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Low-energy electron elastic scattering from Mn, Cu, Zn, Ni, Ag and Cd atoms

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Abstract

Electron elastic total cross sections (TCSs) for ground and excited Mn, Cu, Zn, Ni, Ag and Cd atoms have been investigated in the electron-impact energy range $0 \leq E \leq 1$ eV. The near-threshold TCSs for both the ground and excited states of these atoms are found to be characterized by Ramsauer-Townsend minima, shape resonances and extremely sharp resonances corresponding to the formation of stable bound negative ions. The recently developed Regge-pole methodology wherein is embedded the crucial electron-electron correlations is employed for the calculations. From the close scrutiny of the imaginary parts of the complex angular momenta, we conclude that these atoms form stable weakly bound ground and excited negative ions as Regge resonances through slow electron collisions. The extracted electron binding energies from the elastic TCSs of these atoms are contrasted with the available experimental and theoretical values.

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I. Introduction

There is a great need for a fundamental understanding of the mechanism of the near-threshold electron attachment to the atoms Mn, Cu, Zn, Ni, Ag and Cd, particularly the identification and characterization of the attendant resonance structures in the electron elastic total cross sections (TCSs). The atoms Mn, Zn, Y, Ru and Cd with peculiar closed-shell electronic configurations are expected to yield negative ions as intermediate resonances in low-energy electron collisions, with values of their electron affinities (EAs) near zero or even negative. Recently, the low-energy scattering of electrons from many simple and complex atoms has been found to be characterized by sharp long-lived resonances identified as signatures of the stable bound states of the relevant negative ions formed during the elastic collisions between the incident electron and the target neutral atom as Regge resonances [1, 2]. The imaginary part of the complex angular momentum, L, Im L has been used to distinguish between the stable bound states of the negative ions (long-lived resonances) thus formed during the collision and the shape resonances (short-lived resonances). Im L for the former is several orders- of- magnitude smaller than that for the latter.

In this paper we have selected the atoms Mn,Cu, Zn, Ni, Ag and Cd and investigated their near-threshold electron elastic scattering cross sections to identify and delineate the resonance structures and minima in the electron collision cross sections and extract their EAs where possible. These data are needed for the realization of the electron spectroscopy of tenuously and weakly bound negative ions [3]. The transition metal elements have very rich chemistry, with applications varying from materials science through catalysis, biology and problems of the environment. In recent years Cd because of its toxicity, like Pb has entered the equation of air, food and water concerns since it is now mined as part of the Zn deposits. So, its resonance structure when compared with that of Zn should be interesting and informative. The accurate description of these elements is very challenging for *ab initio* electronic structure theory. Thus considerable theoretical efforts have been devoted to the determination of accurate electron affinities for the 4d and 5d transition metal atoms using various theoretical methods, such as the CCSD(T), MP2 and density functional theory [4] and references therein. These methods obtained results that are riddled with uncertainties and lack definitiveness. The obtained theoretical EAs vary from negative values through about 2.2 eV, while the experimental data lie between 0 and about 2.3 eV (see Table 2 of [4]). For instance, the calculated EA values for the Y, Ru and Hf atoms are respectively -0.205 eV, -0.564 eV and -0.347 eV, contrary to the measurements which give all positive values. Furthermore, for the atoms Mn, Zn and Cd the theory and experiment agree on a zero value for their EAs.

Both relativistic and nonrelativistic calculations have been carried out at the CCSD(T) level of theory for the ionization potentials and electronic excitation energies for the 3d elements [5]. However, the most challenging property calculated in that paper was the EA since in the 3d elements the electrons are bound purely by electron correlation effects. The paper [5] concluded that the Mn and Zn atoms do not bind electrons to form stable negative ions. This theoretical prediction has been followed by coupled cluster methods CCSD(T) and CCSDTQ and multireference configuration interaction [6]. The CCSD(T) method was found to achieve accurate atomic excitation energies and ionization potentials, but the electron affinities proved to be more difficult particularly for the late transition metals Mn-Zn. Nevertheless, the conclusion was the same as in [5], namely the atoms Mn and Zn do not form stable negative ions.

Generally, structure-based theoretical methods encounter difficulties when calculating the EAs of atoms because intricate and subtle interactions among the many diverse electron configurations characterize heavy and complex atoms. To date the structure-type calculations have strived to identify the dominant electron configurations associated with the electron attachment process, resulting in the formation of stable negative ions. Their difficulties can be understood in the context of some important facts in the published literature. First and foremost, Johnson and Burrow [7] concluded that given the extent of configuration mixing in the negative-ion states in the theoretical papers it is inappropriate to assign in the elements such as Na, K, Rb and Cs *only a single electron configuration* to each of the various resonances occurring in the threshold region. Secondly, Amusia [8] has remarked that in structure calculations for negative ions performed, only those cases where the extra electron is in an almost pure one electron state have been considered; even in Ca^- the extra electron is not in a pure 4p-orbital, but almost.

Calculating binding energies (BEs) of excited anions is particularly more exacting because excited states are generally weakly bound, BEs < 1 eV, but mostly tenuously bound, BEs < 0.1 eV. Their wavefunctions are more diffuse than those for ground states of negative ions, which translate into the need for an even larger configuration interaction representation (expansion). It is in this context that the recent complex angular momentum (CAM) or Regge-pole methodology [9, 10] has been developed; it calculates the elastic TCSs using the Mulholland formula [11]. The Regge-pole methodology requires no *a priori* knowledge of the experimental or other theoretical data as inputs.
Thus, in the near-threshold electron impact energy region the electron elastic scattering cross sections for the ground and excited states of the 5d transition metal atoms La, Hf, Pt and Au have already been studied carefully [12, 13] using the Regge-pole methodology [9,10]. From the characteristic resonances in the elastic TCSs the EAs and the BEs of the excited anions were extracted and compared with available measurements.

For the complicated La, Pt and Au atoms the obtained EA values were in outstanding agreement with the available measurements [14-20]. However, the DFT calculated EAs for Au and Pt atoms [4] tended to underestimate the measured values. For Pt the calculated EA value [21] overestimated the measurement by approximately a factor of two. The measured BE for the excited state of the La negative ion [14] agreed moderately with the theoretical value of [22], while for Hf recent calculations obtained very good agreement with each other on the BE [22, 23]. Also, recent investigations of near-threshold electron elastic scattering by Hf, Ru and Y revealed neither negative nor zero EAs for these atoms [22]. Electron elastic scattering cross sections for Ag have been investigated both experimentally and theoretically, but at much higher electron impact energies [24]. The electron impact energy for the experiment varied from 10 eV through 100 eV, while the electron impact energy for the calculation was between 100 eV and 10,000 eV.

The recently observed excellent catalytic properties of Au and Pd nanoparticles and the exceptional catalytic activity of the Au-Pd catalyst when catalyzing H_2O_2 [26] have provided a new impetus to study low-energy electron elastic scattering from the above selected atoms. Very recently, the fundamental mechanism of catalysis at the atomic scale has been proposed and demonstrated for Au, Pd and Au-Pd through the scrutiny of the low-energy electron elastic total cross sections [28]. The interplay between the negative ion resonances and Ramsauer-Townsend minima that characterize the low-energy electron elastic TCSs has been proposed as the fundamental mechanism underlying nanoparticle catalysis [28]. In [29] the enhancement of the catalytic activity of the atoms Au, Ag, Y, Ru, Pd and Pt has been investigated when used in various combinations compared to their individual action. For example, the catalytic activity of the Au–Ag–Pd trimetallic nanoparticles was investigated and found to be efficient in catalyzing the Heck reaction [30]. The experiment [31] found that the methanol oxidation current of the ternary Pt-Ru-Ni catalyst increased by as much as a factor of 2.6 in comparison with that of the binary Pt-Ru catalyst. This can contribute to the controlled synthesis and understanding of fuel-cell catalysts [31]. Furthermore, the high efficiency of Ag nanoparticles deposited over activated carbon has been demonstrated in controlling microorganisms in water [32].

II. Calculational Procedure

Jablonski *et al* [25] investigated electron elastic-scattering cross sections for various atoms, including Ag using two commonly used atomic potentials, namely the Thomas–Fermi–Dirac (TFD) potential and the Dirac–Hartree–Fock (DHF) potential. However, their energies were quite high, varying from 100 eV through 10,000 eV. Interestingly, the DHF potential was found to require a considerably larger number of phase shifts than the TFD potential. In contrast to the hundreds of partial waves used in [25], the present Regge pole methodology requires only a few Regge poles. As is well known, Regge poles are singularities of the S-matrix and rigorously define resonances [33]. Clearly, the attractiveness of the approach to the near threshold calculation of electron scattering is evident.

Crucial to the existence and stability of most negative ions are the mechanisms of electron-electron correlations and core-polarization interactions. It should be noted here that the R-T minima manifest the polarization of the atomic core by the scattered electron [35]. These physical effects render understanding the structure and the dynamics of low-energy electron elastic collisions, resulting in the formation of negative ions as resonances, quite challenging for conventional theoretical methods. The absolute cross section measurements for the processes are difficult as well. Here we calculate the electron elastic TCSs for the ground and excited atoms and extract from them the BEs of the negative ions formed during the collisions as Regge resonances. In the CAM description of scattering we use the Mulholland formula [11] in the form [9, 10] (atomic units are used throughout):

$$\begin{aligned}\sigma_{tot}(E) &= 4\pi k^{-2}\int_0^\infty \mathrm{Re}[1-S(\lambda)]\lambda d\lambda \\ &- 8\pi^2 k^{-2}\sum_n \mathrm{Im}\frac{\lambda_n \rho_n}{1+\exp(-2\pi i\lambda_n)} + I(E)\end{aligned} \tag{1}$$

where S is the S-matrix, k = √(2mE), with m being the mass, ρ_n the residue of the S-matrix at the nth pole, λ_n and I(E) contains the contributions from the integrals along the imaginary λ-axis; its contribution has been demonstrated to be negligible [12]. We will consider the case for which Im λ_n<<1 so that for constructive addition, $\mathrm{Re}\lambda_n \approx 1/2,\ 3/2,\ 5/2....$, yielding $\ell = \mathrm{Re}\,L \cong 0,1,2...$ The importance of Eq. (1) is that a resonance is likely to affect the elastic TCS when its Regge pole position is close to a real integer [10].

The calculation of the elastic TCSs and the Mulholland partial cross sections uses the T-F type model potential [36] in the well investigated form [37, 38]

$$U(r) = \frac{-Z}{r(1+aZ^{1/3}r)(1+bZ^{2/3}r^2)}, \tag{5}$$

where Z is the nuclear charge and *a* and *b* are adjustable parameters. For small r, the potential describes the Coulomb attraction between an electron and a nucleus, $U(r) \sim -Z/(r)$, while at large distances it mimics the polarization potential, $U(r) \sim -1/(abr^4)$ and accounts properly for the vital core-polarization interaction at very low energies. The effective potential

$$V(r) = U(r) + L(L+1)/(2r^2), \tag{6}$$

is considered here as a continuous function of the variables r and L. The potential, Eq. (5) has been used successfully with the appropriate values of *a* and *b*. When the TCS as a function of "*b*" has a resonance [12] corresponding to the formation of a stable bound negative ion, this resonance is longest lived for a given value of the energy which corresponds to the electron affinity of the system (for ground state collisions). This was found to be the case for all the systems we have investigated thus far. This fixes the optimal value of "*b*" for Eq. (5).

In the present investigation of the electron scattering from Ag in particular, we have found three such values of "*b*" which still satisfy the T-F equation within a certain error margin. We identify the two smallest values with the presence of excited states and the largest value with the ground state of the corresponding atom. Note that the energies are measured relative to the ground state of the neutral atom. The values used for "*b*" in this paper are tabulated in Table 1 for the six atoms of interest here, while the value of "*a*" was kept fixed at 0.2 for all the atoms. In the study of low-energy electron scattering from Cu atoms, it was demonstrated that the ground and excited states are polarized differently [39] as expected. This explains the use in this paper of different values for the optimal parameter "*b*" for the ground and excited atoms.

For the numerical evaluation of the TCSs and the Mulholland partial cross sections, we solved the Schrödinger equation for complex values of L and real, positive values of E

$$\psi'' + 2\left(E - \frac{L(L+1)}{2r^2} - U(r)\right)\ \psi = 0, \tag{7}$$

with the boundary conditions:

$$\begin{gathered} \psi(0) = 0, \\ \psi(r) \sim e^{+i\sqrt{2E}r},\ r \to \infty. \end{gathered} \tag{8}$$

We note that Eq. (8) defines a bound state when $k \equiv \sqrt{(2E)}$ is purely imaginary positive. In solving Eq. (7) two independent approaches are adopted. The first integrates numerically the radial Schrödinger equation for real integer ℓ = Re L values of L to sufficiently large r values. The S-matrix is then obtained and the TCSs are evaluated as the traditional sum over partial waves, with the index of summation being ℓ. The second part calculates the S-matrix, S(L, k) poles positions and residues of Eq. (7) following a method similar to that of Burke and Tate [40]. In the method the two linearly independent solutions, f_L and g_L, of the Schrödinger equation are evaluated as Bessel functions of complex order and the S-matrix, which is defined by the asymptotic boundary condition of the solution of the Schrödinger equation, is thus evaluated. Further details of the calculation may be found in [40].

Im L is important in distinguishing between the shape resonances (short–lived resonances) and the stable bound, both ground and excited, states of the negative ions (long-lived resonances) formed as Regge resonances in the electron-atom scattering [12, 41]. In the definitions of Connor [41] and the applications [12] the physical interpretation of Im L is given. It corresponds inversely to the angular life of the complex formed during the collision. A small Im L implies that the system orbits many times before decaying, while a large Im L value denotes a short-lived state. For a true bound state, namely E < 0, Im L ≡ 0 and therefore the angular life, 1/[Im L] → ∞, implying that the system can never decay. Im L is also used to differentiate subtleties between the bound and the excited states of the negative ions formed as resonances during the collisions.

Here it is appropriate to explain the great success of the Regge pole methodology in describing low-energy electron elastic scattering. The motivation is to clarify the roles of the Regge pole methodology itself and the T-F type potential. The calculated results hinge on the strength of the Regge pole methodology itself and the philosophy upon which it is based rather than on the potential used, namely the Thomas-Fermi type potential in the present case. To clarify this point, we give a brief summary of the underlying ideas. In our approach, the problem of calculating bound states of negative ions is reduced to that of electron scattering from the corresponding neutral target and the search for long-lived resonances. Here we are using a Thomas-Fermi type potential to represent the neutral atomic target in the electron scattering process. The T-F type potential used here is suitable and attractive because it can be analytically continued into the complex angular momentum plane. The strength of the potential has been investigated further recently through its pole structure and Stokes lines topology and placed on solid theoretical ground [38].

The Schrodinger equation (SE) is solved for the electron in the field of the target, namely the T-F type potential. We fix the energy E and look for a regular solution of the SE which contains at infinity only the outgoing wave by changing $\Lambda=L(L+1)$, with L being the complex angular momentum. This is a Sturm-Liouville problem. Contrary to most basis-set representations of wave functions for quantum systems which employ energy eigenstates of some model Hamiltonian, the eigenfunctions here are exceptional in this regard since they are not energy eigenstates. Instead, they diagonalize the potential and therefore are superior to energy eigenstates for representing waves in regions where the potential is strongest. In other words, all eigenfunctions with fixed energy are well localized in the physically relevant region of the potential. For this reason they often provide rapidly convergent expansions of wave functions for complex systems, for which most structure-based calculations would almost certainly be intractable. Moreover, the superior localization of the basis sets can be effectively employed to describe dynamic atomic and molecular systems characterized by the electronic states that are initially known to be localized around one particular center of force. This property can be especially useful when describing atomic collisions.

Additionally, we take advantage of the powerful but innocent-looking Mulholland formula for the total cross section which was introduced when it was shown that the standard partial wave representation was unable to identify the origin of some oscillation features in the cross sections below 1eV that has no classical counterpart. The Mulholland formula replaces *identically* the partial wave sum with integrals (the smooth background) and the contribution of a few poles which represent any structure in the cross section. It is well known that negative-ion formation in electron-atom scattering exhibits extreme sensitivity to the electron correlation effects and core polarization interaction. Thus, the crucial electron correlation effects are fully accounted for through the Mulholland formula. However, for the near-threshold electron attachment it is also critical that the potential include the dominant core polarization interaction; hence the importance of the Thomas-Fermi type potential which has the required $-1/r^4$ asymptotic behavior.

III. Results

As pointed out in the introduction, the most important physical effects in low energy electron attachment to atoms, resulting in the formation of stable negative ions, both ground and excited, as Regge resonances in the elastic TCSs, are electron-electron correlation effects and core-polarization interactions. These are embedded in the Regge pole methodology and the T-F type potential used here. Rather than present the results in ascending order of Z values, it is more informative to present the results beginning with those of Ag. The reason is that nanoAg is an excellent catalyst and its resonance structure in the TCS has already been investigated recently in the context of the fundamental understanding of nanocatalysts. Just as the electron scattering TCSs for Au was used as a template for nanocatalysts, the TCSs for the electron scattering from Ag will be used as a template here. The results for Ag have been recalculated but remain very nearly the same as those of [29].

Figure 1 presents the low energy electron elastic scattering cross sections for Ag over a wider energy range $0.01 \le E \le 7$ eV compared to the rest of the results presented here. It is hoped these results will lead to a better understanding of why the atoms Mn, Zn and Cd are believed to have zero EAs. The long-dashed, dashed and solid curves represent respectively data for the ground state, first excited state and second excited state of Ag. The TCSs are rich in R-T minima, shape resonance and the dramatically sharp resonances, representing the stable bound states of the negative ions formed during the collision as Regge resonances. Notably, the ground state TCS is characterized by two R-T minima, with the second one much deeper than the first one. The configuration of these R-T minima, the shape resonances and the bound state, represented by the very sharp resonance, characterizes good nanocatalysts [29]. We note that this interesting structure appears in the energy range $1 \leq E \leq 7$ eV, essentially outside the energy region of interest of this paper.

The investigation of the TCSs in the energy range $0 \leq E \leq 1$ eV for the selected atoms is dictated by the fact that the EAs of Mn, Zn and Cd are believed to be zero. The second curve represents the TCS for the first excited state of Ag. This curve is characterized by a deep broad R-T minimum, followed by a shape resonance and, eventually by the sharp resonance at the second very shallow minimum. This sharp line at the minimum corresponds to the stable bound state of the first excited state of the Ag negative ion. The importance of the bound state at the minimum of the TCS has already been discussed in the context of nanoscale catalysis of Au, Pd and the Au-Pd mixture [28]. It is noted that this structure resembles that of the electron-Hf scattering TCS for the ground state [22].

The solid curve in Fig. 1 represents the TCS for the second excited state of Ag. It is characterized by a broad shape resonance that is followed by a sharp line, manifesting the existence of a stable bound excited negative ion. The parameters for the three curves are summarized in Table 1.

The electron elastic TCSs for Mn are presented in Fig. 2. The long-dashed curve represents the TCS for the ground state of Mn, while the second curve is for the first excited state. We note that the ground state curve resembles that for the first excited state of Ag. It is characterized by a deep, broad R-T minimum near threshold, followed by a broad shape resonance and eventually by the very sharp resonance which defines the stable bound state of the Mn negative ion formed as a Regge resonance during the collision. Contrary to all previous theoretical and experimental investigations, Mn is seen to form a stable negative ion through low energy electron scattering. Its EA is found to be 0.703 eV, a fairly large value. This first prediction, to our knowledge, calls for immediate experimental and theoretical verification. The values of the remaining parameters are summarized in Table 1. The dashed curve of Fig. 2, representing the TCS for the first excited state of Mn, also has a sharp resonance that correspond to the stable bound negative ion formed as a Regge resonance during the collision. The configuration of the two deep minima in the ground and excited states TCSs could be important in the design of nanocatalysts.

The TCSs for atomic Ni are displayed in Fig. 3. Here the long-dashed and the dashed curves represent respectively the TCSs for the first and the second excited states of Ni. In both the first and the second excited states the Ni atom forms stable negatives ions as Regge resonances. The values of the various parameters are given in Table 1. We note that the EAs of Ni and Cu are well established; their values are respectively 1.15 eV and 1.23 eV [42].

Figure 4 presents the data for electron scattering from Cu. The results resemble those of Ni and the values of the various parameters are also given in Table 1. As pointed out above, the EA of Cu resembles that of Ni and is well established [42]. From Table 1 the values of the various parameters of Cu are seen to be comparable to those of Ni and the EAs of Cu and Ni are almost equal in value [42].

Like Mn and Cd atomic Zn is considered to have zero EA value. In our careful search for the EA of Zn, we found only one stable bound state of Zn, as shown in Fig. 5. Namely, low energy electron collisions with Zn leads to a stable bound negative ion as a Regge resonance. The sharp resonance represents the bound state of the negative ion of Zn formed as a Regge resonance. This resonance has a value of 0.137 eV and corresponds to the EA of Zn. This is the first prediction to our knowledge of a nonzero EA value for Zn; it also calls for both experimental and theoretical verification.

In Fig. 6 the TCSs for electron scattering from Cd are presented. The long-dashed curve represents the result for the ground state of Cd. Just as in Mn the cross section is characterized by a broad R-T minimum at 0.0634 eV, followed by a shape resonance at 0. 225 eV and, subsequently by the thin line. This line is the signature of the presence of a stable bound state of the Cd negative ion formed during the collision as a Regge resonance. Cd is one of the atoms that are believed to have zero EA values. Our result is the first ever, to our knowledge, to predict a nonzero EA value for Cd, which is 0.394 eV. This value is relatively large and should lend itself readily to experimental verification. Experiments such as those of Johnston and Burrow [7] should be able to determine the EAs of Mn, Zn and Cd readily.

The dashed curve in Fig. 6, characterized by the very sharp resonance, corresponds to the first excited state of Cd and resembles those of Cu, Ni and Zn. Clearly, low energy electron attachment to Cd yields a stable bound excited state of the Cd negative ion with a BE of 0.113 eV. The parameters of the two curves are also summarized in Table 1.

For the atoms Mn, Zn and Cd the tabulated EA values are all zero [15, 42]. However, on the contrary, this calculation has obtained the values of 0.703 eV, 0.137 eV and 0.394 eV, respectively. To us the nonzero EAs obtained here are not surprising. These cases are similar to that of Ca, where obtaining reliable theoretical EA is very exacting for structure-based calculations. With the Regge pole methodology we were able to obtain a reliable EA value for Ca, even for Sr. The atoms Cu, Ni and Ag have well established EAs and their values are greater than unity [15]. So, they are of no particular interest to this paper, except for their TCSs near threshold.

IV. Summary and Conclusion

In this paper we have used the recent Regge pole methodology wherein is embedded the vital electron-electron correlation effects, to investigate low energy electron elastic scattering from the atoms Mn, Cu, Zn, Ni, Ag and Cd. The objective was to identify and delineate the resonance structures in their elastic TCSs. The presence of dramatically sharp resonances in their TCSs is a manifestation of the existence of stable bound states of negative ions formed during the collision as Regge resonances. Through the close scrutiny of the Im L we have identified shape resonances and the stable bound states of the negative ions (both ground and excited states). For the latter, Im L is several orders of magnitude smaller than that for the former.

We found that the elastic TCSs for these atoms are generally characterized by R-T minima, shape resonances and very sharp resonances that correspond to the existence of stable bound states of the negative ions formed during the collision as Regge resonances. Most important, we also found contrary to general beliefs, that Mn and Cd have non-zero EAs. These first ever predictions, to our knowledge, of non-zero EA values for these atoms call for immediate experimental and theoretical verifications. Furthermore, these atoms are also characterized by the formation of stable excited negative ions. Of particular interest is that Zn also forms through slow electron collision a single stable bound negative ion; we have not found others despite careful searching.

In conclusion, low energy electron elastic scattering from the atoms Mn, Cu, Zn, Ni, Ag and Cd has been found to lead to the formation of stable negative ions, in both ground and excited states, as Regge resonances from which their BEs can be extracted. The results obtained here are also important for the realization of the electron spectroscopy of tenuously and weakly bound negative ions and in the determination of nanocatalysts.

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Table 1 Calculated Binding Energies EAs, E1 and E2 (in eV), positions of Ramsauer-Townsend (RT) minima and shape resonances (SR) (in eV), and *b* parameters for Mn, Ni, Cu, Zn, Ag and Cd atoms

Z	Symbol	b	E2	SR	RT	b	E1	SR	RT	b	EA	SR	RT
25	Mn					0.0354	0.068	n/a	0.048	0.0418	0.703	0.441	0.041
28	Ni	0.0441	0.027	n/a	0.024	0.0304	0.133	0.029	n/a				
29	Cu	0.0473	0.021	n/a	0.019	0.0329	0.176	0.034	n/a				
30	Zn									0.0352	0.137	0.034	n/a
47	Ag	0.0410	0.152	0.0394	n/a	0.0305	0.760	0.244	0.054	0.0486	2.240	1.772	0.970
48	Cd					0.0426	0.113	0.039	n/a	0.0314	0.394	0.225	0.0634

'n/a' stands for 'not available' and indicates that no RT-minimum or shape resonance was found in the energy range presented here.

Figure Captions

Figure 1: Total cross sections, in atomic units, for electron elastic scattering versus E (eV) for Ag, are contrasted on a log x log plot. The long-dashed, dashed and solid curves correspond respectively to ground, first and second excited states. The characteristic R-T minima and resonances are clearly exhibited.

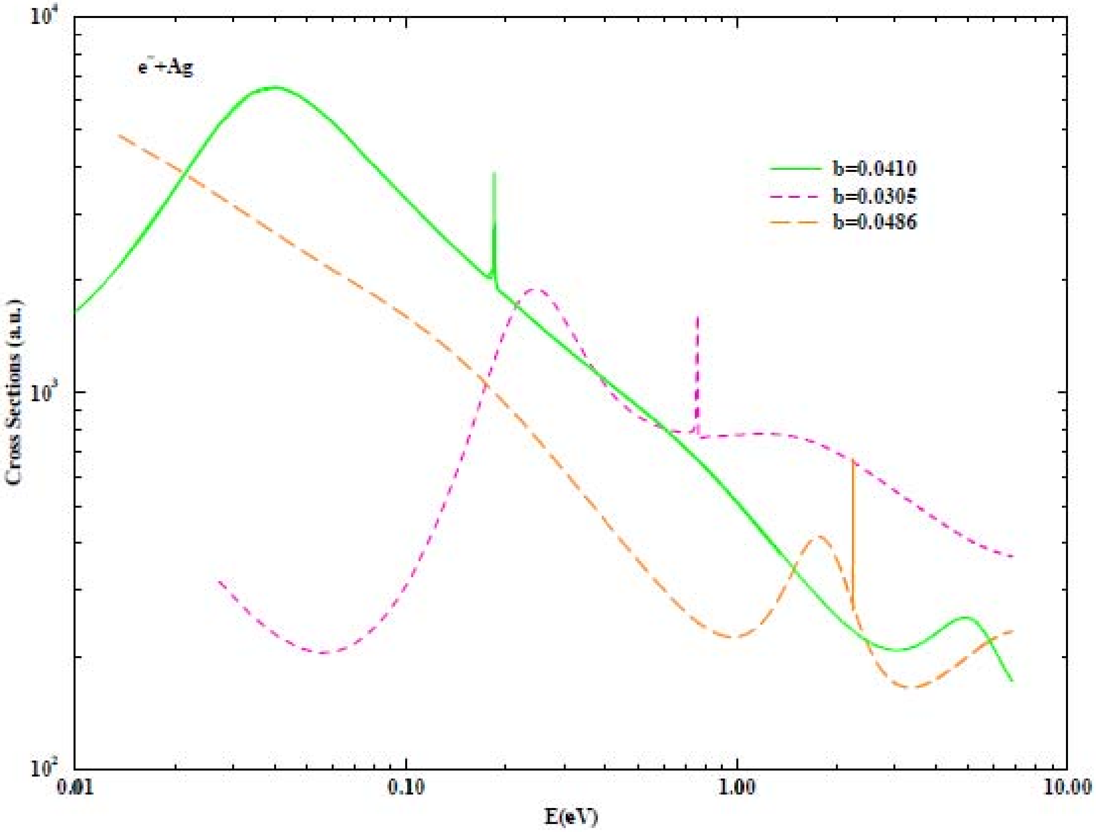
Figure 2: The same as for Fig. 1 except that the results are for electron scattering from ground (long-dashed curve) and first excited (dashed curve) states of the Mn atom.

Figure 3: The same as for Fig. 2 except that the results are for electron scattering from first excited (long-dashed curve) and second excited (dashed curve) states of the Ni atom.

Figure 4: The same as for Fig. 2 except that the results are for electron scattering from first excited (long-dashed curve) and second excited (dashed curve) states of the Cu atom.

Figure 5: The same as for Fig. 2 except that the results are for electron scattering from the only bound state found for the Zn atom.

Figure 6: The same as for Fig. 2 except that the results are for electron scattering from ground (long-dashed curve) and first excited (dashed curve) states of the Cd atom.



e⁻+Ag
b=0.0410
b=0.0305
b=0.0486
Cross Sections (a.u.)
10⁴
10³
10²
0.01
0.10
1.00
10.00
E(eV)

FIG. 1

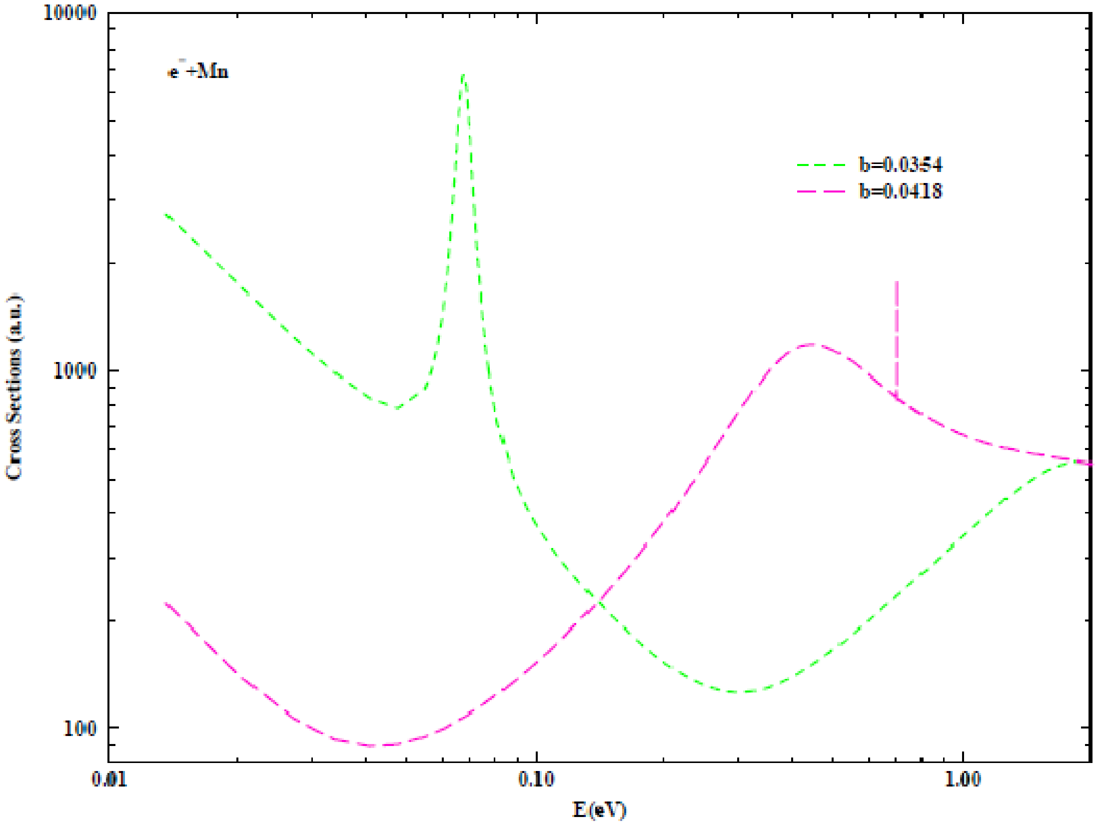
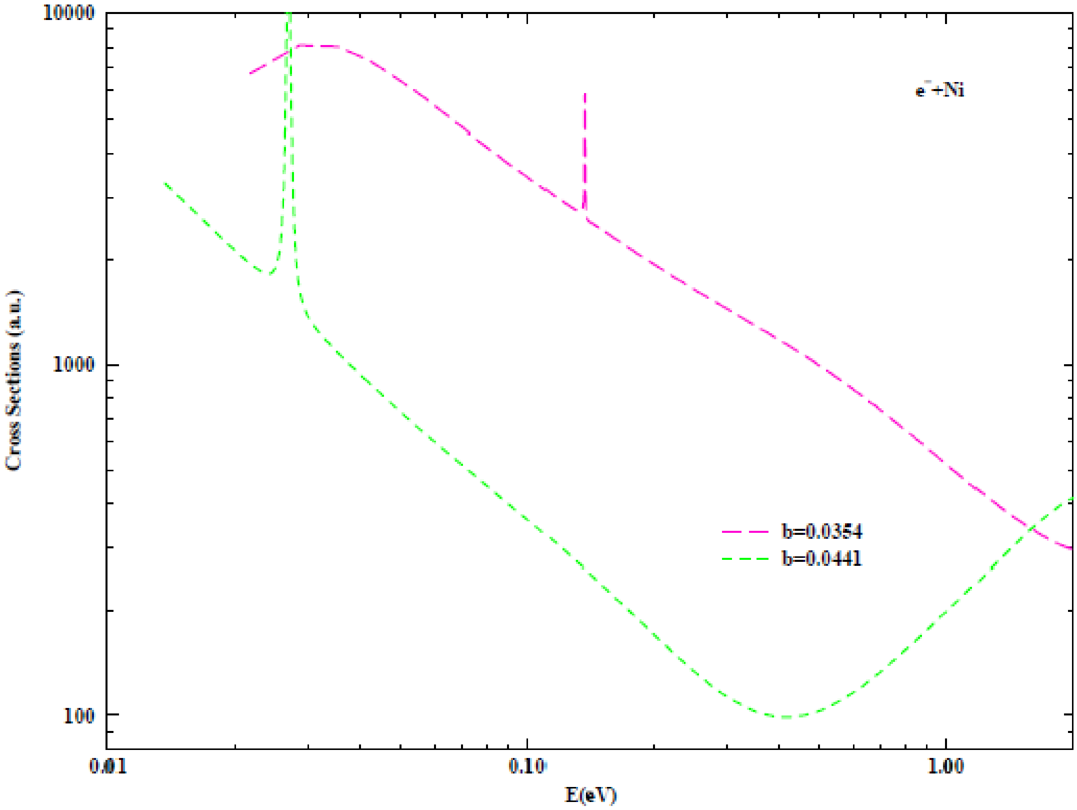

e⁻+Mn
b=0.0354
b=0.0418
Cross Sections (a.u.)
10000
1000
100
0.01
0.10
1.00
E(eV)

FIG. 2



Cross Sections (a.u.)
10000
1000
100
0.01
0.10
1.00
E(eV)
e^-+Ni
b=0.0354
b=0.0441

FIG. 3

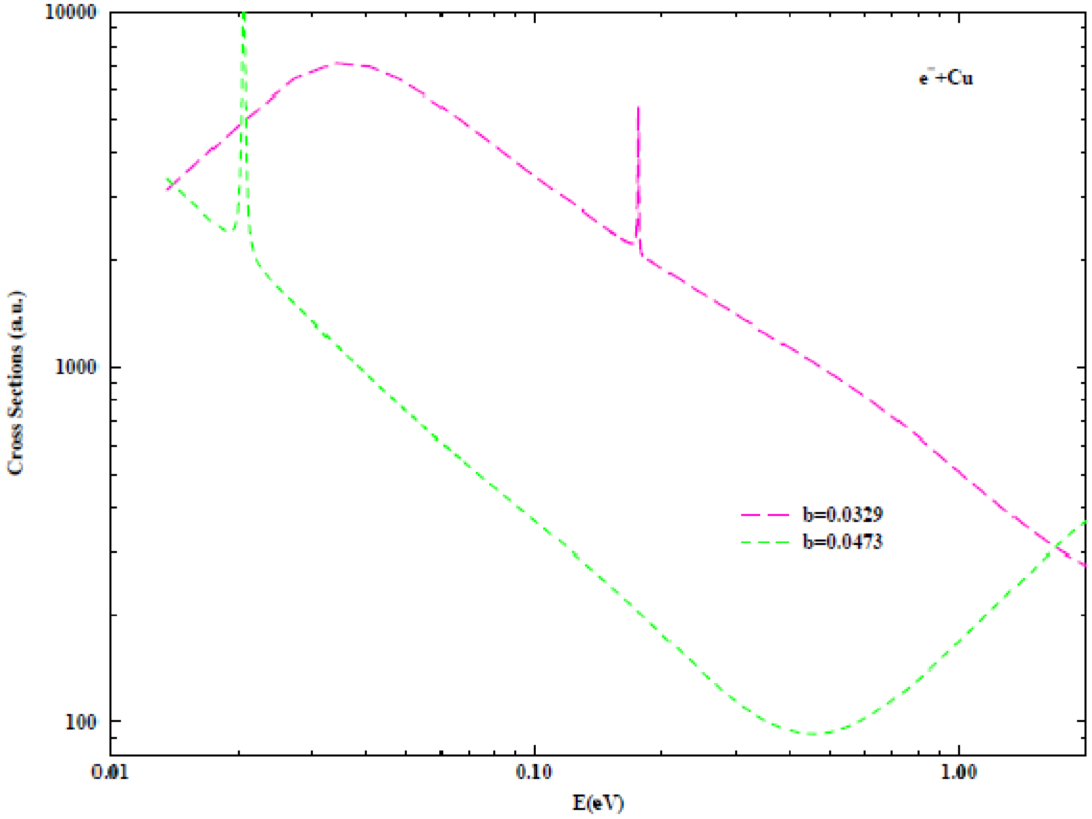

10000
1000
100
Cross Sections (a.u.)
0.01
0.10
1.00
E(eV)
e⁻+Cu
b=0.0329
b=0.0473

FIG. 4

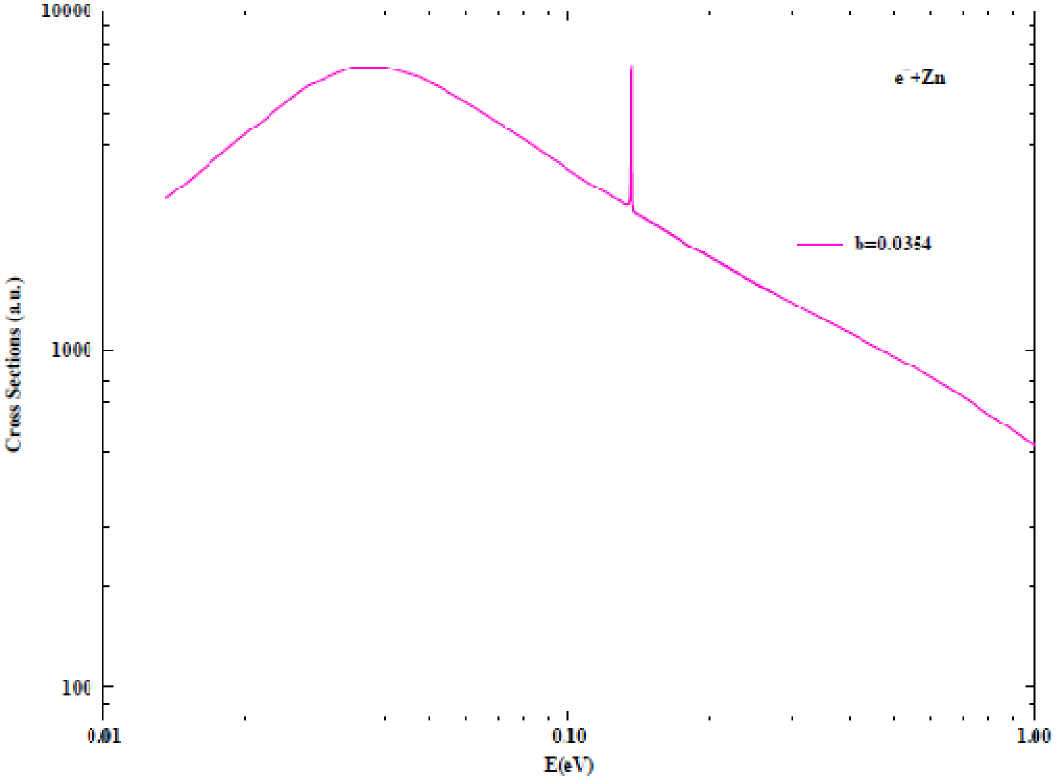


FIG. 5

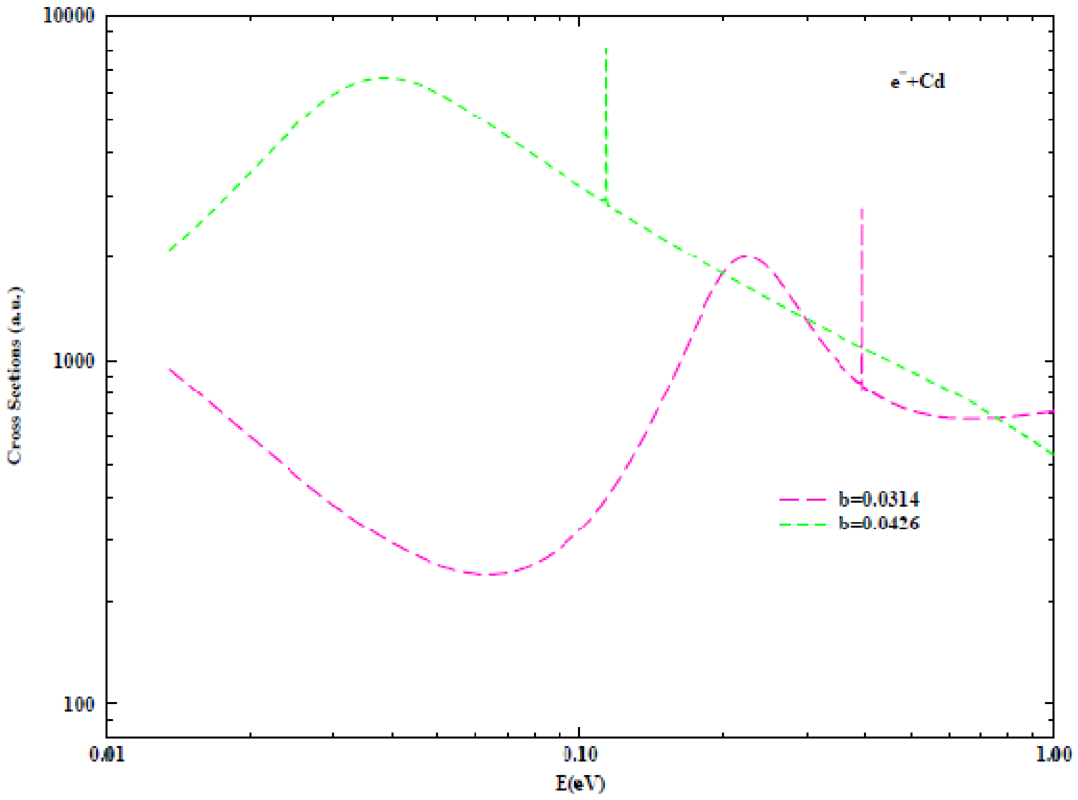

10000
1000
100
Cross Sections (a.u.)
0.01
0.10
1.00
E(eV)
e⁻+Cd
b=0.0314
b=0.0426

FIG. 6