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Using Least squares methods and nonlinear regression Methods to Calculate the Approximate Value of Ionicity in Terms of the Energy Gap

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1. Introduction

The rationale of this research is to find solution for some physical problems mainly the electronic features of the hexagonal structures of the semiconductors. More specifically, the research tries to solve the physical problem of calculating the ionicity factor based on energy gap (E_g) for hexagonal structure semiconductors. To achieve this objective, mathematical models are formulated counting on the process of the mathematical modelling. In this study, the numerical analysis method and statistical regression method are used to establish mathematical models that help solve realistic problems in physics. The method of the analytical expression is applied to find the solution of linear and nonlinear problems. It provides new and efficient computational procedure for solving large classes of nonlinear equations. Essentially the method provides a systematic computational procedure for equations containing any nonlinear terms of physical significance.[1]

Based on the information available in the specified libraries, this study is considered a recent and innovative one in mathematics and physics. In recent years, there have been many studies on the subject of estimation. Arif studied the Mathematical Modeling of Physical Properties for Hexagonal Binaries, and he found a relationship between ionicity and energy gap throughout constructing a mathematical model

ABSTRACT

The objective of the current study is to find the best mathematical models to calculate the estimated value of the ionization for the physical compounds of semiconductors based on the energy gap throughout using some numerical analysis methods as the least squares method. The best of its branches obtained is a nonlinear method of the second degree, we compare the new result with other methods and we obtained our new method is more accurate and efficiency. Another side we using some regression analysis methods as the regression method. The best of its branches obtained is a nonlinear method of the quadratic regression model.

depending on manual attempts [2,3,4]. While, in this study, a mathematical model is formed by depending on numerical analysis and statistical method to find the ionicity factor in terms of energy gap.

Our objective is to find a solution to the physical problem of ionicity factor basing on energy gap of hexagonal structure semiconductors. Through the research, new mathematical models have been built based on numerical analysis and statistical regression methods. The obtained calculated values are in accordance with experimental and theoretical results.[5,6]

2. Numerical Analysis Methods: the least squares method

By applying the numerical analysis method, which is named the least squares method, we take three types of methods: the first method is linear, the second one is polynomial nonlinear of second order, while the third method is the exponential nonlinear.

2.1. The least squares method, linear method:[7,8]

The estimated mathematical model is derived by

$$I_c = a E_{pi} + b$$

the rule can be written as follows:

$$a \sum_{i=1}^{31} E_{pi} + n b = \sum_{i=1}^{31} I_{ci} \quad (1)$$

$$a \sum_{i=1}^{31} E_{pi}^2 + b \sum_{i=1}^{31} E_{pi} = \sum_{i=1}^{31} E_{pi} I_{ci} \quad (2)$$

Where $E_{pi} = E_p(\text{Exp.})$, and $I_{ci} = I_c(\text{Exp.})$ in table 1

Where $i=1,2,\dots,31$

$$\sum_{i=1}^{31} E_{pi}^2 = 1232.351, \quad \sum_{i=1}^{31} I_{ci} = 26.97, \quad \sum_{i=1}^{31} E_{pi} = 172.37,$$

$$\sum_{i=1}^{31} E_{pi} I_{ci} = 154.821$$

We substitute the values above in equations (1) and (2) we get :

$$a(172.37) + b(31) = 26.97 \quad (3)$$

$$(1232.351) + b(172.37) = 154.821 \quad (4) \quad a$$

the equation (3) and (4) we get the values of the constants a, b as :

$$a = 0.01773933418, \quad b = 0.775483871$$

Then

$$I_c = a E_{pi} + b$$

Then the approximate formula is

$$I_c = 0.017 E_{pi} + 0.775 \quad (5)$$

By applying the steps of building the mathematical model such as verification, validation, and evaluation, we obtained the mathematical model (5) [1-3]. The values of iconicity factor are mentioned in Table 1.

Table 1. Comparison of the Results of Iconicity factor I_c (Det.) in Terms of E_p with the Exp. and Theo.

No.	Comp.	E_p (Exp.)	I_c (Exp.)	I_c (Theo.) [2]	I_c (Det.)	Error	Error ²
1	AgF	2.8 ^a	0.894 ^b	0.80	0.822	0.02-	0.0004
2	AgCl	3.249 ^a	0.856 ^b	0.821	0.830	0.009-	0.000081
3	AgBr	2.69 ^a	0.850 ^b	0.790	0.820	0.03-	0.0009
4	AgI	2.62 ^a	0.770 ^b	0.771	0.819	-0.04	0.0016
5	CaO	5.93 ^b	0.913 ^b	0.904	0.875	0.02	0.0004
6	CdO	2.5 ^b	0.785 ^b	0.763	0.817	0.03-	0.0009
7	CuCl	3.35 ^c	0.746 ^b	0.813	0.831	0.01-	0.0001
8	CaS	4.10 ^d	0.902 ^b	0.856	0.844	0.01	0.0001
9	CuBr	2.91 ^d	0.735 ^b	0.789	0.824	0.03-	0.0009
10	CdSe	1.751 ^d	0.699 ^b	0.696	0.804	-0.1	0.01
11	CaTe	1.50 ^e	0.894 ^b	0.682	0.800	0.09	0.0081
12	MgS	3.9 ^d	0.828 ^b	0.837	0.841	0.004-	0.000016
13	MgO	7.16 ^b	0.841 ^b	0.905	0.896	0.009	0.000081
14	SrO	6.7 ^f	0.926 ^b	0.910	0.888	0.02	0.0004
15	SrS	4.1 ^d	0.914 ^b	0.857	0.844	0.01	0.0001
16	ZnS	3.68 ^d	0.764 ^c	0.828	0.837	0.009-	0.000081
17	ZnSe	2.70 ^d	0.740 ^d	0.776	0.820	0.04-	0.0016
18	KF	10 ^c	0.955 ^b	0.948	0.945	0.003	0.000009
19	KBr	6.840 ^c	0.952 ^b	0.911	0.891	0.02	0.0004
20	KCl	7.834 ^c	0.953 ^b	0.925	0.908	0.01	0.0001
21	KI	5.890 ^c	0.950 ^b	0.893	0.875	0.01	0.0001
22	LiF	13.09 ^c	0.915 ^b	0.970	0.997	0.02-	0.0004
23	LiCl	9.4 ^a	0.903 ^b	0.943	0.934	0.001	0.000001
24	LiBr	7.6 ^a	0.899 ^b	0.922	0.904	-0.005	0.000025
25	LiI	5.8 ^d	0.890 ^b	0.891	0.873	0.01	0.0001
26	NaF	10.70 ^c	0.946 ^b	0.954	0.956	0.002-	0.000004
27	NaCl	8.025 ^c	0.935 ^b	0.928	0.911	0.01	0.0001
28	NaBr	7.1 ^a	0.934 ^b	0.928	0.895	0.03	0.0009
29	NaI	5.666 ^c	0.927 ^b	0.888	0.871	0.01	0.0001
30	RbF	10.3 ^d	0.960 ^b	0.958	0.950	0.008	0.000064
31	CdS	2.485 ^c	0.794 ^c	0.762	0.817	-0.02	0.0004

Note. ^a[9], ^b[10]; ^c[11]; ^d[12]; ^e[13]; ^f[14].

Figure 1 displays a comparison between the iconicity factor values which are obtained out of equation (3) in terms of energy gap, and the experimental data

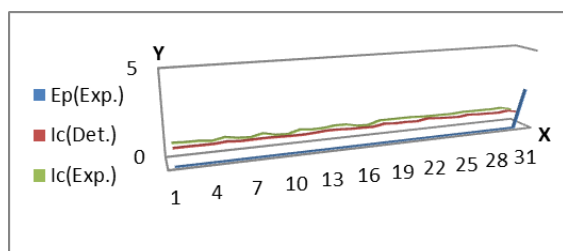


Fig. 1: The determined iconicity factor values compared with the experimental and theoretical values for different hexagonal semiconductors.

2.2. The least squares method polynomial nonlinear of second order [7,8]

The estimated mathematical model is derived by

$$I_c = a E_p^2 + b E_p + c$$

Where a,b,c are constant

the rule can be written as follows

$$\sum_{i=1}^{31} I_{ci} = a \sum_{i=1}^{31} E_{pi}^2 + b \sum_{i=1}^{31} E_{pi} + nc \quad (4)$$

$$\sum_{i=1}^{31} E_{pi} I_{ci} = a \sum_{i=1}^{31} E_{pi}^3 + b \sum_{i=1}^{31} E_{pi}^2 + c \sum_{i=1}^{31} E_{pi} \quad (5)$$

$$\sum_{i=1}^{31} E_{pi}^2 I_{ci} = a \sum_{i=1}^{31} E_{pi}^4 + b \sum_{i=1}^{31} E_{pi}^3 + c \sum_{i=1}^{31} E_{pi}^2 \quad (6)$$

$$(1232.351) + b(172.37) + c(31) = 26.97 \quad (7) \quad a$$

$$a(10443.771) + b(1232.351) + c(172.37) = 154.821 \quad (8)$$

$a (98350.968) + b (10443.771) + c (1232.351) = 1128.8$ (9)

When solving the equations (1), (2) and (3) we get the values of the constants a, b and c as

$a = -0.0031074073$ $b = 0.0570740149$, $c = 0.6723225806$

$$I_c = a E_p^2 + b E_p + c$$

Then the approximate formula is $I_c = -0.0031074073 E_p^2 + 0.0570740149 E_p + 0.6723225806$ (10)

In the same way followed in contracting the mathematical model (3), we verified the construction of the mathematical model (10). The values for iconicity factor are mentioned in Table 2.

Table 2. Comparison of the Results of Iconicity factor I_c (Det.) in Terms of E_p with the Exp. and Theo.

No.	Comp.	E_p (Exp.)	I_c (Exp.)	I_c (Theo.) [2]	I_c (Det.)	Error	Error ²
1	AgF	2.8 ^a	0.894 ^b	0.80	0.808	-0.008	0.000064
2	AgCl	3.249 ^a	0.856 ^b	0.821	0.826	-0.005	0.000025
3	AgBr	2.69 ^a	0.850 ^b	0.790	0.804	-0.01	0.0001
4	AgI	2.62 ^a	0.770 ^b	0.771	0.801	-0.03	0.0009
5	CaO	5.93 ^b	0.913 ^b	0.904	0.905	-0.001	0.000001
6	CdO	2.5 ^b	0.785 ^b	0.763	0.796	-0.01	0.0001
7	CuCl	3.35 ^c	0.746 ^b	0.813	0.829	-0.01	0.0001
8	CaS	4.10 ^d	0.902 ^b	0.856	0.855	0.001	0.000001
9	CuBr	2.91 ^d	0.735 ^b	0.789	0.812	-0.02	0.0004
10	CdSe	1.751 ^d	0.699 ^b	0.696	0.762	-0.06	0.0036
11	CaTe	1.50 ^e	0.894 ^b	0.682	0.751	-0.06	0.0036
12	MgS	3.9 ^d	0.828 ^b	0.837	0.849	-0.01	0.0001
13	MgO	7.16 ^b	0.841 ^b	0.905	0.927	-0.02	0.0004
14	SrO	6.7 ^f	0.926 ^b	0.910	0.919	0.007	0.000049
15	SrS	4.1 ^d	0.914 ^b	0.857	0.855	0.002	0.000004
16	ZnS	3.68 ^d	0.764 ^c	0.828	0.841	0.01	0.0001
17	ZnSe	2.70 ^d	0.740 ^d	0.776	0.804	-0.02	0.0004
18	KF	10 ^c	0.955 ^b	0.948	0.942	0.006	0.000036
19	KBr	6.840 ^c	0.952 ^b	0.911	0.921	-0.01	0.0001
20	KCl	7.834 ^c	0.953 ^b	0.925	0.934	-0.009	0.000081
21	KI	5.890 ^c	0.950 ^b	0.893	0.903	-0.01	0.0001
22	LiF	13.09 ^c	0.915 ^b	0.970	0.904	0.01	0.0001
23	LiCl	9.4 ^a	0.903 ^b	0.943	0.942	0.001	0.000001
24	LiBr	7.6 ^a	0.899 ^b	0.922	0.932	-0.01	0.0001
25	LiI	5.8 ^d	0.890 ^b	0.891	0.902	-0.01	0.000001
26	NaF	10.70 ^c	0.946 ^b	0.954	0.938	0.008	0.000064
27	NaCl	8.025 ^c	0.935 ^b	0.928	0.936	-0.001	0.000001
28	NaBr	7.1 ^a	0.934 ^b	0.928	0.925	0.003	0.000009
29	NaI	5.666 ^c	0.927 ^b	0.888	0.898	-0.01	0.000009
30	RbF	10.3 ^d	0.960 ^b	0.958	0.941	0.01	0.0004
31	CdS	2.485 ^c	0.794 ^c	0.762	0.795	-0.001	0.000001

Figure 2 displays a comparison between the iconicity factor values which are obtained out of equation (10) in terms of energy gap, and the experimental data.

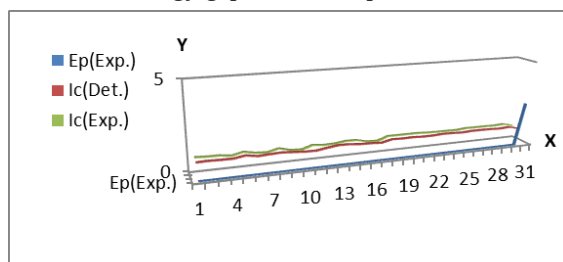


Fig. 2: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

2.3. Exponential nonlinear method [7,8]

The estimated mathematical model is derived by

$$I_c = a * e^{A E_{pi}}$$

Where $i=1,2,3 \dots n$, $n=31$

the rule can be written as follows

$$A \sum_{i=1}^{31} E_{pi} + n B = \sum_{i=1}^{31} I_{ci} \quad (11)$$

$$A \sum_{i=1}^{31} E_{pi}^2 + B \sum_{i=1}^{31} E_{pi} = \sum_{i=1}^{31} E_{pi} I_{ci} \quad (12)$$

$$A (172.37) + B (31) = -4.433 \quad (13)$$

$$A (1232.351) + B (172.37) = -18.881 \quad (14)$$

When solving the equations (13) and (14) we get:

$$A = 0.021 \quad B = -0.259,$$

$$I_c = a * e^{A E_{pi}}$$

We find the values of constants a and b

$$\ln I_c = \ln a + E_{pi} \ln b$$

Where

$$\ln I_c = I_c, \ln b = A, \ln a = B, E_{pi} = E_{pi}$$

$$b = e^A \quad \ln b = A, a = e^B$$

$$\ln b = (0.021), e^{\ln b} = e^{(0.021)} \quad b = e^{(0.021)},$$

$$b = 1.021, a = (-0.259), \quad a = 0.771, \quad \ln a = B,$$

$$e^{\ln a} = e^{(-0.259)}, a = e^{(-0.259)}$$

$$I_c = a e^{A E_{pi}}$$

Then the approximate formula is

$$I_c = (0.771)e^{(0.021)E_p} \quad (15)$$

In the same way that is followed in establishing the mathematical model (3) we created the mathematical model (15). The values for iconicity factor are mentioned in Table 3.

Table 3. Comparison of the Results of Iconicity factor I_c (Det.) in Terms of E_p with the Exp. and Theo.

No.	Comp.	E_p (Exp.)	I_c (Exp.)	I_c (Theo.) [2]	I_c (Det.)	Error	Error ²
1	AgF	2.8 ^a	0.894 ^b	0.80	0.817	-0.01	0.0001
2	AgCl	3.249 ^a	0.856 ^b	0.821	0.824	-0.003	0.000009
3	AgBr	2.69 ^a	0.850 ^b	0.790	0.815	-0.02	0.0004
4	AgI	2.62 ^a	0.770 ^b	0.771	0.814	-0.04	0.0016
5	CaO	5.93 ^b	0.913 ^b	0.904	0.872	0.03	0.0009
6	CdO	2.5 ^b	0.785 ^b	0.763	0.812	-0.02	0.0004
7	CuCl	3.35 ^c	0.746 ^b	0.813	0.826	-0.01	0.0001
8	CaS	4.10 ^d	0.902 ^b	0.856	0.839	0.01	0.0001
9	CuBr	2.91 ^d	0.735 ^b	0.789	0.819	-0.03	0.0009
10	CdSe	1.751 ^d	0.699 ^b	0.696	0.799	-0.1	0.01
11	CaTe	1.50 ^e	0.894 ^b	0.682	0.795	0.09	0.0081
12	MgS	3.9 ^d	0.828 ^b	0.837	0.836	0.001	0.000001
13	MgO	7.16 ^b	0.841 ^b	0.905	0.894	0.01	0.0001
14	SrO	6.7 ^f	0.926 ^b	0.910	0.886	0.02	0.0004
15	SrS	4.1 ^d	0.914 ^b	0.857	0.839	0.01	0.0001
16	ZnS	3.68 ^d	0.764 ^c	0.828	0.832	-0.004	0.000016
17	ZnSe	2.70 ^d	0.740 ^d	0.776	0.815	-0.03	0.0009
18	KF	10 ^c	0.955 ^b	0.948	0.949	-0.001	0.000001
19	KBr	6.840 ^c	0.952 ^b	0.911	0.888	0.02	0.0004
20	KCl	7.834 ^c	0.953 ^b	0.925	0.907	0.01	0.0001
21	KI	5.890 ^c	0.950 ^b	0.893	0.871	0.02	0.0004
22	LiF	13.09 ^c	0.915 ^b	0.970	1.012	-0.04	0.0016
23	LiCl	9.4 ^a	0.903 ^b	0.943	0.937	0.006	0.000036
24	LiBr	7.6 ^a	0.899 ^b	0.922	0.902	-0.003	0.000009
25	LiI	5.8 ^d	0.890 ^b	0.891	0.869	0.02	0.0004
26	NaF	10.70 ^c	0.946 ^b	0.954	0.963	-0.009	0.000081
27	NaCl	8.025 ^c	0.935 ^b	0.928	0.910	0.01	0.0001
28	NaBr	7.1 ^a	0.934 ^b	0.928	0.893	0.04	0.0016
29	NaI	5.666 ^c	0.927 ^b	0.888	0.867	0.02	0.0004
30	RbF	10.3 ^d	0.960 ^b	0.958	0.955	0.003	0.000009
31	CdS	2.485 ^c	0.794 ^c	0.762	0.811	-0.01	0.0001

Figure 3 displays a comparison between the iconicity factor values which are obtained out of equation (15) in terms of energy gap, and the experimental data.

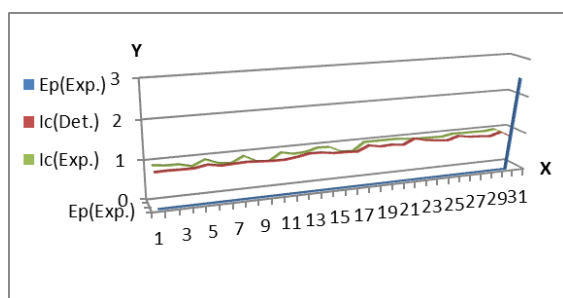


Fig. 3: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

3. Statistical nonlinear regression methods

By applying the statistical nonlinear regression method, we take three kind methods; first method is logarithm nonlinear regression, second method is

quadratic nonlinear regression and three method is cubic nonlinear regression.[15]

3.1. Logarithm nonlinear regression:[16,17]

The estimated mathematical model is derived by

$$\ln I_c = \ln A + B \ln E_p \quad (16)$$

Where $a = 0.716$, $b = 0.098$, In SPSS

A, B constant

, where $\ln I_c = I_c$, $\ln I_c = \ln(0.716) + 0.098 \ln E_p$,

, $B = b$, $\ln E_p = E_p$, $\ln A = a$, $A = 0.716$

$$\ln I_c = \ln A + B \ln E_p$$

Then the approximate formula is

$$\ln I_c = 0.716 + 0.098 \ln E_p \quad (17)$$

In the same way followed in building the mathematical model (3) we verified the construction of the mathematical model (17). The values for iconicity factor are mentioned in Table 4.

Table 4. Comparison of the Results of Iconicity factor I_c (Det.) in Terms of E_p with the Exp. and Theo.

No.	Comp.	E_p (Exp.)	I_c (Exp.)	I_c (Theo.) [2]	I_c (Det.)	Error	Error ^2
1	AgF	2.8 ^a	0.894 ^b	0.80	0.82	0.02-	0.0004
2	AgCl	3.249 ^a	0.856 ^b	0.821	0.83	0.009-	0.000081
3	AgBr	2.69 ^a	0.850 ^b	0.790	0.81	0.02-	0.0004
4	AgI	2.62 ^a	0.770 ^b	0.771	0.81	0.03-	0.0009
5	CaO	5.93 ^b	0.913 ^b	0.904	0.89	0.01	0.0001
6	CdO	2.5 ^b	0.785 ^b	0.763	0.81	0.02-	0.0004
7	CuCl	3.35 ^c	0.746 ^b	0.813	0.83	0.01-	0.0001
8	CaS	4.10 ^d	0.902 ^b	0.856	0.85	0.006	0.000036
9	CuBr	2.91 ^d	0.735 ^b	0.789	0.82	0.03-	0.0009
10	CdSe	1.751 ^d	0.699 ^b	0.696	0.77	0.07-	0.0049
11	CaTe	1.50 ^e	0.894 ^b	0.682	0.76	0.07-	0.0049
12	MgS	3.9 ^d	0.828 ^b	0.837	0.85	0.01-	0.0001
13	MgO	7.16 ^b	0.841 ^b	0.905	0.91	0.005-	0.000025
14	SrO	6.7 ^f	0.926 ^b	0.910	0.90	0.01	0.0001
15	SrS	4.1 ^d	0.914 ^b	0.857	0.85	0.007	0.000049
16	ZnS	3.68 ^d	0.764 ^c	0.828	0.84	0.01-	0.0001
17	ZnSe	2.70 ^d	0.740 ^d	0.776	0.81	0.03-	0.0009
18	KF	10 ^c	0.955 ^b	0.948	0.94	0.008	0.000064
19	KBr	6.840 ^c	0.952 ^b	0.911	0.90	0.01	0.0001
20	KCl	7.834 ^c	0.953 ^b	0.925	0.92	0.005	0.000025
21	KI	5.890 ^c	0.950 ^b	0.893	0.89	0.003	0.000009
22	LiF	13.09 ^c	0.915 ^b	0.970	0.97	0	0
23	LiCl	9.4 ^a	0.903 ^b	0.943	0.94	0.003	0.000009
24	LiBr	7.6 ^a	0.899 ^b	0.922	0.91	0.01	0.0001
25	LiI	5.8 ^d	0.890 ^b	0.891	0.89	0	0
26	NaF	10.70 ^c	0.946 ^b	0.954	0.95	0.004	0.000016
27	NaCl	8.025 ^c	0.935 ^b	0.928	0.92	0.008	0.000064
28	NaBr	7.1 ^a	0.934 ^b	0.928	0.91	0.01	0.0001
29	NaI	5.666 ^c	0.927 ^b	0.888	0.89	0.002-	0.000004
30	RbF	10.3 ^d	0.960 ^b	0.958	0.94	0.01	0.0001
31	CdS	2.485 ^c	0.794 ^c	0.762	0.81	0.01	0.0001

Figure 4 displays a comparison between the iconicity factor values which are obtained out of equation (17) in terms of energy gap, and the experimental data.

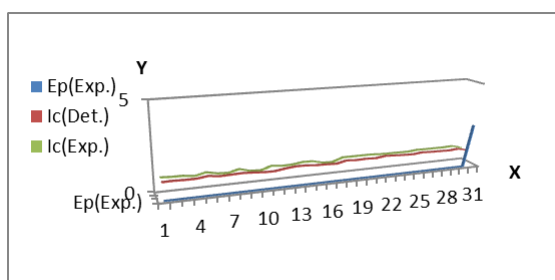


Fig. 4: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

3.2. Quadratic nonlinear regression method [16,17]

The estimated mathematical model is derived by

$$I_c = a + b_1 E_p + b_2 E_p^2 \quad (18)$$

Where $a = 0.690, b_1 = 0.050, b_2 = -0.002$

Then the approximate formula is

$$I_c = 0.690 + 0.050 E_p + (-0.002) E_p^2 \quad (19)$$

In the same way followed in constructing the mathematical model (3) we created the mathematical model (19). The values for iconicity factor are mentioned in Table 5.

Table 5. Comparison of the Results of Iconicity factor I_c (Det.) in Terms of E_p with the Exp. and Theo.

No.	Comp.	E_p (Exp.)	I_c (Exp.)	I_c (Theo.) [2]	I_c (Det.)	Error	Error ^2
1	AgF	2.8 ^a	0.894 ^b	0.80	0.81	0.01-	0.0001
2	AgCl	3.249 ^a	0.856 ^b	0.821	0.83	0.009-	0.000081
3	AgBr	2.69 ^a	0.850 ^b	0.790	0.81	-0.02	0.0004
4	AgI	2.62 ^a	0.770 ^b	0.771	0.81	0.03-	0.0009
5	CaO	5.93 ^b	0.913 ^b	0.904	0.92	0.007-	0.000049
6	CdO	2.5 ^b	0.785 ^b	0.763	0.80	-0.01	0.0001
7	CuCl	3.35 ^c	0.746 ^b	0.813	0.84	0.02-	0.0004
8	CaS	4.10 ^d	0.902 ^b	0.856	0.86	0.004-	0.000016
9	CuBr	2.91 ^d	0.735 ^b	0.789	0.82	0.03-	0.0009
10	CdSe	1.751 ^d	0.699 ^b	0.696	0.77	0.07-	0.0049
11	CaTe	1.50 ^e	0.894 ^b	0.682	0.76	0.07-	0.0049
12	MgS	3.9 ^d	0.828 ^b	0.837	0.85	0.01-	0.0001
13	MgO	7.16 ^b	0.841 ^b	0.905	0.95	-0.04	0.0016
14	SrO	6.7 ^f	0.926 ^b	0.910	0.94	0.01-	0.0001
15	SrS	4.1 ^d	0.914 ^b	0.857	0.86	0.003-	0.000009
16	ZnS	3.68 ^d	0.764 ^c	0.828	0.85	0.02-	0.0004
17	ZnSe	2.70 ^d	0.740 ^d	0.776	0.81	0.03-	0.0009
18	KF	10 ^c	0.955 ^b	0.948	0.99	0.03-	0.0009
19	KBr	6.840 ^c	0.952 ^b	0.911	0.94	0.01	0.0001
20	KCl	7.834 ^c	0.953 ^b	0.925	0.96	0.007-	0.000049
21	KI	5.890 ^c	0.950 ^b	0.893	0.92	0.02-	0.0004
22	LiF	13.09 ^c	0.915 ^b	0.970	1.00	-0.03	0.0009
23	LiCl	9.4 ^a	0.903 ^b	0.943	0.98	0.03-	0.0009
24	LiBr	7.6 ^a	0.899 ^b	0.922	0.95	0.02-	0.0004
25	LiI	5.8 ^d	0.890 ^b	0.891	0.91	0.01-	0.0001
26	NaF	10.70 ^c	0.946 ^b	0.954	1.00	0.04-	0.0016
27	NaCl	8.025 ^c	0.935 ^b	0.928	0.96	0.02-	0.0004
28	NaBr	7.1 ^a	0.934 ^b	0.928	0.94	0.006-	0.000036
29	NaI	5.666 ^c	0.927 ^b	0.888	0.91	0.01	0.0001
30	RbF	10.3 ^d	0.960 ^b	0.958	0.99	-0.03	0.0009
31	CdS	2.485 ^c	0.794 ^c	0.762	0.80	0.006-	0.000036

Figure 5 displays a comparison between the iconicity factor values which are obtained out of equation (19) in terms of energy gap, and the experimental data.

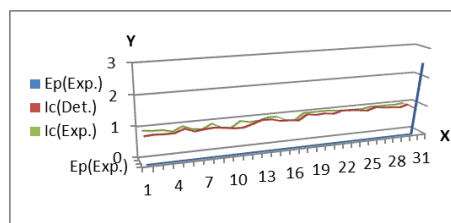


Fig. 5: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

3.3. Cubic nonlinear regression method [16,17]

The estimated mathematical model is derived by

$$I_c = a + b_1 E_p + b_2 E_p^2 + b_3 E_p^3 \quad (20)$$

Where $a = 0.721, b_1 = 0.031, b_2 = 0.001, b_3 = 0.000$

Then the approximate formula is

$$I_c = 0.721 + 0.031 E_p + 0.001 E_p^2 + 0.000 E_p^3 \quad (21)$$

In the same way followed in establishing the mathematical model (3) we verified the construction of the mathematical model (21). The values for iconicity factor are mentioned in Table 6.

Table 6. Comparison of the Results of Iconicity factor I_c (Det.) in Terms of E_p with the Exp. and Theo.

No.	Comp.	E_p (Exp.)	I_c (Exp.)	I_c (Theo.) [2]	I_c (Det.)	Error	Error ²
1	AgF	2.8 ^a	0.894 ^b	0.80	0.82	0.02-	0.0004
2	AgCl	3.249 ^a	0.856 ^b	0.821	0.83	0.009-	0.000081
3	AgBr	2.69 ^a	0.850 ^b	0.790	0.81	0.02-	0.0004
4	AgI	2.62 ^a	0.770 ^b	0.771	0.81	0.03-	0.0009
5	CaO	5.93 ^b	0.913 ^b	0.904	0.94	0.02-	0.0004
6	CdO	2.5 ^b	0.785 ^b	0.763	0.80	0.01-	0.0001
7	CuCl	3.35 ^c	0.746 ^b	0.813	0.84	0.02-	0.0004
8	CaS	4.10 ^d	0.902 ^b	0.856	0.86	0.004-	0.000016
9	CuBr	2.91 ^d	0.735 ^b	0.789	0.82	0.03-	0.0009
10	CdSe	1.751 ^d	0.699 ^b	0.696	0.78	0.08-	0.0064
11	CaTe	1.50 ^e	0.894 ^b	0.682	0.77	0.08-	0.0064
12	MgS	3.9 ^d	0.828 ^b	0.837	0.86	0.02-	0.0004
13	MgO	7.16 ^b	0.841 ^b	0.905	0.99	0.08-	0.0064
14	SrO	6.7 ^f	0.926 ^b	0.910	0.97	0.04-	0.0016
15	SrS	4.1 ^d	0.914 ^b	0.857	0.86	0.003-	0.000009
16	ZnS	3.68 ^d	0.764 ^c	0.828	0.85	0.02-	0.0004
17	ZnSe	2.70 ^d	0.740 ^d	0.776	0.81	0.03-	0.0009
18	KF	10 ^c	0.955 ^b	0.948	1.13	0.1-	0.01
19	KBr	6.840 ^c	0.952 ^b	0.911	0.98	0.02-	0.000004
20	KCl	7.834 ^c	0.953 ^b	0.925	1.03	0.07-	0.0049
21	KI	5.890 ^c	0.950 ^b	0.893	0.94	0.01	0.0001
22	LiF	13.09 ^c	0.915 ^b	0.970	1.30	0.3-	0.09
23	LiCl	9.4 ^a	0.903 ^b	0.943	1.10	0.1-	0.01
24	LiBr	7.6 ^a	0.899 ^b	0.922	1.01	0.08-	0.0064
25	LiI	5.8 ^d	0.890 ^b	0.891	0.93	0.03-	0.0001
26	NaF	10.70 ^c	0.946 ^b	0.954	1.17	0.2-	0.04
27	NaCl	8.025 ^c	0.935 ^b	0.928	1.03	0.09-	0.0081
28	NaBr	7.1 ^a	0.934 ^b	0.928	0.99	0.05-	0.0025
29	NaI	5.666 ^c	0.927 ^b	0.888	0.93	0.003-	0.000009
30	RbF	10.3 ^d	0.960 ^b	0.958	1.15	0.1-	0.01
31	CdS	2.485 ^c	0.794 ^c	0.762	0.80	0.006-	0.000036

Figure 6 displays a comparison between the iconicity factor values which are obtained out of equation (21) in terms of energy gap, and the experimental data.

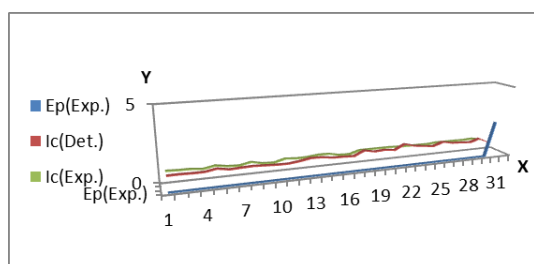


Fig. 6: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

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4. Conclusion and results

By applying the numerical analysis methods, the optimal mathematical model that is obtained from the three methods is the nonlinear second-order equation. In the three nonlinear regression methods, we found that the estimated mathematical model of nonlinear quadratic regression is optimal.

The optimal mathematical model among all methods in numerical analysis and statistical is the estimated mathematical model of the quadratic nonlinear regression. Where we obtained results similar to previous studies and that the error rates are very few and almost nonexistent.

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استخدام طرق المربعات الصغرى وطرق الانحدار الغير خطية لحساب القيمة التقريبية للتأين بدلالة فجوة الطاقة

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قسم الرياضيات , كلية التربية للعلوم الصرفة , جامعة تكريت , تكريت , العراق

الملخص

الهدف من البحث ايجاد افضل النماذج الرياضية لحساب القيمة التقديرية لمقدار التأين للمركبات الفيزيائية لاشباه الموصلات بالاعتماد على فجوة الطاقة باستخدام بعض طرق التحليل العددي كطريقة المربعات الصغرى وحصلنا على احسن فروعها طريقة معادلة متعددة الحدود اللاخطية من الدرجة الثانية وقارنا النتائج الجديدة مع الطرق الاخرى وحصلنا على طرق اخرى اكثر كفاءة ومن جهة اخرى استخدمنا بعض طرق التحليل الاحصائي كطريقة الانحدار وحصلنا على احسن فروعها نموذج الانحدار اللاخطي التربيعي.