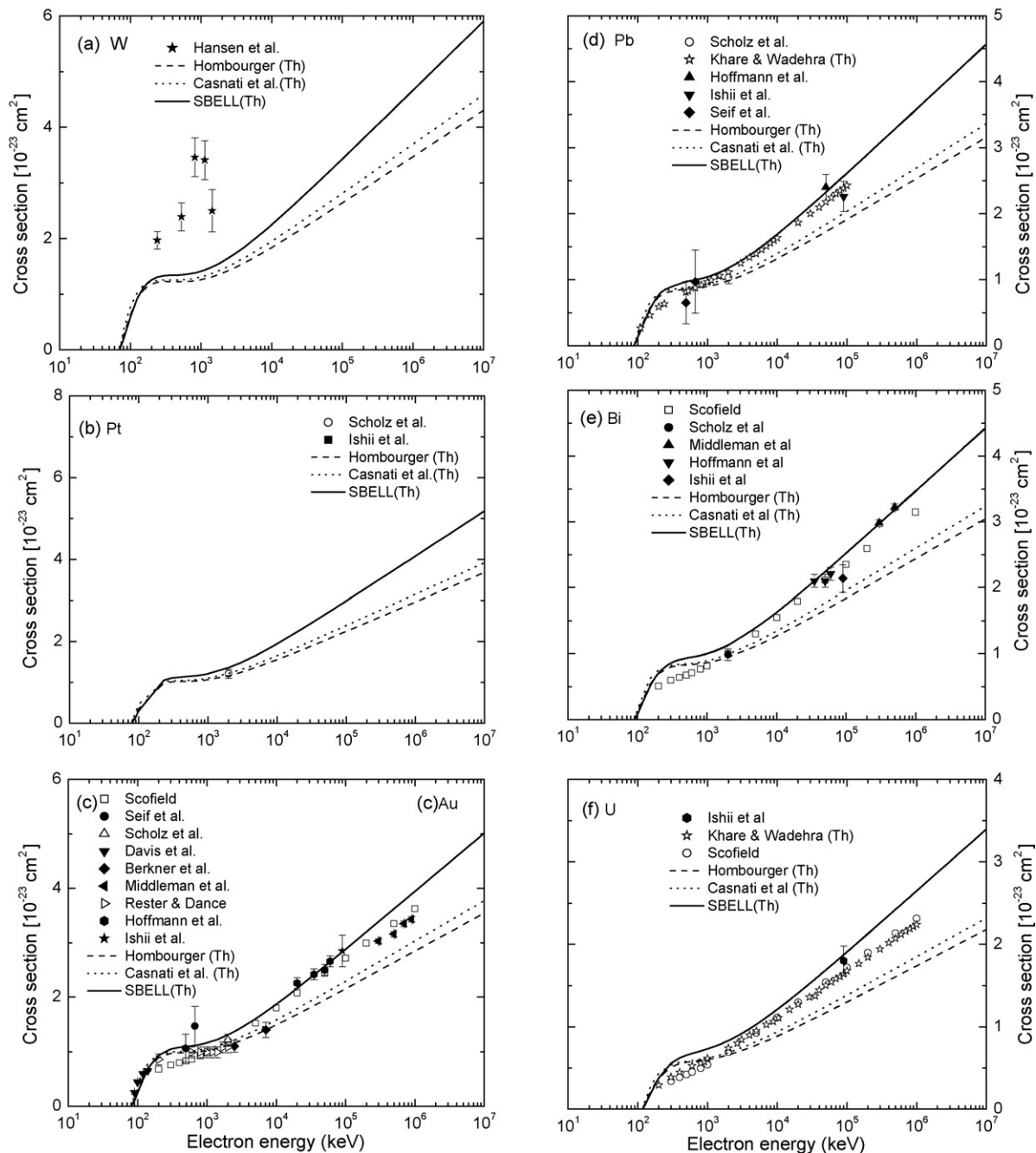


Fig. 10. Electron impact ionization cross sections of *K*-shell for: (a) W, (b) Pt, (c) Au, (d) Pb, (e) Bi, and (f) U.

as compared to the Hombourger [8], Casnati et al. [7], and Bell et al. [9] models, the EII cross sections for *K*-shell not only over the wide incident energies, from low to ultra-relativistic ranges, but also for the wide variety of targets for $Z=H-U$ except for Xe at relativistic energies.

Moreover, the prediction of EII cross sections of *K*-shell by SBELL model are compared with the available quantal PWBA calculations of Kare and Wadehra [3], perturbation calculations, with exchange effect, of Luo and Joy [2], the relativistic PWBA calculations of Scofield [4], and the relativistic DWBA calculations of Segui et al. [5], as can be seen from Figs. 1–10. It is clearly evident that the SBELL model, proposed in the present work, provides a reasonably good agreement over the wide range of energies from threshold to ultra-relativistic for 60 atomic targets from H to U.

4. Conclusion

A simple model is proposed, simplifying BELL formula by incorporating in it both the ionic and relativistic corrections, for the calculation of EII cross sections of *K*-shell neutral atoms. The predicted cross sections are compared with the experimental data. The results of the proposed SBELL model achieve a level of agreement with experimental data those are better than the predictions from the existing theoretical methods and empirical models not only over the wide incident energies within $1 \leq EII_k \leq 10^7$ but also for the large number of targets from $Z=H-U$. This model is very simple-to-use than other empirical or semi-empirical models for implementing in different applied fields. Since this model may be a prudent choice, for the practitioners of applied sciences, due to its simple inherent structure.

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