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NON-RELATIVISTIC CALCULATION OF EXCITED-STATE IONIZATION POTENTIALS FOR LI-LIKE IONS USING WEAKEST BOUND ELECTRON POTENTIAL MODEL THEORY

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In this study, a well-known Weakest Bound Electron Potential Model (WBEPM) was used to determine the exited-state ionization potential of lithium-like elements for different iso-spectrum series such as $1s^2 2p^1\ P_{1/2}$, $1s^2 3s^2\ S_{1/2}$, $1s^2 3d^2\ D_{1/2}$, $1s^2 4s^2\ S_{1/2}$, $1s^2 4p^2\ P_{1/2}$, and $1s^2 4d^2\ D_{1/2}$ having nuclear charges from Z = 3 to Z = 18. On the other hand, to utilize relativistic correction, Briet-Pauli approximation has also been applied to the ionization potential using a fourth-order polynomial expression in the nuclear charge Z. The deviation within the range of 0.1% has been observed between estimated and experimental values that are quite remarkable. Furthermore, new ionization potentials were proposed for iso-series with Z ranging from 19 to 30.
Keywords: *non-relativistic ionization potential; Ionization Potentials; Breit-Pauli approximation; Weakest bound electron potential model (WBEPMT); nuclear charges*
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INTRODUCTION

The application and properties of excited states of many electron systems have great implications in many fields of research. The spectroscopic data signify research areas in both theoretical and experimental fields like fine structure, transition probabilities, Rydberg levels, ionization potentials, etc. In 2022 the full core plus correlation and the Rayleigh-Ritz variation methods were used to study the non-relativistic energies wave functions and fine structures of high-angular-momentum states of lithium-like ions by Xin Liu and Jingchao Zhang [1].In 2019 V. Malyshev and his group use quantum electrodynamics theory to developed a technique to calculate the two-electron recoil contributions for the $1s^2$ state in helium (He) like ions and the $1s^2 2s$ and $1s^2 2p_{1/2}$ states in lithium (Li) like ions [2]. In 2018 Shabaev et al. evaluated nuclear recoil effect on the g factor of highly charged Li-like ions by using 1/Z perturbation theory [3]. In 2017 by using relativistic configuration interaction (CI) method V.A. Yerokhin and his team calculated energy levels of the $1s^2 2l$ and $1s2l2l'$ states of Li like ions for Z=6-17, their theory is more accurate for the core excited states [4]. In 2016 V. A. Yerokhin et.al. reported a method to calculate more accurate value for fine structure constant y by employing the weighted difference of the g factors of the H- and Li-like ions (light element) [5]. In order to gain insight into the electronic structure of various systems, accurate determination of ionization potentials has been the subject of considerable research efforts in physics, chemistry and related fields. Reliable data on the ionization potentials for the lithium-like sequence is particularly important as it facilitates the interpretation of physical and chemical processes. To calculate ionization potentials for ionic or atomic systems, several methods have been employed, such as the 'R-matrix method', 'relativistic configuration interaction (CI) method', 'multi-configuration Hartree Fock (MCHF) method', 'multi-configuration Dirac Fock (MCDF) methods' and 'relativistic many-body perturbation theory (MBPT)' [6-13]. In recent past, a new method has been introduced by Zheng et al. known as the weakest bound electron potential model theory (WBEPMT) for ionization potential, transition probabilities, life time, quantum defects etc. The group also reported transition probability of Lithium atom and lithium like ions by using the same theory [14-19]. In 2022, R. Siddiq et al. studied the four series of Li, by using WBEPMT they calculated energies and transition probabilities of the series [20]. Saeed et al. evaluated transition probabilities and lifetimes of the lithium levels, and found new lifetimes using polynomial of each of the ns, np, nd and nf series [21]. In 2007, Yildiz et al. reported excited state ionization potential for Li by using the same theory [22]. In this work, WBEPMT, Breit-Pauli approximation and the concept of iso-spectrum-level series have been used for the precise extrapolation of ionization potentials as a function of the nuclear charge Z. The calculated ionization potential has been compared to Yildiz's findings, and it was discovered that they are in satisfactory conformity. This study is a continuation of Yildiz's work. Overall, these calculations are important in understanding the behavior of atoms and their properties.

THEORY

In this work, weakest bound electron potential model theory was used, that were developed on the basis of separation of weakest bound electron (WBE) and non-weakest bound electron (NWBE). In atomic and ionic system innermost electrons containing multiple electrons or atomic core electrons are NWBE, and others that are less tightly or outermost

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electrons are known as WBE [17 new 18]. By using this model many electron systems reduce to Li-like atom, which have a single electron in their outermost shell as WBE and the core with combination of nucleus and inner electrons become NWBE. The electronic configuration is identical for all atomic or ionic terms within an iso-electronic series. However, this concept alone cannot accurately determine the ionization potentials of excited states. To address this limitation, the iso-electronic series concept is used to calculate ionization potentials. This series consists of energy levels that share the same level symbol within a known iso-electronic series. The electronic configuration, spectrum terms, and energy levels are all identical in this concept, except for the variable of nuclear charge Z [15].

The total energy of atomic and ionic systems can be calculated as the sum of relativistic energy and non-relativistic energy [15-17].

$$\mathrm{I(Z)} = \mathrm{I_r(Z)} + \mathrm{I_{nr}(Z)}. \tag{1}$$

The symbol $I(Z)$ is used for total energy of atomic and ionic systems, $I_r(Z)$ for relativistic energy and symbol $I_{nr}(Z)$ for non-relativistic energy. For calculation of non-relativistic energy WBEPMT is used, likewise Breit-Pauli approximation is used for relativistic energy.

NON-RELATIVISTIC IONIZATION POTENTIAL$I_{nr}(Z)$

According to WBEPM theory [18] the weakest electron under the non-relativistic condition moves in an orbit that has a larger period, due to which the coupling between WBE and NWBE reduces to Schrodinger equation of the weakest electron in a similar way as the hydrogen atom. The Schrodinger equation of the ith weakest electron can be written as

$$[-\tfrac{1}{2}\nabla_i^2 + \mathrm{V(r_i)}]\varphi_i = \mathrm{E_i}\varphi_i, \tag{2}$$

$$\mathrm{V(r_i)} = \tfrac{\mathrm{d(d+1)+2dl}}{2{r_i}^2} + (-\tfrac{\mathrm{Z^*}}{\mathrm{r_i}}). \tag{3}$$

The first term in equation (3) represents polarization potential which is formed due to dipole formation of ionic core and WBE, and the second term is Columbic potential. Z*is the effective nuclear charge and defined as:

$$\mathrm{Z^*} = \sqrt{(\mathrm{Z}-\sigma)^2 + \mathrm{g(Z-Z_o)}} \tag{4}$$

Here Zo is nuclear charge, σ is screening constant and symbol g is used for relative increase factor. The ionization potential of an atom or ion can be calculated using equation (5) [16-18]:

$$\mathrm{I_{nr}} = \tfrac{\mathrm{Z^*}}{2\mathrm{n^{*2}}} = \tfrac{(\mathrm{Z}-\sigma)^2+\mathrm{g(Z-Z_o)}}{2\mathrm{n^{*2}}} \tag{5}$$

Here $\mathrm{n^*}$ is the effective principal quantum number and can be calculated by using quantum defect.

RELATIVISTIC IONIZATION POTENTIAL $\mathrm{I_r(Z)}$

To calculate the relativistic effect the Breit-Pauli approximation is applied. The relativistic corrections of the iso-spectrum-level series could be determined by fitting fourth-order polynomial in nuclear charge. The method used to calculate $\mathrm{I_r(Z)}$ is the same as in [16]:

$$\mathrm{Ir} = \textstyle\sum_{i=0}^{4} \mathrm{a_i Z^i} \tag{6}$$

The Value of $\mathrm{Z^i}$ is used in the computation of the relativistic contribution and effective nuclear charge of an atom. The parameters $\mathrm{a_i}$ can be determined by using the experimental values of ionization potential $\mathrm{I_{exp}}$ and non-relativistic ionization potential $\mathrm{I_{nr}}$ by using equation (1). The value of $\mathrm{I_{exp}}$ is obtained from NIST (National Institute of Standards and Technology) website [23]. Now the total ionization potential of the iso-spectrum-level series is given by equation number (7).

$$\mathrm{I} = \tfrac{(\mathrm{Z}-\sigma)^2+\mathrm{g(Z-Z_o)}}{2\mathrm{n^2}} + \textstyle\sum_{i=0}^{4} \mathrm{a_i Z^i} \tag{7}$$

RESULT AND DISCUSSION

The excited state ionization potential for a range of lithium-like series, including $1s^2 2p^1\ P_{1/2}$, $1s^2 3s^2\ S_{1/2}$, $1s^2 3d^2\ D_{1/2}$, $1s^2 4s^2\ S_{1/2}$, $1s^2 4p^2\ P_{1/2}$, and $1s^2 4d^2\ D_{1/2}$ have been determined by using WBEPM theory, and the Breit-Pauli approximation for n = 3 to n = 30 energy levels. It is found that values of ionization potential of Lithium-Like ions are very close to the results available in NIST [23]. WBEPM is used to calculate non relativistic ionization potential I_{nr}, equation (5). To obtain more fine results of Ionization potential, relativistic effect is introduced in the ionization potential using Breit-Pauli approximation, equation (6). In addition to determine total ionization potential, equation (7) is

utilized that is the combination of both relativistic and non-relativistic effect. Since the relativistic effect generally depends on nuclear charge Z of an atom, therefore atoms like lithium to neon the relativistic effects have little impact to total energies [24-25]. The major relativistic contributions to the ionization potential increases up to the fourth power of nuclear charge Z of the iso-spectrum level series [26]. Different parameters of potential, in which the weakest bound electron travels given by equation (3) is reported in Table I. In Table II(a)-II(c) the calculated non relativistic ionization potential is compared with experimental [23] and Yildiz [19] values. First column shows nuclear charge (Z), second column shows experimental ionization Potential (I_{exp}), third column shows Yildiz ionization potential (I_{yildiz}), column IV shows calculated non-relativistic ionization Potential (I_{nr}) and fifth column shows the difference between I_{exp} and I_{nr} Figure I-III shows the graphs between nuclear charge (Z) and non-relativistic ionization potential for different series. The red curve shows the work of Yildiz [22], the blue curve an extension of red curve shows the ionization potential calculated in this work. The two curves in all series perfectly overlap

Table I. The parameters required to calculate the ionization potential of Lithium-Like Sequence by Computer Program

	1st series $1s^22p\ ^2P_{1/2}$	2nd series $1s^23s^2S_{1/2}$	3rd series $1s^23d^2D_{1/2}$	4th series $1s^24s^2S_{1/2}$	5th series $1s^24p^2P_{1/2}$	6th series $1s^24d^2D_{1/2}$
σ	1.9998552	1.998069833	2.000027255	2.000272688	2.000034471	2.000033207
n*	1.9905805	2.992304883	2.999200319	3.992108353	3.991755353	3.998513662
g	0.1830223	0.51920133	0.002941923	0.386424563	0.096351577	0.000799136
a0	12.401682	4.45E+00	6.04E+00	2.74E+00	3.24E+00	3.40E+00
a1	-1.33E+01	-5.37E+00	-6.05E+00	-3.12E+00	-3.35E+00	-3.40E+00
a2	3.43E+00	1.52E+00	1.51E+00	8.54E-01	8.54E-01	8.51E-01
a3	1.67E-08	-2.37E-07	3.14E-08	6.90E-08	-1.54E-07	1.14E-07
a4	1.14E-13	5.84E-09	-2.36E-10	-1.46E-09	3.39E-09	-3.05E-09

Table II (a). A Comparison between non-relativistic values of ionization potential with other results for series $1s^22p\ ^2P_{1/2}$ and $1s^23s^2S_{1/2}$

1st series ($1s^22p\ ^2P_{1/2}$)					**2nd series** ($1s^23s^2S_{1/2}$)				
Z	**I_{exp}[20]**	**I_{yildiz} [19]**	**I_{nr} (eV)**	**$I_{exp} - I_{nr}$**	**Z**	**I_{exp}**	**I_{yildiz}[19]**	**I_{nr} (eV)**	**$I_{exp} - I_{nr}$**
3	3.54344	3.54344	3.543443	-2.79E-06	3	2.01833	2.01833	2.018324	5.70E-06
4	14.25066	14.32546	14.32546	-2.09E-06	4	7.27085	7.28714	7.287146	-5.95E-06
5	31.93084	31.97487	31.97487	3.62E-06	5	15.58641	15.59502	15.59503	-7.10E-06
6	56.49166	56.49166	56.49166	4.32E-06	6	26.94195	26.94197	26.94197	2.24E-06
7	87.90269	87.87583	87.87583	2.95E-08	7	41.33234	41.32797	41.32797	2.07E-06
8	126.15448	126.12739	126.1274	7.35E-07	8	58.75740	58.75303	58.75303	2.40E-06
9	171.24633	171.24633	171.2463	-3.56E-06	9	79.21710	79.21715	79.21715	3.22E-06
10	223.18138	223.23266	223.2327	-2.85E-06	10	102.71914	102.7203	102.7203	4.54E-06
11	281.96689	282.08638	282.0864	2.85E-06	11	129.25182	129.2626	129.2626	-3.65E-06
12	347.61269	347.80748	347.8075	3.56E-06	12	158.84802	158.8439	158.8439	-1.35E-06
13	420.12125	420.39596	420.396	-7.36E-07	13	191.47027	191.4642	191.4642	1.44E-06
14	499.54365	499.85183	499.8518	-2.90E-08	14	227.20910	227.1236	227.1236	-5.27E-06
15	585.84889	586.17508	586.1751	-4.32E-06	15	265.95539	265.8221	265.8221	-1.48E-06
16	679.10256	679.36572	679.3657	-3.62E-06	16	307.72651	307.5597	307.5596	2.79E-06
17	779.27514	779.42375	779.4237	2.09E-06	17	352.60836	352.3362	352.3362	-2.43E-06
18	886.40532	886.34916	886.3492	2.79E-06	18	400.57306	400.1519	400.1519	2.83E-06
19			1000.142		19			451.0066	
20			1120.802		20			504.9004	
21			1248.33		21			561.8332	
22			1382.725		22			621.8051	
23			1523.987		23			684.8161	
24			1672.117		24			750.8661	
25			1827.114		25			819.9551	
26			1988.978		26			892.0833	
27			2157.71		27			967.2505	
28			2333.309		28			1045.457	
29			2515.776		29			1126.702	
30			2705.11		30			1210.986	

Table II(b). A Comparison between non-relativistic values of ionization potential with other results for series $1s^2 3d^2D_{1/2}$and $1s^2 4s^2S_{1/2}$

3rd series ($1s^2 3d^2D_{1/2}$) **[19]**					**4th series** ($1s^2 4s^2S_{1/2}$) **[19]**				
Z	$\mathbf{I_{exp}}$**[20]**	$\mathbf{I_{yildiz}}$	$\mathbf{I_{nr}}$ **((eV)**	$\mathbf{I_{exp} - I_{nr}}$	**Z**	$\mathbf{I_{exp}}$**[20]**	$\mathbf{I_{yildiz}}$	$\mathbf{I_{nr}}$ **((eV)**	$\mathbf{I_{exp} - I_{nr}}$
3	1.51291	1.51291	1.512914	-4.30E-06	3	1.05064	1.05064	1.0506407	-6.86E-07
4	6.05316	6.05379	6.05379	1.40E-07	4	3.89488	3.90338	3.9033829	-2.85E-06
5	13.61943	13.61977	13.61977	3.16E-06	5	8.45868	8.46357	8.4635681	1.86E-06
6	24.21083	24.21085	24.21085	4.77E-06	6	14.73119	14.7312	14.731197	3.44E-06
7	37.82680	37.82702	37.82703	-5.05E-06	7	22.70955	22.70627	22.706268	1.91E-06
8	54.46972	54.46831	54.46831	3.72E-06	8	32.39465	32.38878	32.388783	-2.75E-06
9	74.13465	74.13469	74.13469	1.07E-06	9	43.78560	43.77874	43.778741	-5.35E-07
10	96.81329	96.82617	96.82617	-2.99E-06	10	56.87938	56.87614	56.876141	-1.44E-06
11	122.55134	122.5428	122.5428	1.52E-06	11	71.68095	71.68099	71.680985	4.53E-06
12	151.31074	151.2845	151.2844	4.62E-06	12	88.19848	88.19327	88.193273	-2.62E-06
13	183.08382	183.0512	183.0512	-3.70E-06	13	106.52100	106.413	106.413	-2.90E-06
14	217.92139	217.8431	217.8431	-3.44E-06	14	126.39435	126.34018	126.34018	3.70E-06
15	255.80362	255.6601	255.6601	-4.60E-06	15	148.01319	147.97479	147.97479	-2.82E-06
16	296.67349	296.5022	296.5022	2.82E-06	16	171.41096	171.31685	171.31685	-2.47E-06
17	340.55864	340.3694	340.3694	-1.17E-06	17	196.51987	196.36636	196.36636	4.76E-06
18	387.53903	387.2617	387.2617	3.42E-06	18	223.33434	223.1233	223.1233	-1.13E-06
19			437.1791		19			251.58769	
20			490.1216		20			281.75952	
21			546.0892		21			313.6388	
22			605.0819		22			347.22552	
23			667.0997		23			382.51968	
24			732.1426		24			419.52128	
25			800.2106		25			458.23033	
26			871.3037		26			498.64682	
27			945.4219		27			540.77075	
28			1022.565		28			584.60213	
29			1102.734		29			630.14095	
30			1185.927		30			677.38722	

Table II (c). A Comparison between non-relativistic values of ionization potential with other results for series $1s^2 4p^2P_{1/2}$and $1s^2 4d^2D_{1/2}$

5th series ($1s^2 4p^2P_{1/2}$)					**6th series** ($1s^2 4d^2D_{1/2}$)				
Z	$\mathbf{I_{exp}}$**[20]**	$\mathbf{I_{yildiz}}$**[19]**	$\mathbf{I_{nr}}$ **((eV)**	$\mathbf{I_{exp} - I_{nr}}$	**Z**	$\mathbf{I_{exp}}$**[20]**	$\mathbf{I_{yildiz}}$**[19]**	$\mathbf{I_{nr}}$ **((eV)**	$\mathbf{I_{exp} - I_{nr}}$
3	0.86995	0.86996	0.869955	4.55E-06	3	0.85088	0.85089	0.850888	1.54E-06
4	3.48627	3.49489	3.494892	-1.90E-06	4	3.40437	3.40427	3.404271	-9.26E-07
5	7.82257	7.82757	7.827573	-3.48E-06	5	7.65991	7.65963	7.659631	-5.19E-07
6	13.86799	13.868	13.868	-1.74E-07	6	13.61696	13.61697	13.61697	2.77E-06
7	21.61960	21.61617	21.61617	-1.99E-06	7	21.27555	21.27628	21.27628	-1.07E-06
8	31.07590	31.07209	31.07209	1.07E-06	8	30.63627	30.63757	30.63757	-2.03E-06
9	42.24083	42.23575	42.23575	-9.97E-07	9	41.70082	41.70084	41.70084	-1.07E-07
10	55.10167	55.10716	55.10716	1.82E-06	10	54.46076	54.46608	54.46609	-5.31E-06
11	69.68630	69.68631	69.68631	-4.93E-07	11	68.96604	68.93331	68.93331	2.37E-06
12	86.02284	85.97321	85.97321	2.08E-06	12	85.26550	85.10251	85.10251	2.92E-06
13	103.98956	103.9679	103.9679	-4.78E-07	13	102.99906	102.9737	102.9737	-3.64E-06
14	123.74763	123.6702	123.6702	1.85E-06	14	122.60092	122.5468	122.5468	2.67E-06
15	145.64399	145.0804	145.0804	-9.53E-07	15	143.86521	143.822	143.822	1.86E-06
16	168.27704	168.1983	168.1982	1.13E-06	16	166.84025	166.7991	166.7991	3.92E-06
17	193.14794	193.0239	193.0239	-1.92E-06	17	191.56114	191.4782	191.4782	-1.13E-06
18	219.73678	219.5572	219.5572	-8.57E-08	18	217.96899	217.8592	217.8592	-3.31E-06
19			247.7984		19			245.9423	
20			277.7472		20			275.7273	
21			309.4038		21			307.2143	
22			342.7682		22			340.4032	
23			377.8403		23			375.2942	

5th series ($1s^2 4p^2 P_{1/2}$)					**6th series** ($1s^2 4d^2 D_{1/2}$)				
24			414.6201		24			411.8871	
25			453.1077		25			450.182	
26			493.303		26			490.1789	
27			535.2061		27			531.8778	
28			578.8169		28			575.2786	
29			624.1355		29			620.3814	
30			671.1618		30			667.1862	

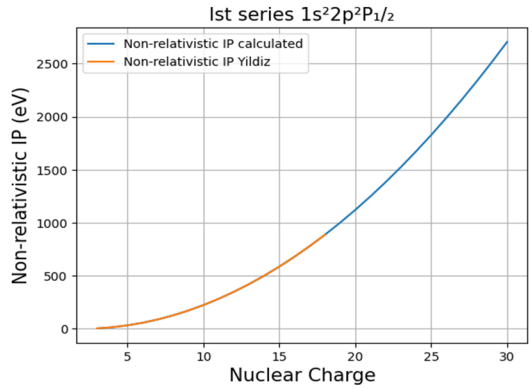

Figure I. Graphs between nuclear charge (Z) and non-relativistic ionization potential for 1st series $1s^2 2p^1\ P_{1/2}$

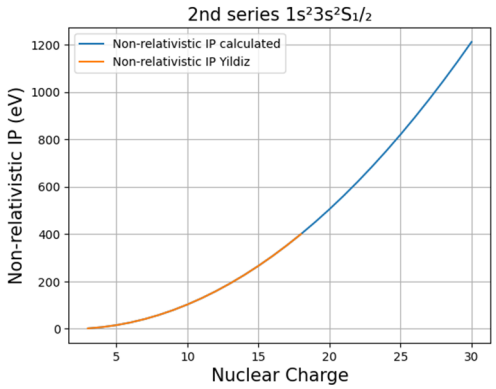

Figure II. Graphs between nuclear charge (Z) and non-relativistic ionization potential for series $1s^2 3s^2\ S_{1/2}$

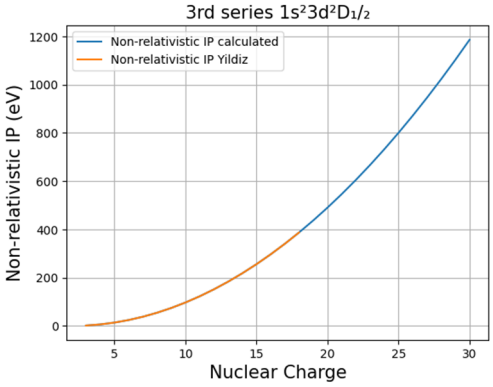

Figure III. graphs between nuclear charge (Z) and non-relativistic ionization potential for series$1s^2 3d^2\ D_{1/2}$

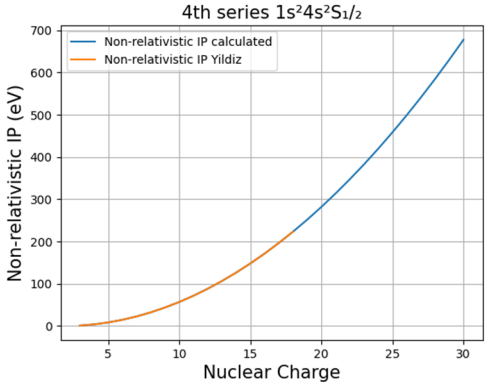

Figure IV. graphs between nuclear charge (Z) and non-relativistic ionization potential for series $1s^2 4s^2\ S_{1/2}$

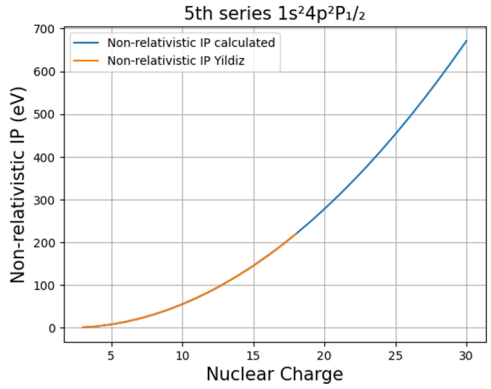

Figure V. graphs between nuclear charge (Z) and non-relativistic ionization potential for series $1s^2 4p^2\ P_{1/2}$

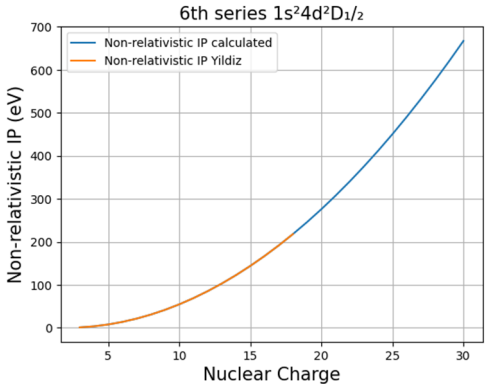

Figure VI. Graphs between nuclear charge (Z) and non-relativistic ionization potential for series $1s^2 4d^2\ D_{1/2}$

CONCLUSION

The Weakest Bound Electron Potential Model Theory the Breit–Pauli approximation is used to calculate the ionization potentials of lithium-like series. The constants in Eq. 7 are determined by using experimental data from the

National Institute of Standards and Technology (NIST) website [23] and reported in Table I. These constants are then used to calculate non-relativistic ionization potentials from n = 3 to n = 30 for each individual series, as shown in Table II. The experimental values from NIST are close to the calculated values for series. The non-relativistic potential for six series has also been compared with the work of Yildiz [22]. The agreement in the overlap area of the two works is excellent, as can be seen in Figure I-VI. An excellent agreement with previously reported data shows the reliability of calculation. The blue curve an extension of red curve in Fig. I-VI shows the new relativistic ionization potential calculated in this work. This work is an extension of Yildiz's findings.

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НЕРЕЛЯТИВІСТСЬКИЙ РОЗРАХУНОК ПОТЕНЦІАЛІВ ІОНІЗАЦІЇ У ЗБУДЖЕНОМУ СТАНІ ДЛЯ ЛІТІЙ-ПОДІБНИХ ІОНІВ З ВИКОРИСТАННЯМ ТЕОРІЇ МОДЕЛІ СЛАБШОГО ЗВ'ЯЗАНОГО ЕЛЕКТРОННОГО ПОТЕНЦІАЛУ

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У цьому дослідженні добре відома модель потенціалу найслабшого зв'язку електронів (WBEPM) була використана для визначення потенціалу іонізації збудженого стану літієподібних елементів для різних серій ізоспектру, таких як $1s^2 2p^1\ P_{1/2}$, $1s^2 3s^2\ S_{1/2}$, $1s^2 3d^2\ D_{1/2}$, $1s^2 4s^2\ S_{1/2}$, $1s^2 4p^2\ P_{1/2}$, та $1s^2 4d^2\ D_{1/2}$, які мають заряди ядра від Z = 3 до Z = 18. З іншого боку, для використання релятивістської поправки до іонізації також було застосовано наближення Бріє-Паулі потенціал, використовуючи поліноміальний вираз четвертого порядку в заряді ядра Z. Відхилення в діапазоні 0,1% спостерігалося між розрахунковими та експериментальними значеннями, що є досить примітним. Крім того, були запропоновані нові потенціали іонізації для ізо-рядів із Z в діапазоні від 19 до 30.

Ключові слова: *нерелятивістський потенціал іонізації; потенціали іонізації; апроксимація Брейта-Паулі; модель потенціалу найслабшого зв'язку електронів (WBEPMT); ядерні заряди*