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QED effects in 1s and 2s single and double ionization potentials of the noble gases

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We present calculations on the quantum electrodynamics (QED) effects in 1s and 2s single and double ionization potentials of noble gases from Ne to Rn as perturbations on relativistic four-component Dirac-Fock wavefunctions. The most dominant effect originates from the self-energy of the core-electron that yields corrections of similar order as the transverse interaction. For 1s ionization potentials, a match within few eV against the known experimental values is obtained, and our work reveals considerable QED effects in the photoelectron binding energies across the periodic table—most strikingly even for Ne. We perform power-law fits for the corrections as a function of Z and interpolate the QED correction of ∼−0.55 eV for S1s. Due to this, the K-edge electron spectra of the third row and below need QED for a match in the absolute energy when using state-of-the-art instrumentation. *Published by AIP Publishing.* [http://dx.doi.org/10.1063/1.4979991]

I. INTRODUCTION

For producing accurate predictions of core-electron binding energies, several relativistic mechanisms need to be accounted for: spin-orbit coupling, Dirac-level one-electron effects (e.g., Darwin term), and retarded electron-electron interactions as recently reviewed by Fischer *et al.*[1] In core-level spectroscopy, the number of relativistic electrons in the system changes and therefore these effects step into transition energies and state couplings that can have a significant magnitude.[2–4] Spectroscopic simulations are often carried out at most on the Dirac-Coulomb-Breit level, leaving quantum electrodynamics (QED) out. However there also is evidence of significant QED effects from X-ray emission calculations.[5,6] Studies of QED corrections begun from the measurements of the Lamb shift in the fine-structure of hydrogen[7] and since then these corrections have been the target of numerous papers considering especially heavy atoms and hydrogen-like ions (see, e.g., References 8–12 and references therein). The dominant radiative QED effects are vacuum-polarization (VP) and self-energy (SE) corrections.

The simplest experimental measure of relativistic effects in core-levels is the ionization potential (IP) of the electrons on the orbital. Whereas traditional electron spectroscopy for chemical analysis[13] (ESCA) and derived techniques probe single-hole states, it is also possible to record a multitude of electrons from an ionization event in coincidence using magnetic bottle time-of-flight spectrometers,[14] which allows direct studies of double-core-hole states.[15] For the $2s^{-2}$ states, double IPs (DIPs) can also be obtained by subtracting the KL_1L_1 Auger-electron kinetic energy from the known 1s IP. In addition, due to the availability of X-ray free-electron sources, it is becoming possible to generate previously inaccessible states of matter by sequential multiphoton processes in the hard X-ray region. However, even normal single photoemission, near-edge absorption fine structure, X-ray emission spectroscopy, and resonant inelastic X-ray scattering carry their respective relativistic and QED effects in the involved energy levels.

In this work we study the QED effects in IPs and DIPs as perturbations on the Dirac-Fock (DF) wavefunction. We report calculations for the noble gases from Ne to Rn and investigate the Z-scaling of these effects. By using approximate formulation implemented in a published atomic structure package, we obtain agreement within few eV with the experimental values and find the role of QED corrections significant. We show that especially the effect of self-energy correction can be similar to the transverse-photon interaction, or even exceed it in magnitude, and that detectable QED effects can be observed in binding energies of the third-row elements. This has consequences to the simulation of core-level spectra, as absolute energies can not be expected to be correct in any calculation ignoring relativistic electron-electron effects or the first few QED corrections.

II. THEORY AND CALCULATIONS

We calculated several corrections to single and double ionization initial and final states and then for the resulting (D)IPs. In this work we included a vacuum-polarization correction in the approximation of Fullerton and Rinker[16] and evaluated a self-energy correction estimate formulated by Fritzsche.[17] The

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self-energy correction is based on shift for a point nucleus, close to which the charge distribution is obtained from many-electron calculations. As non-QED effects we included a transverse electron-electron interaction correction[18] and studied the effects due to nuclear motion, titled as normal and specific mass shifts.[19] The corrections were evaluated as perturbations on a Dirac-Fock (DF) four-component wavefunction. The calculations were done using single-determinant wavefunctions, but also the effect of the electron-electron correlation for Ar and Xe was examined by carrying out multiconfiguration (MC) simulations. These calculations included all 1-electron and 2-electron excitations from 3s and 3p orbitals to 3d, 4s, and 4p, and from 5s and 5p to 4f, 5d, 6s, and 6p, respectively. In the single-determinant model, the perturbations are additive, whereas in multiconfiguration calculations the effects were piled up adding interactions in their strength order of the single determinant case. The effect of non-additivity was, however, found to be minor.

The Dirac-Fock wavefunctions were evaluated using the GRASP2K[20] software package. All corrections, except for self-energy, were calculated as implemented in the CI-module RCI of the package[20] (original implementation can be found in Ref. 21). The self-energy corrections were evaluated using the RELCI program[17] because it was found to provide more consistent, smooth behaviour of the corrections. We understand this to originate from a better implementation of the model, as described in Ref. 17.

III. RESULTS

In this work we refer to contributions in binding energies rather than contributions to state energies, since the experiment probes only the net effect. Because the effect of the corrections is smaller in magnitude for the hole states, the contribution of the correction to (D)IPs is of a different sign than to the state energies. The results for 1s IPs and DIPs are presented in Table I. The QED corrections (self-energy, vacuum polarization) are ordered similarly in magnitude over the whole range with opposite signs. Both mass-shift contributions remain small throughout the series. The results for 2s orbital are given in Table II.

Noble gases have ground state and core-hole states of a strong single-reference character. Argon, however, due to the presence of mixing of especially 3*d* orbital with the valence makes a clear exception. The electron-electron correlation effects from the MC model yield considerably different results, by lowering Ar 1s IP 2.3 eV (result 3203.5 eV) and 2s IP by 0.89 eV (result 236.3 eV) without changing the corrections. For Ar 1s DIP, the change is 3.7 eV (result 6649.85 eV) and 2s DIP 1.37 eV (result 694.06 eV). Similar effects could be expected for Xe, due to the mixing of 4f and 5d with the valence. However, the MC calculation shows only a 120-meV improvement. These findings indicate that the disagreement between the experiment and calculations arises, at least partly, from an insufficient treatment of the electron-electron

TABLE I. The calculated 1s IPs and DIPs in Dirac-Fock level. The transverse interaction (TR) correction, the QED corrections, and the nuclear-motion corrections were evaluated as perturbations. The experimental values are from the literature. Energies are in eV.

DF/correction	Ne	Ar	Kr	Xe	Rn
1s IP					
Dirac-Coulomb	869.79	3209.17	14 358.99	34 686.87	98 981.35
Transverse	−0.33	−2.34	−22.05	−81.71	−379.94
Self-energy	−0.13	−1.08	−12.06	−48.51	−260.93
Vacuum polarization	0.01	0.08	1.28	7.04	62.89
Normal mass shift	−0.02	−0.04	−0.10	−0.16	−0.31
Specific mass shift	0.00	0.01	0.04	0.07	0.15
Total	869.32	3205.80[a]	14 326.10	34 563.61	98 403.20
Experiment	866.9 ± 0.3[b]	3202.9 ± 0.3[b]	14 327.26 ± 0.04[c]	34 561.4 ± 1.1[b]	98 404 ± 12[b]
	870.21 ± 0.05[d]	3206.3 ± 0.3[e]	14 327.2 ± 0.8[e]	34 565.4[f]	
		3205.9[g]			
1s DIP					
Dirac-Coulomb	1862.79	6658.60	29 232.78	70 206.01	19 9501.04
Transverse	−0.39	−2.92	−28.64	−108.08	−508.68
Self-energy	−0.28	−2.24	−24.60	−98.32	−526.67
Vacuum polarization	0.01	0.16	2.62	14.27	127.01
Normal mass shift	−0.05	−0.09	−0.21	−0.32	−0.63
Specific mass shift	0.01	0.03	0.09	0.15	0.31
Total	1862.10	6653.54[a]	29 182.03	70 013.72	198 592.38
Experiment	1863[h]	–	–	–	–

[a]For Ar IP, MC calculation yields 3203.50 eV. For Ar DIP, MC calculation yields 6649.85 eV.
[b]Bearden and Burr in Ref. 22.
[c]Dragoun *et al.* in Ref. 23.
[d]Pettersson *et al.* in Ref. 24.
[e]Breinig *et al.* in Ref. 25.
[f]Deutsch and Kizler in Ref. 26.
[g]Thompson *et al.* in Ref. 27.
[h]Pelicon *et al.* in Ref. 28.

TABLE II. The calculated 2s IPs and DIPs in Dirac-Fock level. The transverse interaction correction, the QED corrections, and the nuclear-motion corrections were evaluated as perturbations. The experimental values are from the literature. Energies are in eV.

DF/correction	Ne	Ar	Kr	Xe	Rn
2s IP					
Dirac-Coulomb	49.45	327.21	1933.61	5 472.01	18 139.01
Transverse	−0.01	−0.11	−1.69	−7.81	−45.41
Self-energy	−0.01	−0.09	−1.36	−6.27	−42.07
Vacuum polarization	0.00	0.01	0.13	0.82	9.35
Normal mass shift	−0.00	−0.00	−0.01	−0.03	−0.06
Specific mass shift	−0.00	−0.00	−0.00	0.00	0.01
Total	49.43	327.02[a]	1930.68	5 458.71	18 060.83
Experiment	48.475[b]	326.25 ± 0.05[c]	1921.4 ± 0.3[d]	5 452.8 ± 0.4[e]	18 049 ± 38[e]
			1 924.6 ± 0.8[f]	5 452.9 ± 0.5[g]	
2s DIP					
Dirac-Coulomb	121.95	695.42	3948.69	11 087.12	36 555.27
Transverse	−0.01	−0.21	−3.25	−15.01	−86.53
Self-energy	−0.02	−0.19	−2.74	−12.59	−84.10
Vacuum polarization	0.00	0.01	0.27	1.66	18.85
Normal mass shift	−0.00	−0.01	−0.03	−0.06	−0.13
Specific mass shift	−0.00	−0.00	−0.00	0.00	0.01
Total	121.92	695.02[a]	3942.93	11 061.12	36 403.37
Experiment	118.6[h]	694[i]	3920 ± 2[j]	11 037.5 ± 4.6[k]	–
	121.9[l]	697.4[m]			
		697[n]			

[a]For Ar IP, MC calculation yields 236.32 eV. For Ar DIP, MC calculation yields 694.06 eV.
[b]Calculated based on the works of Saloman and Sansonetti in Ref. 29 and Kramida and Nave in Ref. 30.
[c]Glans *et al.* in Ref. 31.
[d]Dragoun *et al.* in Ref. 23.
[e]Bearden and Burr in Ref. 22.
[f]Sevier in Ref. 32.
[g]Breinig *et al.* in Ref. 25.
[h]Derived based on the works of Bearden and Burr in Ref. 22 and Leväsalmi *et al.* in Ref. 33.
[i]Derived based on the works of Bearden and Burr in Ref. 22 and Asplund *et al.* in Ref. 34.
[j]Derived based on the works of Dragoun *et al.* in Ref. 23, Breinig *et al.* in Ref. 25, and Kovalík *et al.* in Ref. 35.
[k]Derived based on the works of Bearden and Burr in Ref. 22, Deutsch and Kizler in Ref. 26, and Kovalík *et al.* in Ref. 36.
[l]Derived based on the works of Pettersson *et al.* in Ref. 24 and Leväsalmi *et al.* in Ref. 33.
[m]Derived based on the works of Breinig *et al.* in Ref. 25 and Asplund *et al.* in Ref. 34.
[n]Derived based on the works of Thompson *et al.* in Ref. 27 and Asplund *et al.* in Ref. 34.

correlation both in the single-determinant calculations and in the MC calculations.

To provide transferable estimates over the whole range of elements, we studied the scaling of the QED effects as a function of Z. We assumed a power-law dependence for correction x(Z),

$$x(\mathrm{Z}) = aZ^n, \tag{1}$$

where parameters a and n were optimized in a least squares fitting procedure to best describe each correction: transverse photon interaction, self-energy, vacuum polarization, and their sum. The results are presented in Table III and the plots in the Appendix.

It is known that the required removal energy of two core electrons from the same orbital is not in general double the magnitude of the removal energy of one electron. Similarly, the relativistic and QED effects for DIPs are not twice those of IPs. Figure 1 shows the ratio (DIP/IP) of the corrections for the studied QED effects and reveals that the behaviour is very similar to both vacuum polarization and self-energy corrections. As a function of increasing Z, the corrections are more additive, which is expected due to the heavier systems containing more relativistic electrons.

IV. DISCUSSION

Noble gases are good systems to study relativistic and QED effects because they have a large band gap and a closed-shell ground-state electron structure. Thus neither the electron-electron correlation nor the multiplet structure significantly complicates obtaining values for corrections from the variationally optimized single-configuration N-electron system. This also means that the single and double hole states are given by a single spectral line with clear interpretation, which in cases of IPs is confirmedly close to the experimental values.

The calculated 1s IPs are in total in better agreement with the experiment than the 2s IPs. For the previous, few-eV deviations are observed, whereas almost 10-eV deviation not within the error limit is observed for the Kr $2s^{-1}$ state. Even more severe mismatch is seen for the Kr $2s^{-2}$ and Xe $2s^{-2}$ states, where experimental values are derived using the 1s IPs and

TABLE III. Z-scaling parameters a (in eV) and n of the power-law fits for the corrections in 1s and 2s (D)IPs. Mass-shift corrections are not included in total.

Correction	a (eV)	n
1s IP		
Transverse	$-1.611\,980 \times 10^{-4}$	3.294 040
Self-energy	$-3.191\,392 \times 10^{-5}$	3.573 111
Vacuum polarization	$2.134\,480 \times 10^{-6}$	3.858 735
Total	$-2.217\,869 \times 10^{-4}$	3.316 597
1s DIP		
Transverse	$-1.914\,536 \times 10^{-4}$	3.320 920
Self-energy	$-6.303\,802 \times 10^{-5}$	3.578 065
Vacuum polarization	$4.669\,252 \times 10^{-6}$	3.841 028
Total	$-3.167\,359 \times 10^{-4}$	3.338 112
2s IP		
Transverse	$-4.820\,384 \times 10^{-6}$	3.604 424
Self-energy	$-4.592\,577 \times 10^{-6}$	3.597 120
Vacuum polarization	$1.457\,483 \times 10^{-6}$	3.513 968
Total	$-5.151\,210 \times 10^{-6}$	3.711 522
2s DIP		
Transverse	$-7.015\,001 \times 10^{-6}$	3.664 618
Self-energy	$-4.590\,706 \times 10^{-6}$	3.753 399
Vacuum polarization	$1.820\,876 \times 10^{-6}$	3.621 956
Total	$-1.149\,376 \times 10^{-5}$	3.680 526

the KL_1L_1 Auger electron kinetic energies. The mismatch can be partially explained by the experimental arrangement. These two Auger energies result from experiments done by the K-shell electron capture of radioactive Rb and Cs, which leaves the outermost ns (n = 5 or 6) electron screening the decay. According to our calculations, such screening results in 6.5 eV and 5.8 eV higher Auger-electron kinetic energies for Kr and Xe, respectively. Thus the reported experimental KL_1L_1 energies are higher than the unscreened ones. The DIPs with unscreened decay would thus increase by 6.5 eV and 5.8 eV for Kr and Xe, respectively. Moreover, the experimental KL_1L_1 kinetic energies are reported with respect to the Fermi level, not with respect to the vacuum level like the calculations are. The

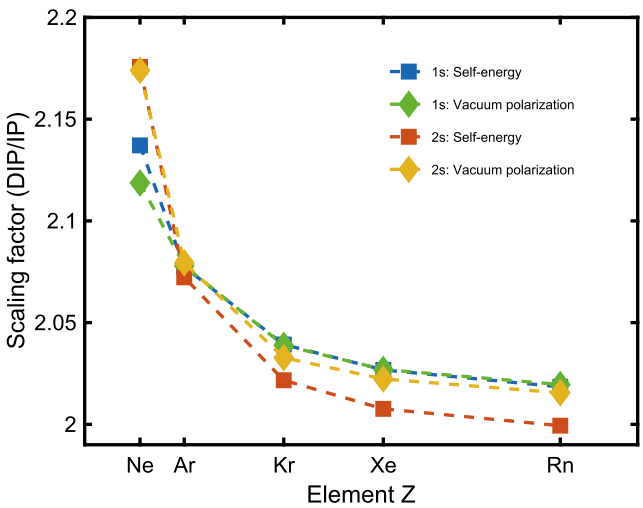

FIG. 1. The ratio of corrections as a function of Z (DIP/IP) for 1s and 2s hole states. Value 2 means direct additivity.

chosen model is not an exact representation of the addressed physical problem. Known factors for the mismatch include the approximative formulation of the corrections and the lack of the complete treatment of the electron-electron correlation. Furthermore, it remains an open question, how large contributions would originate from more complete formulations of relativistic-QED Hamiltonians[37,38] or other mechanisms of elementary particle physics. Therefore the present results should be viewed as a benchmark, rather than a complete solution. We also point out that there are considerable deviations in the experimental 1s and 2s binding energies reported in the present literature. Therefore continuation of the theoretical work in understanding the fine details defining these binding energies requires new high precision measurements.

QED effects are not usually considered in studies of core-level photoionization or core-level excitations. However from Tables I and II it becomes obvious that relativistic electrons can have QED effects of similar magnitude as the relativistic electron-electron interaction corrections. Table III shows that the power-law fits of the QED effects have larger exponents than those of the transverse interaction correction for 1s (D)IPs, which results in a relative increase along Z. Moreover, for the 1s DIP of Rn, the value of the correction from self-energy exceeds that of the transverse interaction. The relativistic one-electron effects from the Dirac Hamiltonian always dominate in the noble gases and vary from ~1 eV to ~11 keV for IP from Ne to Rn.[4] For DIP the corresponding range is from ~2.5 eV to ~22 keV.[4] However, with the contemporary spectrometers and synchrotron sources, detection is completely feasible with the resolution similar to or better than the magnitude of the QED effects. The 1s IPs demonstrate that the approximated self-energy correction makes a significant correction to a desired direction and is balanced by the vacuum-polarization correction.

The contributions brought by the QED and electron-electron relativistic effects for Ar remain the same regardless of the treatment of the electron-electron correlation. We expect the same to happen for other atoms in the series, and that the electron-electron correlation possibly has few-eV effects in the results. To exclude these effects completely would require studies using hydrogen-like heavy ions that are very difficult to produce for experiments.

Direct additivity (value 2) is achieved for the self-energy of the 2s orbital of Rn. This observation is related to the dependence of the orbital shape and relaxation. Indeed, a calculation performed with frozen orbitals produces always a value of 2 for the additivity, which is expected for one-electron correction effects. Thus the additivity of perturbative corrections is a measure of orbital relaxation: the 2s orbital overlap integral with the ground state form is 0.995 37 and 0.982 12 for Ne $1s^{-1}$ and $1s^{-2}$ states, respectively. For Rn $1s^{-1}$ and $1s^{-2}$ states, the corresponding values were 0.999 94 and 0.999 77. This is in agreement with the view that the validity of frozen-orbital approach increases with increasing Z.

The relative contribution of the corrections (absolute value) to the (D)IP is presented in Figure 2. The relative self-energy (SE) or vacuum-polarization (VP) correction contributions are the same in the IPs and DIPs, but the transverse interaction (TR) shows a differing relative magnitude. This

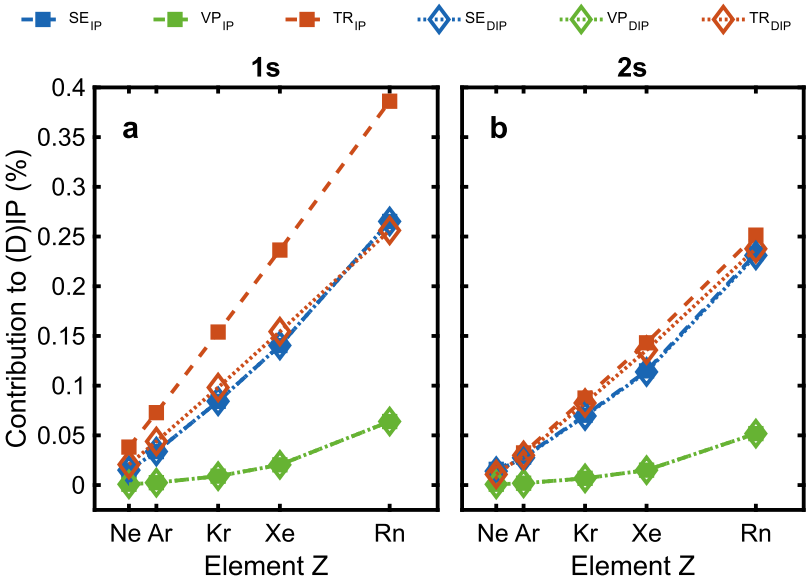

FIG. 2. The relative contribution of the absolute value of corrections in the Z for (a) 1s and (b) 2s hole states for transverse interaction (TR), self-energy (SE), and vacuum polarization (VP).

is due to the one-electron nature of the two aforementioned corrections, whereas transverse photon interaction is a correction to electron-electron interactions. Thus emptying the 1s orbital completely reduces the number of relativistic electrons that are needed for the correction to be significant. The behavior of the relative magnitude of the corrections is close to linear, perhaps apart from vacuum polarization that seems more quadratic-like as a function of Z.

The results obtained in this work manifest the need for QED corrections in atomic photoionization, when correct absolute values are desired. Especially striking is that even for Ne and Ar that are reachable with soft/tender X-ray photons, self-energy contributions in both single and double ionization are detectable. Thus any simulation reproducing third-row K-edge spectra better than by ∼1 eV accuracy does this due to the cancellation of errors. For example, using the values of Table III, combined self-energy and vacuum polarization correction of −0.55 eV is obtained for S 1s IP. Luckily for the interpretation of the experiments, the effect can be approximated to remain as a constant shift in changes of the chemical environment.

V. CONCLUSIONS

The calculated QED corrections for 1s and 2s single and double ionization potentials of noble gases from Ne to Rn show significant contributions from QED. The effects may even exceed those from relativistic electron-electron interaction corrections. With the corrections studied on top of Dirac-Fock calculations, the available experimental single and double ionization potentials are well reproduced apart from Kr 2s and Xe 2s. We presented power-law fits over the Z-range, and, for example, for S 1s ionization potential a QED correction of ∼−0.55 eV was obtained. We also emphasize that without the cancellation of errors, calculated absolute energies for K-edge spectra in any non-QED calculation of the third-row elements can not match with experimental values.

APPENDIX: POWER-LAW FITS TO THE DATA

To fit the data using the model of Equation (1), we applied least-squares fitting procedure. The quasi-Newton algorithm implemented in MATLAB function fminunc was used for

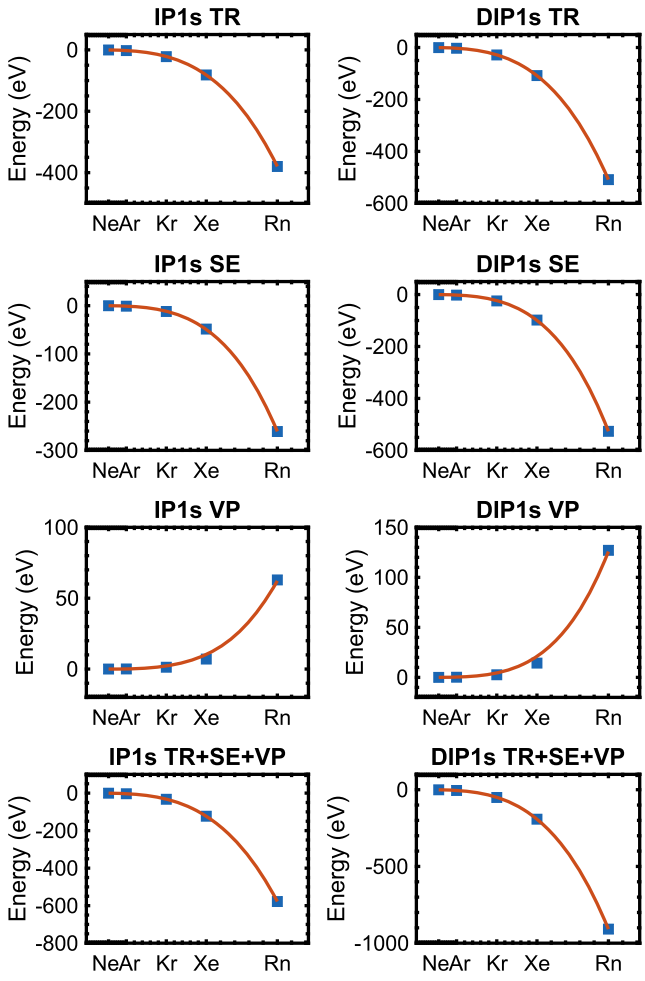

FIG. 3. The corrections and the least-squares fit of the power-law model for 1s. The fit is shown in red and the data points in blue for transverse interaction (TR), self energy (SE), vacuum polarization (VP), and their sum.

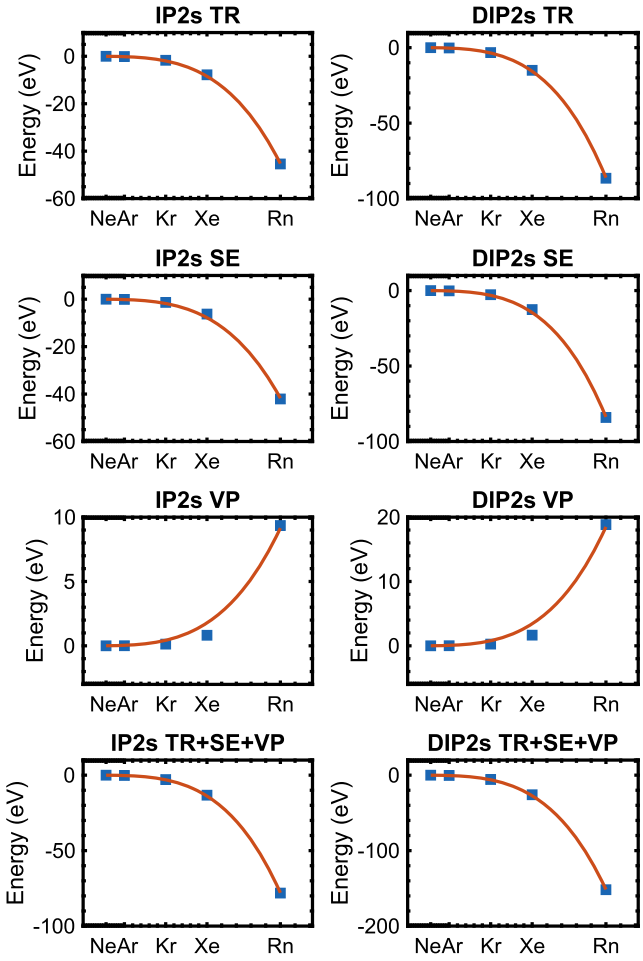

FIG. 4. The corrections and the least-squares fit of the power-law model for 2s. The fit is shown in red and the data points in blue for transverse interaction (TR), self energy (SE), vacuum polarization (VP), and their sum.

minimizing the quadratic cost function in terms of parameters a and n. The resulting curves are presented in Figures 3 and 4 together with the data points.

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