Rydberg Energy Levels and Quantum Defects of some Semiconductor Elements

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Abstract: Weakest bound Electron Potential Model Theory has turned out to be a successful theory in explaining many atomic properties, namely, energy levels, transition probabilities and oscillator strengths. The theory has also been used to calculate Rydberg energy levels and quantum defects. In this paper we studied semiconductor elements Boron and Silicon. We calculated energy levels of Rydberg atoms of Boron and Silicon up to n = 50 levels using WBEPMT. We also calculated quantum defects in principle quantum number for various configurations of these elements.

Keywords: Weakest bound Electron Potential Model Theory, Rydberg Atoms, Rydberg energy levels, Boron, Silicon.

INTRODUCTION

Weakest bound Electron Potential Model Theory has turned out to be a successful theory in explaining many atomic properties, namely, energy levels, transition probabilities and oscillator strengths. The theory has also been used to calculate Rydberg energy levels and quantum defects. In the following section we have given a brief introduction of WBEPMT [1-2]. One atom System energy of an atom system can be expressed as;

T = T(ionization limit) + E(energy of the weakest bound electron) (WBE)

$$T = T_{limit} + E \tag{1}$$

$$\frac{1}{2}\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \left[E - V(r) - \frac{l(l+1)}{2r^2}\right] - R = 0 \tag{2}$$

The potential by Weakest Bound electron as [3]

$$V(r) = -\frac{Z'}{r} + \frac{k(k+1)+2kl}{2r^2} \tag{3}$$

By comparative & substitutive sketch of eq-3 & eq-2, the new format of radial equation turns out to be;

$$\frac{1}{2}\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \left[E - \frac{Z'}{r} - \frac{l(l+1)}{2r^2}\right] - R = 0 \tag{4}$$

Where

$$l' = l + K \tag{5}$$

The equation-4 can be simplified as

$$R_{nl}(r) = A\exp\left(-\frac{Z'r}{n'}\right)L_{n-l-1}^{2l'+1}\left(\frac{2Z'r}{n'}\right) \tag{6}$$

$$E = -R\left(\frac{Z'}{n'}\right)^2 \tag{7}$$

where “R” is Rydberg constant

$$\frac{Z'}{n'} = \frac{Z_{net}}{n - \delta_n} \tag{8}$$

Where Z_{net} represents the Net-charge # of Atomic Kernel and its value is one for atoms and δn

Represents the quantum defect;

$$T = T_{limit} + E = T_{limit} + \left(\frac{Z_{net}}{n - \delta_n}\right)^2 \tag{9}$$

Where δ_n can be represented as; by the reference of Martin’s formula

$$\delta_n = \sum_{i=0}^{3} \frac{a_i}{(n - \delta_o)^{2i}} \tag{10}$$

Where δ_o represents quantum defect of lowest energy level, and a_i are the parameters, these parameters can be obtained by the minimum possible square fitting of equation (9) using minimal experienmental data obtained at first reading of the given spectrum series. [3]

Boron in a chemical element is symbolically represented by “B” and has atomic number” 5”. It is completely produced by spallation of Cosmic rays, having low abundance in Solar system including

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Earth's Crust. It is metalloid that originated in small quantities in meteoroids but chemically uncombined boron cannot be found naturally on Earth's Crust. Technologically, very pure boron is formed with trouble because of stubborn pollution by carbon or other components. This element was discovered by L.J. Gay-Lussac and L.J. Thénard in city of France and H.D. in London, UK in 1808. It belongs to group thirteen, Period two and block P. It is a solid state at temperature of 20 degree, and has electronic configuration (He) $2s^2 2p^1$.

Theoretical investigation, numerical reproduction and tests of hot making for ultra-high forte boron steel were studied. The hot making effect of boron steel is examined and the best temperature variety 750~800^o for hot making was attained [4]. Then the design of the armor-plated beam's dies, the chilling system and method of processing were applied by the approaches of numerical simulation, optimization and experiments. The experimental results of boron steel components formed by the designed die showed that the rigidity value presents a similar distribution and the Vickers rigidity is higher than 430,the yield limitation of the warm forming material is 11 000 MPa, the strength limitation is 1 430 MPa and that the martensite is similar. These results indicate the possibility of the methods [5]. The role of boron in providing flame retardancy to wood is studied. Different loading levels of borax-boric acid, ranging from O% to 20% addition by weight, were applied to Southern Pine. There were two types of fire tests used to assess flame retardancy. Study of Flame retardants for wood alters the burning characteristics of wood to reduction of surface flame blowout. Flame retardant chemicals cause acid catalyzed dehydration reactions in wood to facilitate the formation of char and decrease the effective heat of burning, resulting in lower heat release and flame spread [6]. High quality boron doped synthetic were studied by infrared absorption and photo-thermal ionization spectroscopies. Some excited states in bound hole were found to follow Rydberg Series [7]. To deal with nonorthogonalities in transition calculations a new method was proposed, multiconfiguration Hartree Fock method was used to study ionic line 1362 A^o of Boron [8].

Silicon is well known semiconductor that belongs to group 4. Carbon and germanium are other two important elements of the same group. It has an atomic number 14. Normally it is crystalline solid with grey-bluish luster. The electron affinity of silicon is high for oxygen but is less reactive than germanium. By mass it acquires number eight in the list of elements. It is mostly found in compound form; the most common compound of silicon is SiO_2. In 1823, Mr. Jöns Jakob Berzeliusit prepared and characterized Silicon in pure form [9]. Density-functional theory was employed to study low lying energy levels of silicon cluster. First principle method was also used to verify the result [10]. Takahashi *et al*. performed the fabrication, performance, and applications of a-Si solar cells. They investigated characteristics of Si and its solar cell to reduce the cost of solar cells [11]. Botti, S. *et al*. studied the optical and electronic properties of Si using first principle method. They also investigated characteristics of Si based thin film solar cells [12].

RESULT AND DISCUSSION

T. F. Gallagher *et al*. determined the radiative lifetimes of s and d states of Na for n =5 to13. They used two photon spectroscopy; with the help of two dye lasers. The results were found to be in good agreement with Coulomb-approximation calculations [13]. The energy levels using Linear Combination of Atomic Orbital- Molecular Orbitals with Self Consistent field method found Rydberg series in Nitrogen molecule. They found only one 1Σu+ level around 104 000 cm^{-1}. The calculations confirmed the configurations previously suggested for the upper states of Worley's third and Hopfield's Rydberg series [14-21]. Configuration interaction functions were used to calculate Rydberg excited levels of 1Σ+, 3Σ+, 1Π, and 3Π symmetry. The comparison of their results with experimental data converge to the 2Σ+ ground state of CO+. A simple Rydberg formula was used to calculate quantum defect [22]. The 6snd $1D^2$(n = 17-35) and 6snd $3D^2$ (n = 17-28) were studied to find Rydberg levels of Ba I using two-step laser excitation in an atomic beam. They also calculated the lifetimes of 5d7d $1D^2$ level. The measured values have been satisfactorily interpreted by a parametric method based upon the wave functions previously obtained from a multichannel quantum defect analysis of the energies [23]. T. Trickl studied Kr in=5, 6, 7 $4p^5ns$ using high-resolution hyperfine studies and isotope shifts for energy determination of Rydberg levels. Two-photon spectroscopy was used with an extreme-ultraviolet. They improved 12 wavenumber of energy levels by more than one order of magnitude. They found that the $4p^56s$ and $4p^57s$ states are a pure jj-coupling scheme states. They also determined life times of $4p^56s$ and $4p^57s$ states [24]. An effective potential method was used to study the electrostatic fine structure for singly excited lithium. Using variational wave functions some

Table 1: Rydberg Energy Levels and Quantum Defects for $^2D_{5/2}$ Term of Boron

n	QD	E (NIST) cm^{-1}	E (cal.)	ΔE cm^{-1}	n	QD	E (NIST) cm^{-1}	E (cal.) cm^{-1}	ΔE cm^{-1}
10	0.038641	65822.14	65822.14	0	30	0.048872	66805.67	66805.71	0.04
11	0.039404	66014.59	66014.59	0	31	0.049009	66813.69	66813.49	-0.2
12	0.039467	66160.94	66160.94	0	32	0.049132	66821.07	66820.55	-0.52
13	0.040141	66274.68	66274.68	0	33	0.049243	66827.07	66826.97	-0.1
14	0.041121	66364.91	66364.85	-0.06	34	0.049343	66832.74	66832.84	0.1
15	0.042157	66437.64	66437.57	-0.07	35	0.049434	66838.36	66838.21	-0.15
16	0.043133	66497.16	66497.06	-0.1	36	0.049517	66843.32	66843.13	-0.19
17	0.044007	66546.49	66546.35	-0.14	37	0.049593	66847.83	66847.67	-0.16
18	0.044771	66587.8	66587.65	-0.15	38	0.049662	66852.03	66851.85	-0.18
19	0.045432	66622.73	66622.6	-0.13	39	0.049726	66855.6	66855.71	0.11
20	0.046002	66652.54	66652.43	-0.11	40	0.049784		66859.28	
21	0.046494	66678.18	66678.1	-0.08	41	0.049838		66862.6	
22	0.046919	66700.43	66700.34	-0.09	42	0.049887		66865.68	
23	0.047288	66719.81	66719.74	-0.07	43	0.049933		66868.55	
24	0.047609	66736.87	66736.77	-0.1	44	0.049976		66871.23	
25	0.04789	66752.05	66751.79	-0.26	45	0.050015		66873.73	
26	0.048137	66765.21	66765.1	-0.11	46	0.050052		66876.07	
27	0.048355	66777.09	66776.97	-0.12	47	0.050086		66878.26	
28	0.048547	66787.68	66787.58	-0.1	48	0.050118		66880.31	
29	0.048719	66797.31	66797.12	-0.19	49	0.050148		66882.24	
					50	0.050176		66884.06	

Table 2: Rydberg Energy Levels and Quantum Defects for $^2D_{3/2}$ Term of Boron

n	QD	E (NIST) cm^{-1}	E (cal.)	ΔE cm^{-1}	n	QD	E (NIST) cm^{-1}	E (cal.) cm^{-1}	ΔE cm^{-1}
3	-0.00403	54767.69	54767.69	0	27	0.040136		66777.06	
4	0.021987	59993.45	59993.45	0	28	0.040155		66787.67	
5	0.029946	62485.5	62485.5	0	29	0.040172		66797.19	
6	0.033636	63845.32	63845.32	0	30	0.040187		66805.78	
7	0.035666	64665.35	64665.51	0.16	31	0.0402		66813.55	
8	0.036902	65197.29	65197.47	0.18	32	0.040212		66820.61	
9	0.03771		65561.84		33	0.040223		66827.03	
10	0.038268		65822.22		34	0.040234		66832.89	
11	0.038668		66014.71		35	0.040243		66838.25	
12	0.038965		66161		36	0.040251		66843.18	
13	0.039192		66274.78		37	0.040259		66847.71	
14	0.039369		66365		38	0.040266		66851.88	
15	0.039509		66437.74		39	0.040273		66855.74	
16	0.039623		66497.25		40	0.040279		66859.32	
17	0.039716		66546.55		41	0.040285		66862.63	

(Table 2). Continued.

n	QD	E (NIST) cm^{-1}	E (cal.)	ΔE cm^{-1}	n	QD	E (NIST) cm^{-1}	E (cal.) cm^{-1}	ΔE cm^{-1}
18	0.039793		66587.84		42	0.04029		66865.71	
19	0.039857		66622.78		43	0.040295		66868.58	
20	0.039912		66652.6		44	0.040299		66871.25	
21	0.039959		66678.25		45	0.040304		66873.75	
22	0.039999		66700.48		46	0.040307		66876.09	
23	0.040034		66719.87		47	0.040311		66878.28	
24	0.040065		66736.89		48	0.040315		66880.33	
25	0.040092		66751.9		49	0.040318		66882.26	
26	0.040115		66765.21		50	0.040321		66884.07	

Table 3: Rydberg Energy Levels and Quantum Defects for $^4F^o_{5/2}$ Term of Boron

n	QD	E (NIST) cm^{-1}	E (cal.) cm^{-1}	ΔE cm^{-1}	n	QD	E (NIST) cm^{-1}	E (cal.) cm^{-1}	ΔE cm^{-1}
4	0.01115	60031.076	60031.076	0.00	28	0.01482		66787.921	
5	0.01248	62516.559	62516.559	0.00	29	0.01482		66797.423	
6	0.01321	63866.326	63866.326	0.00	30	0.01483		66805.989	
7	0.01366	64679.745	64679.745	0.00	31	0.01483		66813.740	
8	0.01395	65207.380	65207.403	0.02	32	0.01484		66820.776	
9	0.01416		65568.990		33	0.01484		66827.181	
10	0.01430		65827.525		34	0.01484		66833.029	
11	0.01441		66018.742		35	0.01484		66838.383	
12	0.01449		66164.134		36	0.01485		66843.297	
13	0.01455		66277.253		37	0.01485		66847.817	
14	0.01460		66366.988		38	0.01485		66851.985	
15	0.01464		66439.367		39	0.01485		66855.837	
16	0.01467		66498.593		40	0.01485		66859.403	
17	0.01469		66547.670		41	0.01486		66862.712	
18	0.01472		66588.791		42	0.01486		66865.787	
19	0.01473		66623.587		43	0.01486		66868.650	
20	0.01475		66653.292		44	0.01486		66871.319	
21	0.01476		66678.853		45	0.01486		66873.813	
22	0.01477		66701.006		46	0.01486		66876.146	
23	0.01478		66720.331		47	0.01486		66878.331	
24	0.01479		66737.289		48	0.01487		66880.382	
25	0.01480		66752.253		49	0.01487		66882.308	
26	0.01481		66765.522		50	0.01487		66884.119	
27	0.01481		66777.344						

Table 4: Rydberg Energy Levels and Quantum Defects for $^1P^o$ Term of Silicon

n	QD	E (NIST) cm^{-1}	E (cal.) cm^{-1}	ΔE cm^{-1}	n	QD	E (NIST) cm^{-1}	ΔE cm^{-1}
3	0.020387	53387.33	53387.33	0	27	0.039043		65596.79
4	0.025322	58801.53	58801.53	0	28	0.039067		65607.4
5	0.029697	61305.67	61305.67	0	29	0.039089		65616.92
6	0.032468	62666.25	62666.25	0	30	0.039109		65625.51
7	0.034242		63486.16		31	0.039126		65633.28
8	0.035427		64017.83		32	0.039143		65640.33
9	0.036251		64382		33	0.039157		65646.75
10	0.036845		64642.26		34	0.039171		65652.61
11	0.037287		64834.66		35	0.039183		65657.98
12	0.037623		64980.9		36	0.039194		65662.9
13	0.037885		65094.63		37	0.039204		65667.43
14	0.038094		65184.82		38	0.039214		65671.61
15	0.038261		65257.54		39	0.039223		65675.47
16	0.038399		65317.03		40	0.039231		65679.04
17	0.038512		65366.32		41	0.039239		65682.35
18	0.038608		65407.61		42	0.039246		65685.43
19	0.038688		65442.54		43	0.039252		65688.3
20	0.038757		65472.35		44	0.039258		65690.98
21	0.038816		65498		45	0.039264		65693.47
22	0.038867		65520.23		46	0.039269		65695.81
23	0.038911		65539.61		47	0.039274		65698
24	0.038951		65556.62		48	0.039279		65700.05
25	0.038985		65571.63		49	0.039283		65701.98
26	0.039016		65584.94		50	0.039287		65703.8

properties of singly excited lithium were determined [25]. A literature review was carried out and published data of B I was assembled. Classification of 164 lines in the range 36010−993 Å with corresponding intensities and wavenumbers of 92 levels were reported [26].

In this study, we used WBEPMT to calculate energy of Rydberg atoms of Boron & Silicon. The results are shown in Tables **1** to **4**, where Tables (**1** to **3**) show Rydberg energies and Quantum defects (n= 4-50) for Boron and Table **4** shows the same for 1Po of Silicon. Experimental data was obtained from NIST site. The data was processed to change it into a suitable format. A computer program was developed to do the theoretical calculations on the basis of WBEPMT. This program uses four experimental values to calculate the coefficient "$\mathbf{a}_i$" (see eqn-10). Then the energy up to n=50 levels is calculated by the software. The theoretical results are compared with available data. In most of the cases a small amount of data was available so we calculated Rydberg energies and Quantum defects for those states for which data was available and in most cases we found the new results for Rydberg energies and Quantum defects.

CONCLUSION

Weakest Bound Electron Potential Model has been employed to calculate Rydberg energy levels. The experimental data was obtained from NIST (National Institute of Standard and Technology) site. The experimental data was used to find the constants a_i in eq. (10) and the constants are used to find Rydberg energies for the levels having principal quantum number 4-50. There was good agreement in theoretically calculated energies of Rydberg levels and experimental values obtained from NIST. In this work we calculated Rydberg energies for semiconducting

elements for the states $^2D_{5/2}$, $^2D_{3/2}$, $^4F^o_{5/2}$, of boron and $^1P^o$ of silicon. For the same principal quantum defects were also calculated.

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