IASJ
المجلات الاكاديمية العراقية

Tikrit Journal of Pure Science
ISSN: 1813 – 1662 (Print) --- E-ISSN: 2415 – 1726 (Online)

Journal Homepage: http://tjps.tu.edu.iq/index.php/j

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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https://doi.org/10.25130/tjps.v24i5.424

ARTICLE INFO.

Article history:

-Received: 10 / 4 / 2018

-Accepted: 7 / 5 / 2018

-Available online: / / 2018

Keywords: Mathematical model, the least squares method, nonlinear statistical regression method, ionization, energy gap.

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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.

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 iconicity and energy gap throughout constructing a mathematical 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 iconicity factor in terms of energy gap.

Our objective is to find a solution to the physical problem of iconicity 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 $Ep_i = Ep(Exp.)$,and $Ic_i = Ic(Exp.)$ in table 1

Where i=1,2,…,31

$\sum_{i=1}^{31} Ep_i^2 = 1232.351$, $\sum_{i=1}^{31} Ic_i = 26.97$, $\sum_{i=1}^{31} Ep_i = 172.37$,

$\sum_{i=1}^{31} Ep_i Ic_i = 154.821$

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

a (172.37)+b (31)=26.97 (3)

(1232.351)+b (172.37) =154.821 (4) a

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

a = 0.01773933418, b = 0.775483871

Then

$I_c = a E_{pi} + b$

Then the approximate formula is

$I_c = 0.017 E_{pi} + 0.775$ (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	*KCI*	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

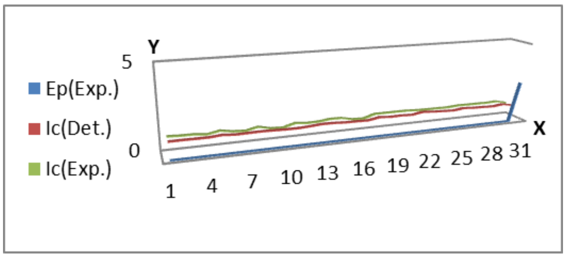

Fig. 1: The determined iconicity factor values compared with the experimental and theoretical values for different hexagonal semiconductors.

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

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

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

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

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

a (10443.771) + b (1232.351) + c (172.37) = 154.821 (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

$I_c = aE_p^2 + bE_p + c$

Then the approximate formula is

$$I_c = -0.0031074073E_p^2 + 0.0570740149E_p + 0.6723225806 \quad (10)$$

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	*KCI*	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.

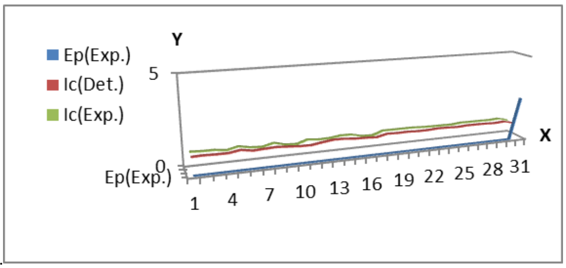

Fig. 2: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

2.3. Exponential nonlinear method [7,8]

The estimated mathematical model is derived by

$Ic = a * e^{A\,Epi}$

Where i=1,2,3…n ,n=31

the rule can be written as follows

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

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

A (172.37) + B (31) = -4.433 (13)

A (1232.351) + B (172.37) = -18.881 (14)

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

A = 0.021 B = -0.259,

$Ic = a * e^{A\,Epi}$

We find the values of constants a and b

$Ln\, I_c = Ln\, a + E_p\, Ln\, b$

Where

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

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

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

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

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

$I_c = a\, e^{A\,Epi}$

Then the approximate formula is

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

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	*KCI*	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.

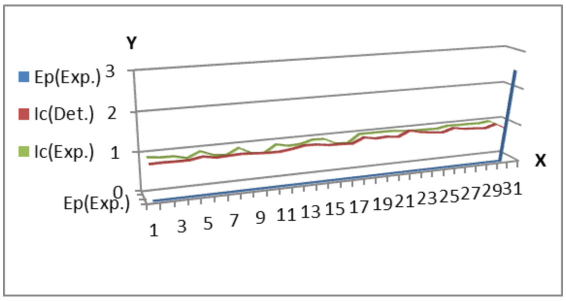

Fig. 3: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

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	*KCI*	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.

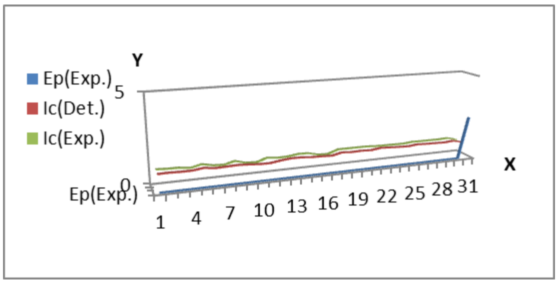

Fig. 4: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

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,b1=0.050,b2=-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.

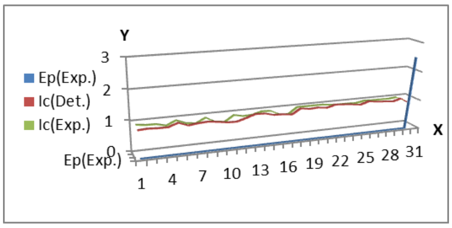

Fig. 5: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

3.3. Cubic nonlinear regression method [16,17]

The estimated mathematical model is derived by

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

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

Then the approximate formula is

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

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	*KCI*	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.

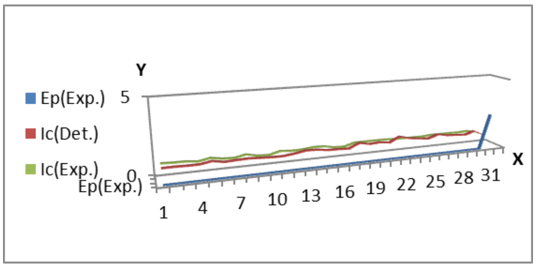

Fig. 6: The determined iconicity factor values compared to experimental and theoretical for different hexagonal semiconductors.

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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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.