Complex angular momentum analysis of low-energy electron elastic scattering from lanthanide atoms

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Electron attachment to the lanthanide and Hf atoms resulting in the formation of stable excited lanthanide and Hf anions as Regge resonances is explored in the near-threshold electron impact energy region, $E < 1.0$ eV. The investigation uses the recent Regge-pole methodology wherein is embedded the electron-electron correlations together with a Thomas-Fermi–type model potential incorporating the crucial core-polarization interaction. The near-threshold electron elastic total cross sections (TCSs) for the lanthanide and Hf atoms are found to be characterized by extremely narrow resonances whose energy positions are identified with the binding energies (BEs) of the resultant anions formed during the collision as Regge resonances. The extracted BEs for excited lanthanide anions are contrasted with those of the most recently calculated electron affinities (ground state BEs). We conclude that the BEs for the Pr⁻, Tb⁻, Dy⁻, Ho⁻, Er⁻, and Tm⁻ anions of O'Malley and Beck [Phys. Rev. A **79**, 012511 (2009)] are not identifiable with the electron affinities as claimed. Formation of bound excited anions is identified in the elastic TCSs of all the lanthanide atoms including Hf, except Eu and Gd. The imaginary part of the complex angular momentum L, ImL is used to distinguish between the shape resonances and the bound excited negative ions. These results challenge both experimentalists and theoreticians alike since the excited anions are very weakly bound, but mostly tenuously bound (BEs < 0.1 eV). Shape resonances and Ramsauer-Townsend minima are also presented.

I. INTRODUCTION

The aim of this paper is to investigate low-energy, $E < 1.0$ eV electron elastic collisions with the lanthanide and Hf atoms, resulting in the possible formation of stable excited negative ions as long-lived resonances. New binding energies (BEs) for excited lanthanide negative ions formed during the collisions as resonances are extracted from the calculated elastic total cross sections (TCSs). Additionally, corrected electron affinities (EAs) for the Tm, Yb, Lu, and Hf atoms, also extracted from the TCSs, are presented. The EA of an atom is defined as the binding energy of the ground state of the corresponding negative ion relative to the ground state of the neutral atom and is taken as a positive number. Note that the BE of an excited state of the negative ion is also measured with respect to the ground state of the corresponding neutral atom. The motivation is twofold: (1) To understand the disturbing disagreements between our recently calculated EA values for the Pr, Tb, Dy, Ho, Er, and Tm atoms [1] and those of O'Malley and Beck [2,3] and correct some of our EA values and (2) To identify and obtain values of shape resonances, Ramsauer-Townsend (RT) minima as well as binding energies for excited lanthanide and Hf⁻ negative ions. For the calculations we use our Regge-pole methodology [4], based on the complex angular momentum description of electron-atom scattering, wherein the electron-electron correlation effects are accounted for through the Mulholland formula. This formula for the total cross section converts the infinite discrete sum into a background integral plus the contribution from a few poles to the process under consideration. The vital core-polarization interaction is incorporated through the well-investigated Thomas-Fermi–type model potential. We limit our calculations to the near-threshold energy

region, keeping below any inelastic thresholds to avoid their effects.

The knowledge of low-energy collisions of atoms and ions is essential for the exploration of the physics of the cooling and trapping of gaseous atomic ensembles and in the investigation of cold plasmas [5], including the creation of new molecules from atoms. Low-energy collisions, resulting in negative ion formation as intermediate resonances, provide a special insight into quantum dynamics [6]. The formation of temporary negative ionic states as resonances and their properties define the mechanism through which low-energy electron scattering deposits energy and induces chemical transitions [7,8]. The understanding of chemical reactions involving negative ions requires accurate binding energies (BEs) [9]. Electron attachment to a neutral atom resulting in the formation of a very weakly bound negative ion produces intershell-type resonances [10]. Crucial to the existence and stability of most negative ions are the mechanisms of electron-electron correlations and core-polarization interactions. Various theoretical investigations have demonstrated through comparisons with measurements the vital importance of the core-polarization interaction in low-energy electron scattering from atoms and molecules [10–15]. In recent years negative ions have attracted significant experimental investigations using various experimental techniques and for various reasons [16–20]. In particular, the experiment [21] concluded that the existence of a large characteristic peak in the measured electron-atom scattering TCS at low energy is a manifestation of the ground state of the negative ion formed during the collision as a resonance. This facilitates considerably the identification of the BEs of negative ions in the electron elastic scattering TCSs.

The near-threshold elastic scattering TCSs of electrons by neutral atoms are generally characterized by the Wigner

threshold law [22], shape resonances and Ramsauer-Townsend minima. The Wigner threshold law is essential in high precision measurements of BEs of valence electrons using photodetachment threshold spectroscopy [23]. Shape resonances are useful for interpreting electron-induced chemical processes resulting in negative ion production [7,8]. The Ramsauer-Townsend minima are important in understanding sympathetic cooling and the production of cold molecules from natural fermions [24]. We note that the RT minima manifest the polarization of the atomic core by the scattered electron [25]. Ground state atoms with low electron affinity values are also required for the quenching of Rydberg atoms through collisions [26]. Consequently, it is important to identify and delineate these physical effects in low-energy electron collisions to guide measurements.

II. CALCULATIONAL PROCEDURE

Heavy and complex atoms are generally characterized by intricate and subtle interactions among the many diverse electron configurations. So, calculating binding energies of excited anions is particularly challenging because excited states are generally weakly bound, BEs < 1 eV or even tenuously bound, BEs < 0.1 eV. Calculational procedures that obtain these values through explicit subtraction of two large numbers can lead to significant errors [27]. For calculating electron attachment or removal processes the electron propagator or one particle Green's function is appropriate since the poles of the propagator are the electron affinities and ionization potentials of the atomic or molecular systems [27]. It is in this context that the present Regge-pole methodology [4] has been developed since Regge-poles, singularities of the S matrix, rigorously define resonances [28,29]. To use the nonrelativistic Regge-pole methodology to investigate the formation of excited negative ions as Regge resonances in low-energy electron collisions with complex atoms, the methodology has already been benchmarked on the accurately measured BEs of excited bound states of the Ge$^-$ and Sn$^-$ anions [16].

The extracted BEs [30] compared excellently with the term averaged values from the measurement of Scheer *et al.* [16] and also very well with the term averaged values [31]. For the bound excited state of the La$^-$ anion the agreement between the measured BE by Covington *et al.* [32] and the Regge-pole calculated value is moderate.

Here we calculate the electron elastic TCSs for the lanthanide and Hf atoms and extract from them the BEs of the resultant negative ions. The imaginary part of the complex angular momentum (CAM), L, ImL is used to distinguish between the bound states of these ions and the attendant shape resonances. For the latter the ImL is several orders-of-magnitude larger than that for the former. In the CAM description of scattering we use the Mulholland formula [33] in the form [4,34] (atomic units are used throughout):

$$\sigma_{\text{tot}}(E) = 4\pi k^{-2} \int_0^\infty \text{Re}[1 - S(\lambda)]\lambda d\lambda$$
$$- 8\pi^2 k^{-2} \sum_n \text{Im} \frac{\lambda_n \rho_n}{1 + \exp(-2\pi i \lambda_n)} + I(E), \quad (1)$$

where $\sigma_{\text{tot}}(E)$ is the total cross section (TCS) at impact energy E, S is the S matrix, $k = \sqrt{(2mE)}$, 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 [1]. Note that λ is related to the complex angular momentum L through $\lambda = L + 1/2$. We will consider the case for which Im $\lambda_n \ll 1$ so that for constructive addition, Re$\lambda_n \approx 1/2, 3/2, 5/2 \ldots$, yielding $\ell = \text{Re}L \cong 0, 1, 2 \ldots$. 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 [4].

The calculation of the elastic TCSs and the Mulholland partial cross sections uses the TF-type model potential [35] in the well investigated form [36]

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

TABLE I. Calculated binding energies, BEs (eV), shape resonances, SRs (eV), Ramsauer-Townsend (RT) minima (eV), and b parameter for excited lanthanide and Hf$^-$ negative ions. "NA" denotes "not available."

Z	Symbol	BEs	b	ReL	ImL	SRs	ReL	ImL	RT
57	La	0.115	0.0304	3	1.6×10^{-5}	0.023	1	3.1×10^{-2}	NA
58	Ce	0.101	0.0315	3	9.0×10^{-6}	0.023	1	3.5×10^{-2}	NA
59	Pr	0.152	0.0328	3	3.3×10^{-5}	0.027	1	4.2×10^{-2}	NA
60	Nd	0.047	0.0459	2	2.0×10^{-4}	NA	NA	NA	0.039
61	Pm	0.052	0.0475	2	2.4×10^{-4}	NA	NA	NA	0.042
62	Sm	0.044	0.0490	2	1.4×10^{-4}	NA	NA	NA	0.036
63	Eu	NA	NA	NA	NA	NA	NA	NA	NA
64	Gd	NA	NA	NA	NA	NA	NA	NA	NA
65	Tb	0.114	0.0400	3	5.6×10^{-6}	0.031	1	4.1×10^{-2}	NA
66	Dy	0.084	0.0412	3	1.7×10^{-6}	0.031	1	3.7×10^{-2}	NA
67	Ho	0.124	0.0426	3	5.9×10^{-6}	0.034	1	4.2×10^{-2}	NA
68	Er	0.119	0.0439	3	4.6×10^{-6}	0.034	1	4.1×10^{-2}	NA
69	Tm	0.016	0.03202	2	3.4×10^{-5}	NA	NA	NA	0.014
70	Yb	0.028	0.0331	2	1.3×10^{-4}	NA	NA	NA	0.024
71	Lu	0.029	0.0341	2	1.4×10^{-4}	NA	NA	NA	0.025
72	Hf	0.017	0.0350	2	3.2×10^{-5}	NA	NA	NA	0.015

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,

$$V(r) = U(r) + L(L+1)/(2r^2), \tag{3}$$

is considered here as a continuous function of the variables r and L. The potential, Eq. (2) has been used successfully with the appropriate values of a and b. When the TCS as a function of b has a resonance [1] 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. (2).

In the case of the lanthanide and Hf atoms studied here, we have found two such values of b which still satisfy the TF equation within a certain error margin. We identify the smaller value of the corresponding resonance energies with the presence of an excited state and the larger with that of the ground state of the relevant negative ion. 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 I for excited lanthanide atoms, 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 [37] as expected. This explains the use in this paper of different values for the
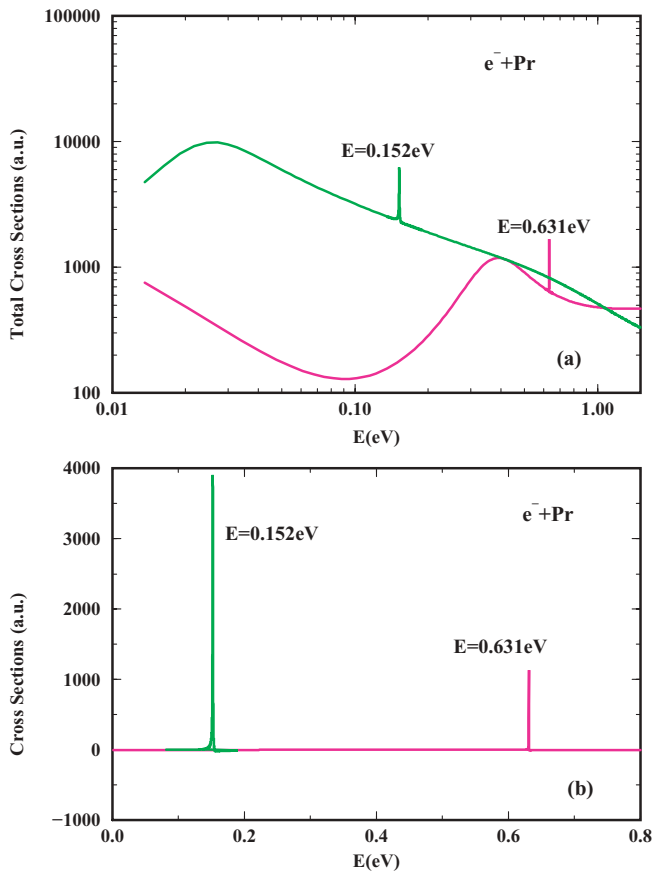

FIG. 1. (Color online) (a) The total cross sections, in atomic units, for e^--Pr elastic scattering versus E (eV), are contrasted, lower curve is for the ground state and the upper curve is for an excited state. The lower curve (ground state) exhibits the characteristic RT minimum at 0.088 eV, a shape resonance at 0.386 eV and a stable ground state of the Pr$^-$ anion at 0.631 eV, formed during the collision as a Regge resonance. The top curve (excited state) shows the shape resonance at 0.027 eV and a stable excited state resonance at 0.152 eV. Note the log-log plot. (b) The Mulholland partial cross sections, in atomic units, for e^--Pr elastic scattering versus E (eV) are displayed on a linear scale, showing the sharp resonances at 0.152 eV and at 0.631 eV. The positions of these resonances correspond respectively to an excited state and the ground state of the negative Pr$^-$ ions formed during the collision as Regge resonances.
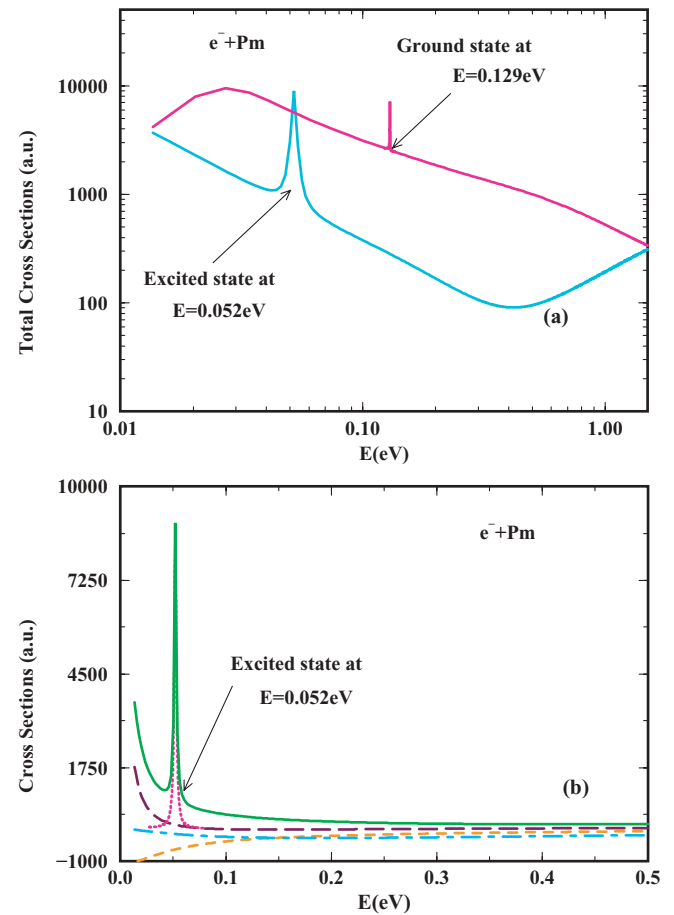

FIG. 2. (Color online) (a) The same as for Fig. 1(a) except that the results are for e^--Pm scattering. Contrary to Fig. 1(a) here the curves for the ground and excited states cross sections have interchanged their positions. (b) Total (solid) and Mulholland partial elastic cross sections, in atomic units, for e^--Pm scattering versus E (eV). The long-dashed, dashed, dot-dashed and dotted curves represent, respectively, the $n = 1, 2, 3$, and 4 Mulholland contributions, as given by the second term on the right-hand side of Eq. (1) (Note that the $n = 4$ partial cross section (dotted) is responsible for the very sharp resonance at 0.052 eV; the latter is identified with a stable excited state of the Pm$^-$ negative ion formed during the collision as a Regge resonance; the RT minimum is clearly visible near threshold.

optimal parameter b for the ground and excited lanthanide and Hf$^-$ anions.

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

$$\psi'' + 2\left(E - \frac{L(L+1)}{2r^2} - U(r)\right)\psi = 0, \qquad (4)$$

with the boundary conditions:

$$\psi(0) = 0,$$
$$\psi(r) \sim e^{+i\sqrt{2E}r}, \quad r \to \infty. \qquad (5)$$

We note that Eq. (5) defines a bound state when $k \equiv \sqrt{(2E)}$ is purely imaginary positive. In solving Eq. (4) two independent

approaches are adopted. The first integrates numerically the radial Schrödinger equation for real integer $\ell = \mathrm{Re}L$ 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. (4) following a method similar to that of Burke and Tate [38]. 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 [38].
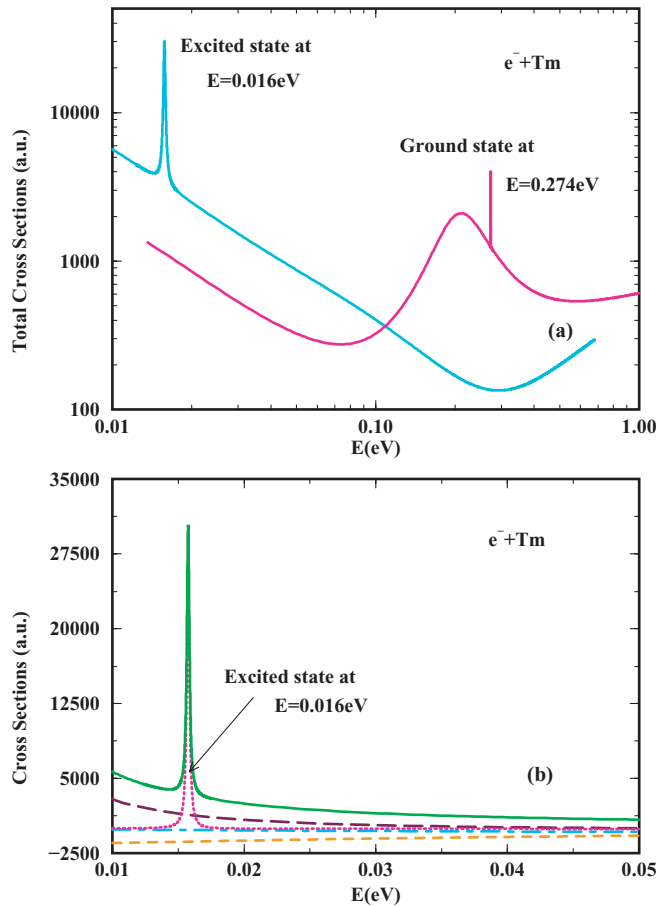

FIG. 3. (Color online) (a) The same as in Fig. 1(a) except that the results are for e^--Tm scattering. The very sharp resonance at 0.016 eV is identified with a stable excited state of the Tm$^-$ negative ion; the RT minimum is clearly visible near threshold. Note the position of the shape resonance in the TCS between the ground and excited state resonances. (b) Total (solid) and Mulholland partial elastic cross sections, in atomic units, for e^--Tm scattering versus E (eV). The long-dashed, dashed, dot-dashed and dotted curves represent, respectively, the $n = 1, 2, 3$, and 4 Mulholland contributions, as given by the second term on the right-hand side of Eq. (1) Note that the $n = 4$ partial cross section (dotted) is responsible for the very sharp resonance at 0.016 eV; the latter is identified with a stable excited state of the Tm$^-$ negative ion formed during the collision as a Regge resonance; the RT minimum is clearly visible near threshold.
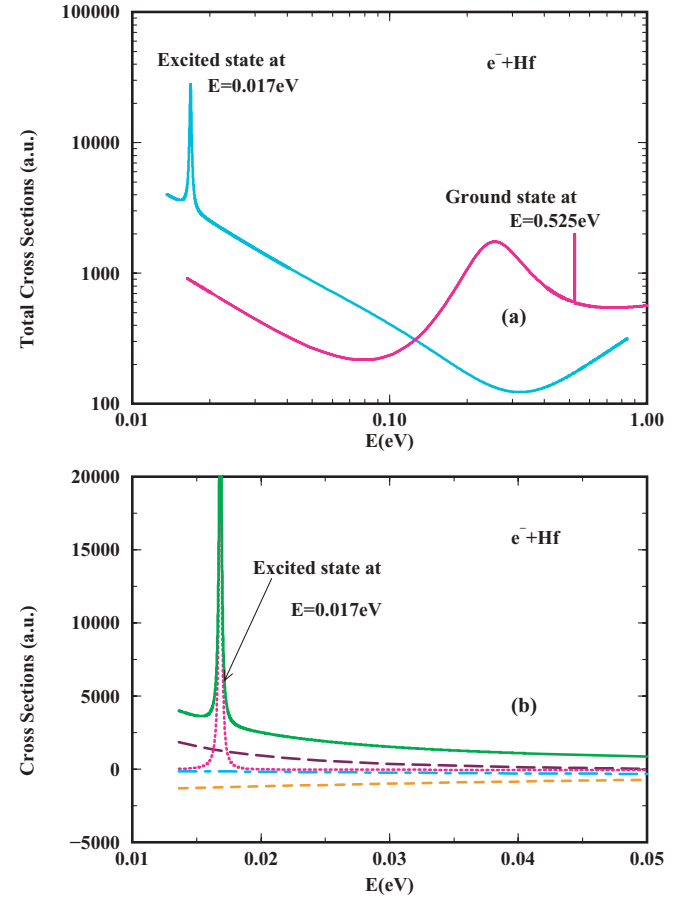
FIG. 4. (Color online) (a) The same as for Fig. 1(a) except that the results are for e^--Hf scattering. The very sharp resonance at 0.017 eV is identified with a stable excited state of the Hf$^-$ negative ion; the RT minimum is clearly visible near threshold. The ground state TCS curve exhibits the characteristic structure. Near threshold the excited state TCS dominates while for $E > 0.2$ eV the ground state TCS is the dominant of the two. (b) Total (solid) and Mulholland partial elastic cross sections, in atomic units, for e^--Hf scattering versus E (eV). The long-dashed, dashed, dot-dashed and dotted curves represent, respectively, the $n = 1, 2, 3$, and 4 Mulholland contributions, as given by the second term on the right-hand side of Eq. (1). Note that the $n = 4$ partial cross section (dotted) is responsible for the very sharp resonance at 0.017 eV; the latter is identified with a stable excited state of the Hf$^-$ negative ion formed during the collision as a Regge resonance; the RT minimum is clearly visible near threshold.

ImL 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 [1,39]. In the definitions of Connor [39] and the applications [1] the physical interpretation of ImL is given. It corresponds inversely to the angular life of the complex formed during the collision. A small ImL implies that the system orbits many times before decaying, while a large ImL value denotes a short-lived state. For a true bound state, namely $E < 0$, Im$L \equiv 0$ and therefore the angular life, $1/(\text{Im}L) \rightarrow \infty$, implying that the system can never decay. ImL is also used to differentiate subtleties between the bound and excited states of the negative ions formed as resonances during the collisions.

III. RESULTS

The primary focus of this paper is to calculate the TCSs and the Mulholland partial cross sections for electron elastic scattering from the lanthanide and Hf atoms, leading to the formation of excited anions during the collisions as Regge resonances and extract their BEs. Comparison of the extracted BEs with the EA values of O'Malley and Beck [2,3] and ours [1], is expected to resolve the source of the disturbing disagreements between some of the former EA values and those of the latter. We must stress here that the Regge-pole methodology assumes no *a priori* knowledge of any experimental data whatsoever. In our paper [1] we pointed out that the significant discrepancy between the O'Malley and Beck [2] EAs and ours [1] of the lanthanide atoms occurred in atoms where the RT minima preceded the shape resonances; otherwise agreement between the two calculations varied from good to outstanding. The electron elastic TCSs for the Pr and Tm atoms were such examples. Consequently, for a better understanding and appreciation of the calculated results, we first discuss the elastic TCSs for e^--Pr and e^--Pm scattering. These are

presented in Figs. 1 and 2, respectively, and will serve as typical results.

Figure 1(a) contrasts using a log-log representation the ground (lower curve) and excited (upper curve) states elastic TCSs for e^--Pr scattering in the energy range $E < 1.0$ eV. The ground state TCS is from [1] and is characterized by a RT minimum, a shape resonance and a very sharp Regge resonance, identified with the stable bound state of the Pr$^-$ negative ion formed during the collision. On the other hand the excited state total cross section is characterized by a shape resonance at 0.027 eV followed by a Regge resonance at 0.152 eV. This resonance is also identified using ImL with the stable bound state of an excited negative ion formed during the collision as a Regge resonance. We note here that the TCS for the excited state is generally higher than that of the ground state and that the shape resonance associated with the ground state is between the excited and ground states of the anion formed during the collision. Figure 1(b) contrasts the Mulholland partial cross sections for the excited and the ground Pr negative ion in the energy region of the Regge resonances. The excited state resonance at 0.152 eV corresponds to a stable excited Pr$^-$ negative anion while the second peak at 0.631 eV defines the EA of the Pr atom.

The results for the electron elastic scattering from the Pm atom are presented in Fig. 2. It is informative to contrast Fig. 2(a) with Fig. 1(a). As was demonstrated in [1] this represents a case where the shape resonance precedes the ground state resonance. Here the ground state TCS generally dominates the excited state TCS, in contrast to the case of the e^--Pr scattering. Furthermore, the excited state resonance is quite strong and appears between the shape resonance and the ground state resonance, again in contrast to the situation in Fig. 1(a). Figure 2(b) presents the TCS and the Mulholland partial cross sections for the excited Pm atom in the energy region of the excited state resonance, corresponding to a stable excited Pm$^-$ negative anion at 0.052 eV. The RT minimum near threshold is also evident in the figure.

TABLE II. Calculated electron affinities, EAs (eV) for the lanthanide and Hf atoms and binding energies, BEs (eV) for excited states of the corresponding negative ions.

Z	Symbol	EAs	ReL	ImL	BEs	ReL	ImL
57	La	0.480	4	7.8×10^{-7}	0.115	3	1.6×10^{-5}
58	Ce	0.610	4	1.9×10^{-6}	0.101	3	9.0×10^{-6}
59	Pr	0.631	4	1.9×10^{-6}	0.152	3	3.3×10^{-5}
60	Nd	0.162	3	3.6×10^{-5}	0.047	2	2.0×10^{-4}
61	Pm	0.129	3	1.4×10^{-5}	0.052	2	2.4×10^{-4}
62	Sm	0.162	3	2.8×10^{-5}	0.044	2	1.4×10^{-4}
63	Eu	0.116	3	7.6×10^{-6}	NA	NA	NA
64	Gd	0.137	3	1.2×10^{-5}	NA	NA	NA
65	Tb	0.436	4	5.0×10^{-6}	0.114	3	5.6×10^{-6}
66	Dy	0.350	4	1.6×10^{-6}	0.084	3	1.7×10^{-6}
67	Ho	0.338	4	1.1×10^{-6}	0.124	3	5.9×10^{-6}
68	Er	0.312	4	6.7×10^{-7}	0.119	3	4.6×10^{-6}
69	Tm	0.274	4	3.2×10^{-7}	0.016[a]	2	3.4×10^{-5}
70	Yb	0.486	4	3.7×10^{-6}	0.028[a]	2	1.3×10^{-4}
71	Lu	0.415	4	1.6×10^{-6}	0.029[a]	2	1.4×10^{-4}
72	Hf	0.525	4	4.0×10^{-6}	0.017	2	3.2×10^{-5}

[a]These were previously identified with the EAs in [1].

Another case of interest and worth discussing is e^--Tm scattering, whose results are displayed in Fig. 3. The reason is that previously, we identified the very sharp and strong resonance at 0.016 eV with the EA of the Tm atom [see Fig. 3(a)] because we did not search sufficiently high on the energy scale and this resonance is very dominant. The characteristic ground state curve is also presented with its RT minimum at 0.085 eV, the shape resonance at 0.22 eV and the EA value at 0.274 eV. At impact energies $Es > 0.15$ eV (approximately) the ground state TCS dominates that of the excited state. Note here also as in Fig. 1(a) that the shape resonance appears between the excited state and the ground state resonances.

The e^--Hf scattering is another example where the identification of the EA requires correction. In Fig. 4(a) the new ground state TCS curve is presented for the first time ever with its characteristic parameters, namely the RT minimum at 0.0857 eV, the shape resonance at 0.25 eV and the EA value at 0.525 eV. It is contrasted with the excited state TCS. The excited state resonance yields the BE of 0.017 eV for the stable Hf$^-$ negative ion. Note here also as in Fig. 1(a) that the shape resonance appears between the excited state and the ground state resonances. Figure 4(b) displays the TCS and the Mulholland partial cross sections for e^--Hf scattering. The position of the huge resonance at 0.017 eV is identified with the BE of an excited Hf$^-$ negative ion formed during the collision as a Regge resonance. The new results for the e^--Hf scattering, including the EA value of Hf are also included in Table II.

From the results of Figs. 1–4, it is clear that as the impact energy approaches threshold the various physical quantities (BEs, EAs, RT minima and shape resonances) characterizing the elastic TCSs begin to appear together [see for example Fig. 1(a)]. This makes their identification quite challenging.
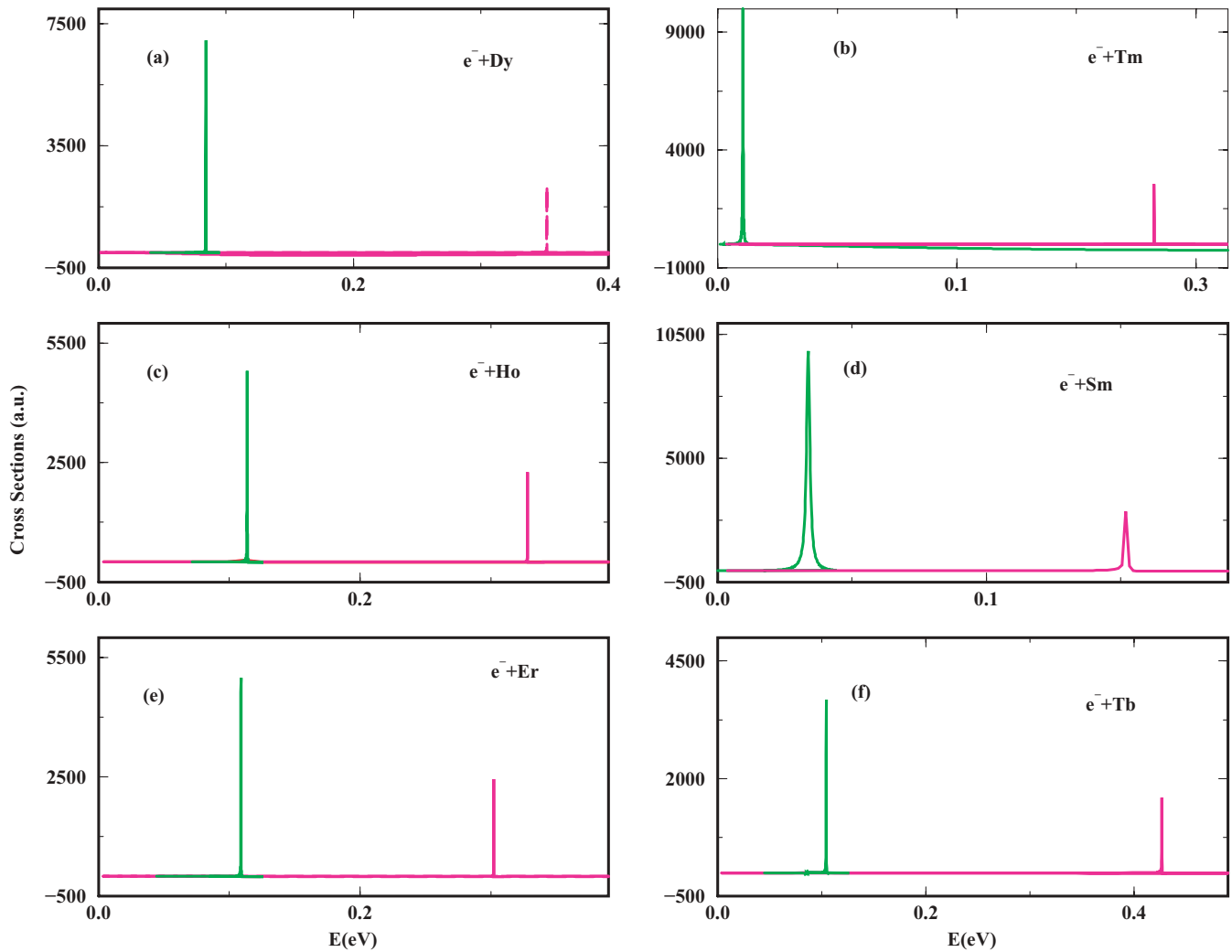

FIG. 5. (Color online) (a) Same as in Fig. 1(b), except that the results are for e^--Dy scattering. The excited state BE and the EA are, respectively, at 0.084 eV and at 0.350 eV. (b) Same as in Fig. 1(b), except that the results are for e^--Tm scattering. The excited state BE and the EA are, respectively, at 0.016 eV and at 0.274 eV. (c) Same as in Fig. 1(b), except that the results are for e^--Ho scattering. The excited state BE and the EA are, respectively, at 0.124 eV and at 0.338 eV. (d) Same as in Fig. 1(b), except that the results are for e^--Sm scattering. The excited state BE and the EA are, respectively, at 0.044 eV and at 0.162 eV. (e) Same as in Fig. 1(b), except that the results are for e^--Er scattering. The excited state BE and the EA are, respectively, at 0.119 eV and at 0.312 eV. (f) Same as in Fig. 1(b), except that the results are for e^--Tb scattering. The excited state BE and the EA are, respectively, at 0.114 eV and at 0.436 eV.

TABLE III. Comparison of electron affinities, EAs (eV) for the lanthanide and Hf atoms and binding energies, BEs (eV) for excited states of the corresponding negative ions.

Z	Symbol	EAs [1]	EAs [2,3]	BEs (Present)
57	La	0.480	0.434	0.115
58	Ce	0.610	0.660	0.101
59	Pr	0.631	0.177	0.152
60	Nd	0.162	0.167	0.047
61	Pm	0.129	0.154	0.052
62	Sm	0.162	0.130	0.044
63	Eu	0.116	0.117	NA
64	Gd	0.137	0.234	NA
65	Tb	0.436	0.085	0.114
66	Dy	0.350	0.063	0.084
67	Ho	0.338	0.050	0.124
68	Er	0.312	0.038	0.119
69	Tm	0.274	0.022	0.016[a]
70	Yb	0.482	–	0.028[a]
71	Lu	0.415	0.353	0.029[a]
72	Hf	0.525	0.110[b]	0.017

[a]These were previously identified with the EAs in [1].
[b]EA (Hf) = 0.110 eV from [40].

However, the representation of the TCSs as in Fig. 1(a) allows the identification to be readily achieved.

The main objective of this paper is to investigate through the calculated elastic cross sections possible electron attachment to the lanthanide and Hf atoms, resulting in the formation of stable excited anions as Regge resonances and extract their BEs for comparison with previous data. Accordingly, in Fig. 5 we display only the Mulholland partial cross sections in the energy region of the stable ground and excited negative ions. This is done to keep the paper compact but yet readily understandable. Figure 5(a), 5(b), 5(c), 5(d), 5(e), and 5(f) represents, respectively, the Mulholland partial cross sections for electron elastic scattering from the Dy, Tm, Ho, Sm, Er, and Tb lanthanide atoms in the energy region of the appropriate resonances. Their positions are identified with the BEs of the ground and excited negative ions formed during the collisions. We note that in the figures the excited states resonances dominate those for the ground states in magnitudes. However, the ground state resonances have longer lifetimes as seen from the ImL in Tables I and II.

All the results of the calculations are summarized in the Tables I and II, particularly the BEs and the EAs. The new BEs are compared in Table III with the EAs of O'Malley and Beck [2,3] and those of [1]. The results demonstrate that the O'Malley and Beck [2,3] BEs for the Pr$^-$, Tb$^-$, Dy$^-$, Ho$^-$, Er$^-$, and Tm$^-$ anions do not correspond to the EA values of the corresponding atoms. The reason is that their magnitudes are not the largest values relative to the ground state of the relevant neutral atoms. It is appropriate to emphasize here that the Regge-pole methodology uses the rigorous definition of resonances and extracts the BEs from the positions of these resonances and requires no *a priori* knowledge of the BE values or the EA values whatsoever. We believe that the results presented here are reliable as has been demonstrated by our recent successful extraction of binding

energies for tenuously bound (BE < 0.1 eV), weakly bound (BE < 1 eV), complicated open-shell and strongly bound (BE > 1 eV) atoms from resonances in the near-threshold elastic scattering cross sections obtained using the Regge-pole methodology.

IV. SUMMARY AND CONCLUSION

In this paper we have investigated low-energy electron elastic scattering from the lanthanide and Hf atoms for a fundamental understanding of electron attachment resulting in the formation of stable ground and excited negative ions as Regge resonances. For the calculations we used our Regge-pole methodology wherein the electron-electron correlation effects are accounted for through the Mulholland formula. The vital core-polarization interaction is incorporated through the well-investigated Thomas-Fermi–type model potential. We limited our calculations to the near-threshold energy region, keeping below any inelastic thresholds to avoid their effects.

We found that the near-threshold electron elastic TCSs for these atoms are characterized by dramatically sharp resonance structures, with those corresponding to excited anions being of greater magnitude than those for the ground anions. From the positions of these resonances, we extracted the EAs (ground state binding energies) and the binding energies of excited anions formed during the collisions as resonances. Where possible we also obtained the RT minima and shape resonances. The ImL was used to differentiate between the shape resonances and the BEs.

With the new BEs for excited lanthanide anions we correct our EA values for Tm, Yb, and Lu given in Table I [1] and provide the corrected EA values in the present Table II, which also includes values for Hf. From the comparison in Table III we conclude that the O'Malley and Beck [2,3] BEs for the negative ions Pr$^-$, Tb$^-$, Dy$^-$, Ho$^-$, Er$^-$, and Tm$^-$ obtained using a relativistic configuration interaction method do not correspond to the EAs of the corresponding atoms as claimed. We note that the O'Malley and Beck calculations assumed a *p*-electron attachment for all the lanthanides they investigated contrary to [1] where no such assumptions were made. The present calculation, like our previous one [1] requires no prior knowledge of the BEs or the EAs; these are extracted from the resonances in the TCSs for elastic scattering. The present results challenge both experimentalists and theoreticians alike since the excited anions are very weakly bound, but mostly tenuously bound (BEs < 0.1 eV). Reliable BEs are also needed in the context of the development of the spectroscopy of tenuously and weakly bound systems for application in the detection and identification of nanomaterials.

In conclusion and most importantly, the data obtained and presented here will now add to the existing body of knowledge on negative ions [16–20], particularly the almost nonexistent binding energies of excited states and low-energy electron elastic scattering cross sections for the important lanthanide atoms.

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