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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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 ionicity 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 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

\[ I_c = aE_p + b \]

the rule can be written as follows:

\[ a \sum_{i=1}^{31} E_{pi} + b \sum_{i=1}^{31} I_{ci} = \sum_{i=1}^{31} I_{ci} \]  

\[ a \sum_{i=1}^{31} E_{pi}^2 + b \sum_{i=1}^{31} E_{pi} = \sum_{i=1}^{31} E_{pi} I_{ci} \]

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

Where i=1,2,...,31
We substitute the values above in equations (1) and (2) we get:

\[ a \begin{pmatrix} 172.37 \end{pmatrix} + b \begin{pmatrix} 31 \end{pmatrix} = 26.97 \]
\[ (1232.351) + b \begin{pmatrix} 172.37 \end{pmatrix} = 154.821 \]

We get the values of the constants \( a, b \) as:

\[ a = 0.01773933418, b = 0.775483871 \]

Then

\[ I_c = a E_p + b \]

Then the approximate formula is

\[ I_c = 0.017 E_p + 0.775 \]  \( 5 \)

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 \( I_c \) 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 2 |
|-----|-------|---------------|----------------|-------------------|----------------|-------|---------|
| 1   | AgF   | 2.8^o         | 0.80           | 0.822             | 0.02           | 0.0004 |
| 2   | AgCl  | 3.249^o       | 0.856^o        | 0.821             | 0.009-       | 0.000081 |
| 3   | AgBr  | 2.69^o        | 0.850^o        | 0.790             | 0.02          | 0.0009 |
| 4   | AgI   | 2.62^o        | 0.770^o        | 0.771             | -0.04         | 0.0016 |
| 5   | CaO   | 5.93^o        | 0.913^o        | 0.904             | 0.02          | 0.0004 |
| 6   | CdO   | 2.5^o         | 0.785^o        | 0.763             | -0.03         | 0.0009 |
| 7   | CuCl  | 3.35^c        | 0.746^o        | 0.813             | 0.01-        | 0.0001 |
| 8   | CuS   | 4.10^d        | 0.902^m        | 0.856             | 0.01          | 0.0001 |
| 9   | CuBr  | 2.91^m        | 0.735^o        | 0.789             | 0.03-        | 0.0009 |
| 10  | CdSe  | 1.751^a       | 0.699^h        | 0.696             | -0.1         | 0.01 |
| 11  | CuTe  | 1.50^f        | 0.894^l        | 0.682             | 0.09         | 0.0081 |
| 12  | MgS   | 3.9^g         | 0.828^l        | 0.837             | 0.04-        | 0.000016 |
| 13  | MgO   | 7.10^h        | 0.841^l        | 0.905             | 0.009        | 0.000081 |
| 14  | SrO   | 6.7^i         | 0.926^l        | 0.910             | 0.02         | 0.0004 |
| 15  | SrS   | 4.1^j         | 0.914^l        | 0.857             | 0.01         | 0.0001 |
| 16  | ZnS   | 3.68^k        | 0.764^l        | 0.828             | 0.03         | 0.000081 |
| 17  | ZnTe  | 2.70^l        | 0.740^m        | 0.776             | 0.04-        | 0.0016 |
| 18  | KF    | 10^o          | 0.955^m        | 0.948             | 0.003        | 0.00009 |
| 19  | KBr   | 6.840^o       | 0.952^m        | 0.911             | 0.02         | 0.0004 |
| 20  | KCl   | 7.834^c       | 0.953^m        | 0.925             | 0.01         | 0.0001 |
| 21  | KI    | 5.890^o       | 0.950^m        | 0.893             | 0.01         | 0.0001 |
| 22  | LiF   | 13.09^c       | 0.915^m        | 0.970             | 0.02-        | 0.0004 |
| 23  | LiCl  | 9.4^d         | 0.903^m        | 0.943             | 0.001        | 0.000001 |
| 24  | LiBr  | 7.6^e         | 0.899^m        | 0.922             | -0.005       | 0.000025 |
| 25  | Li   | 5.8^i         | 0.890^m        | 0.891             | 0.01         | 0.0001 |
| 26  | NaF   | 10.70^i       | 0.946^m        | 0.954             | 0.002-       | 0.000004 |
| 27  | NaCl  | 8.025^d       | 0.935^m        | 0.928             | 0.01         | 0.0001 |
| 28  | NaBr  | 7.1^g         | 0.934^m        | 0.928             | 0.03         | 0.0009 |
| 29  | NaI   | 5.666^f       | 0.927^m        | 0.887             | 0.01         | 0.0001 |
| 30  | RbF   | 10.3^j        | 0.960^m        | 0.958             | 0.008        | 0.000064 |
| 31  | CdS   | 2.485^g       | 0.794^m        | 0.762             | -0.02        | 0.0004 |

Note. [9], [10], [11]; [12]; [13]; [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.](image)

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:

\[ \sum I_c = a \sum E_p^2 + b \sum E_p + n c \]  \( 4 \)

\[ \sum E_p I_c = a \sum E_p^3 + b \sum E_p^2 + c \sum E_p \]  \( 5 \)

\[ \sum E_p^2 I_c = a \sum E_p^4 + b \sum E_p^3 + c \sum E_p^2 \]  \( 6 \)

\[(1232.351) + b \begin{pmatrix} 172.37 \end{pmatrix} + c \begin{pmatrix} 31 \end{pmatrix} = 26.97 \]  \( 7 \)

\[ a = 0.014437.771 + b (1232.351) + c (172.37) = 154.821 \]  \( 8 \)
Then the approximate formula is
\[ I_0 = -0.0031074073 E_p^2 + 0.0570740419 E_p + 0.672325806 \]
(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.

| 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 | 0.0000064 |
| 2   | AgCl  | 3.249 \( b \) | 0.856 \( b \) | 0.821 | 0.826 | -0.005 | 0.000025 |
| 3   | AgBr  | 2.69 \( b \) | 0.850 \( b \) | 0.790 | 0.804 | -0.01 | 0.0001 |
| 4   | AgI   | 2.62 \( b \) | 0.770 \( b \) | 0.771 | 0.801 | -0.03 | 0.0009 |
| 5   | CaO   | 5.93 \( b \) | 0.913 \( b \) | 0.904 | 0.905 | -0.01 | 0.00001 |
| 6   | CdO   | 2.5 \( b \) | 0.785 \( b \) | 0.763 | 0.796 | -0.01 | 0.0001 |
| 7   | CuCl  | 3.35 \( b \) | 0.746 \( b \) | 0.813 | 0.829 | -0.01 | 0.0001 |
| 8   | CuS   | 4.10 \( b \) | 0.902 \( b \) | 0.856 | 0.855 | 0.001 | 0.000001 |
| 9   | CuBr  | 2.91 \( b \) | 0.735 \( b \) | 0.789 | 0.812 | -0.02 | 0.0004 |
| 10  | CdSe  | 1.75 \( b \) | 0.699 \( b \) | 0.696 | 0.762 | -0.06 | 0.0036 |
| 11  | CaTe  | 1.50 \( b \) | 0.894 \( b \) | 0.682 | 0.751 | -0.06 | 0.0036 |
| 12  | MgS   | 3.9 \( b \) | 0.828 \( b \) | 0.837 | 0.849 | -0.01 | 0.0001 |
| 13  | MgO   | 7.18 \( b \) | 0.841 \( b \) | 0.905 | 0.927 | -0.02 | 0.0004 |
| 14  | SrO   | 6.7 \( b \) | 0.926 \( b \) | 0.910 | 0.919 | 0.007 | 0.000049 |
| 15  | SrS   | 4.1 \( b \) | 0.914 \( b \) | 0.857 | 0.855 | 0.002 | 0.000004 |
| 16  | ZnS   | 3.68 \( b \) | 0.764 \( b \) | 0.828 | 0.841 | 0.01 | 0.0001 |
| 17  | ZnSe  | 2.70 \( b \) | 0.740 \( b \) | 0.776 | 0.804 | -0.02 | 0.0004 |
| 18  | KF    | 10 \( b \) | 0.955 \( b \) | 0.948 | 0.942 | 0.006 | 0.000036 |
| 19  | KBr   | 6.84 \( b \) | 0.952 \( b \) | 0.911 | 0.921 | -0.01 | 0.0001 |
| 20  | KCl   | 7.83 \( b \) | 0.953 \( b \) | 0.925 | 0.934 | -0.09 | 0.000081 |
| 21  | KI    | 5.89 \( b \) | 0.950 \( b \) | 0.893 | 0.903 | -0.01 | 0.0001 |
| 22  | LiF   | 13.09 \( b \) | 0.915 \( b \) | 0.970 | 0.904 | 0.01 | 0.0001 |
| 23  | LiCl  | 9.4 \( b \) | 0.903 \( b \) | 0.943 | 0.942 | 0.001 | 0.000001 |
| 24  | LiBr  | 7.6 \( b \) | 0.899 \( b \) | 0.922 | 0.932 | -0.01 | 0.0001 |
| 25  | LiI   | 5.8 \( b \) | 0.890 \( b \) | 0.891 | 0.902 | -0.01 | 0.0001 |
| 26  | NaF   | 10.7 \( b \) | 0.946 \( b \) | 0.954 | 0.938 | 0.008 | 0.000064 |
| 27  | NaCl  | 8.025 \( b \) | 0.935 \( b \) | 0.928 | 0.9366 | -0.001 | 0.000001 |
| 28  | NaBr  | 7.1 \( b \) | 0.934 \( b \) | 0.928 | 0.925 | 0.003 | 0.000009 |
| 29  | NaI   | 5.66 \( b \) | 0.927 \( b \) | 0.888 | 0.898 | -0.01 | 0.000009 |
| 30  | RbF   | 10.3 \( b \) | 0.960 \( b \) | 0.958 | 0.941 | 0.01 | 0.0004 |
| 31  | CdS   | 2.485 \( b \) | 0.794 \( b \) | 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.](image)

2.3. Exponential nonlinear method [7,8]
The estimated mathematical model is derived by
\[ I_c = a \times e^{A E_p} \]
Where \( i = 1, 2, 3, \ldots, n \), \( n = 31 \)
the rule can be written as follows
\[ A \sum_{i=1}^{n} E_p - n B = \sum_{i=1}^{n} I_c \]
(11)
\[ A \sum_{i=1}^{n} E_p^2 - B \sum_{i=1}^{n} E_p = \sum_{i=1}^{n} E_p I_c \]
(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 \( B = -0.259 \),
\[ I_c = a \times e^{A E_p} \]
We find the values of constants a and b
\[ Ln I_c = Ln a + E_p Ln b \]
Where
\[ Ln I_c = I_c, Ln b = A, Ln a = B, E_p = E_p \]
\[ b = e^L n b = A, a = e^L n a \]
\[ Ln b = (0.021) e^{L n a} = e^{0.021} b = e^{0.021} \]
\[ b = 1.021 \times a = (-0.259), a = 0.771, Ln a = B, e^{L n a} = e^{-0.259}, a = e^{-0.259} \]
\[ I_c = a \times e^{A E_p} \]
Then the approximate formula is

\[ I_c = (0.771)e^{-0.021E_p} \quad (15) \]

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

| No. | Comp. | \( E_p \) (Exp.) | \( I_c \) (Exp.) | \( I_c \) (Theo.) | \( I_c \) (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^a          | 0.913^b         | 0.904           | 0.872           | 0.03   | 0.0009  |
| 6   | CdO  | 2.8^a           | 0.785^b         | 0.763           | 0.812           | -0.02  | 0.0004  |
| 7   | CuCl | 3.35^a          | 0.746^b         | 0.813           | 0.826           | 0.01   | 0.0001  |
| 8   | CuS  | 4.10^a          | 0.902^b         | 0.856           | 0.839           | 0.01   | 0.0001  |
| 9   | CuBr | 2.91^a          | 0.735^b         | 0.789           | 0.819           | 0.03   | 0.0009  |
| 10  | CdSe | 1.751^a         | 0.699^b         | 0.696           | 0.799           | -0.1   | 0.0000  |
| 11  | CdTe | 1.50^a          | 0.682^b         | 0.795           | 0.975           | -0.09  | 0.0001  |
| 12  | MgS  | 3.9^a           | 0.828^b         | 0.837           | 0.836           | 0.001  | 0.000001|
| 13  | MgO  | 7.16^a          | 0.841^b         | 0.905           | 0.894           | 0.01   | 0.0001  |
| 14  | SrO  | 6.7^a           | 0.926^b         | 0.910           | 0.886           | 0.02   | 0.0004  |
| 15  | SrS  | 4.1^a           | 0.914^b         | 0.857           | 0.839           | 0.01   | 0.0001  |
| 16  | ZnS  | 3.68^a          | 0.764^b         | 0.828           | 0.832           | -0.004 | 0.000016|
| 17  | ZnSe | 2.70^a          | 0.740^b         | 0.776           | 0.815           | -0.03  | 0.0009  |
| 18  | KF   | 10^d            | 0.955^e         | 0.948           | 0.949           | -0.001 | 0.000001|
| 19  | KBr  | 6.840^d         | 0.952^e         | 0.911           | 0.888           | 0.02   | 0.0004  |
| 20  | KCl  | 7.834^d         | 0.953^e         | 0.925           | 0.907           | 0.01   | 0.0001  |
| 21  | KI   | 5.890^d         | 0.950^e         | 0.893           | 0.871           | 0.02   | 0.0004  |
| 22  | LiF  | 13.09^d         | 0.915^e         | 0.970           | 0.912           | -0.04  | 0.0016  |
| 23  | LiCl | 9.4^d           | 0.903^e         | 0.943           | 0.937           | 0.006  | 0.000036|
| 24  | LiBr | 7.6^d           | 0.899^e         | 0.922           | 0.902           | 0.003  | 0.000009|
| 25  | LiI  | 5.8^d           | 0.890^e         | 0.891           | 0.869           | 0.02   | 0.0004  |
| 26  | NaF  | 10.70^d         | 0.946^e         | 0.954           | 0.963           | -0.009 | 0.000081|
| 27  | NaCl | 8.025^d         | 0.935^e         | 0.928           | 0.910           | 0.01   | 0.0001  |
| 28  | NaBr | 7.1^d           | 0.934^e         | 0.928           | 0.893           | 0.04   | 0.0016  |
| 29  | NaI  | 5.666^d         | 0.927^e         | 0.888           | 0.867           | 0.02   | 0.0004  |
| 30  | RbF  | 10.3^d          | 0.960^e         | 0.958           | 0.955           | 0.003  | 0.000009|
| 31  | CdS  | 2.485^d         | 0.794^e         | 0.762           | 0.811           | -0.01  | 0.0001  |

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

3. Statistical nonlinear regression methods

By applying the statistical nonlinear regression method, we take three kinds of methods; first method is logarithmic nonlinear regression, second method is quadratic nonlinear regression and third method is cubic nonlinear regression.[15]

3.1. Logarithm nonlinear regression:[16,17]

The estimated mathematical model is derived by

\[ \text{Ln } I_c = \text{Ln } A + B \text{ Ln } E_p \quad (16) \]

Where \( a = 0.716, b=0.098 \), In SPSS

A,B constant

\[ \text{Ln } I_c = \text{Ln } I_c - \text{Ln } I_c = \text{Ln } (0.716) + 0.098 \text{ Ln } E_p. \]

Then the approximate formula is

\[ \text{Ln } I_c = \text{Ln } A + B \text{ Ln } E_p \quad (17) \]

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

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

![Graph showing comparison between experimental and theoretical ionicity factor values](image)
The estimated mathematical model is derived by
\[ I_c = a + b_1 E_p + b_2 E_p^2 \] (18)

Then the approximate formula is
\[ I_c = 0.690 + 0.050 E_p + (-0.002) E_p^2 \] (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 $I_i$ (Det.) in Terms of $E_p$ with the Exp. and Theo.

| No. | Comp. | $E_p$ (Exp.) | $I_i$ (Exp.) | $I_i$ (Theo.) [2] | Error | Error ^2 |
|-----|-------|-------------|-------------|-------------------|-------|---------|
| 1   | AgF   | 2.84        | 0.894       | 0.80              | 0.81  | 0.01    |
| 2   | AgCl  | 3.249       | 0.856       | 0.821             | 0.83  | 0.009   |
| 3   | AgBr  | 2.694       | 0.850       | 0.790             | 0.81  | -0.02   |
| 4   | AgI   | 2.621       | 0.770       | 0.771             | 0.81  | 0.03    |
| 5   | CuO   | 5.934       | 0.913       | 0.904             | 0.92  | 0.007   |
| 6   | CdO   | 2.5        | 0.785       | 0.763             | 0.80  | -0.01   |
| 7   | CuCl  | 3.347       | 0.746       | 0.813             | 0.84  | 0.02    |
| 8   | CaS   | 4.103       | 0.902       | 0.856             | 0.86  | 0.004   |
| 9   | CuBr  | 2.914       | 0.735       | 0.789             | 0.82  | 0.03    |
| 10  | CsCl  | 1.751       | 0.699       | 0.696             | 0.77  | 0.07    |
| 11  | CaTe  | 1.596       | 0.894       | 0.682             | 0.76  | 0.07    |
| 12  | MgS   | 3.9        | 0.828       | 0.837             | 0.85  | 0.01    |
| 13  | MgO   | 7.16       | 0.841       | 0.905             | 0.95  | -0.04   |
| 14  | SrO   | 6.7        | 0.926       | 0.910             | 0.94  | 0.01    |
| 15  | SrS   | 4.146       | 0.914       | 0.857             | 0.86  | 0.003   |
| 16  | ZnS   | 3.646       | 0.764       | 0.828             | 0.85  | 0.02    |
| 17  | ZnSe  | 2.707       | 0.740       | 0.776             | 0.81  | 0.03    |
| 18  | KF    | 10         | 0.955       | 0.948             | 0.99  | 0.03    |
| 19  | KBr   | 6.846      | 0.952       | 0.911             | 0.94  | 0.01    |
| 20  | KCl   | 7.834      | 0.953       | 0.925             | 0.96  | 0.007   |
| 21  | KI    | 5.890      | 0.950       | 0.893             | 0.92  | 0.02    |
| 22  | LiF   | 13.096     | 0.915       | 0.970             | 1.00  | -0.03   |
| 23  | LiCl  | 9.44       | 0.903       | 0.943             | 0.98  | 0.03    |
| 24  | LiBr  | 7.64       | 0.899       | 0.922             | 0.95  | 0.02    |
| 25  | Li    | 5.84       | 0.890       | 0.891             | 0.91  | 0.01    |
| 26  | NaF   | 10.706     | 0.946       | 0.954             | 1.00  | 0.04    |
| 27  | NaCl  | 8.025      | 0.936       | 0.928             | 0.96  | 0.02    |
| 28  | NaBr  | 7.13       | 0.934       | 0.928             | 0.94  | 0.006   |
| 29  | NaI   | 5.666      | 0.927       | 0.888             | 0.91  | 0.01    |
| 30  | RbF   | 10.34      | 0.960       | 0.958             | 0.99  | -0.03   |
| 31  | CdS   | 2.4855     | 0.794       | 0.762             | 0.80  | 0.006   |

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.

![Graph showing comparison between experimental and theoretical data for iconicity factor values.](image)

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

$$I_i = a + b_1E_p + b_2E_p^2 + b_3E_p^3$$

(20)

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

Then the approximate formula is

$$I_i = 0.721 + 0.031E_p^2 + 0.000E_p^3$$

(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.) | Error | Error^2 |
|-----|-------|--------------|--------------|---------------|-------|---------|
| 1   | AgF   | 2.84         | 0.894        | 0.80          | 0.02  | 0.0004  |
| 2   | AgCl  | 3.249        | 0.856        | 0.821         | 0.03  | 0.00081 |
| 3   | AgBr  | 2.69         | 0.850        | 0.790         | 0.02  | 0.0004  |
| 4   | AgI   | 2.62         | 0.770        | 0.771         | 0.03  | 0.0009  |
| 5   | CaO   | 5.93         | 0.913        | 0.904         | 0.02  | 0.0004  |
| 6   | CdO   | 2.53         | 0.785        | 0.763         | 0.01  | 0.0001  |
| 7   | CuCl  | 3.35         | 0.746        | 0.813         | 0.02  | 0.0004  |
| 8   | CuS   | 4.10         | 0.902        | 0.856         | 0.04  | 0.0016  |
| 9   | CuBr  | 2.91         | 0.735        | 0.789         | 0.03  | 0.0009  |
| 10  | CdSe  | 1.75         | 0.699        | 0.696         | 0.08  | 0.0064  |
| 11  | CaTe  | 1.50         | 0.894        | 0.682         | 0.08  | 0.0064  |
| 12  | MgS   | 3.99         | 0.828        | 0.837         | 0.02  | 0.0004  |
| 13  | MgO   | 7.16         | 0.841        | 0.905         | 0.09  | 0.0064  |
| 14  | SrO   | 6.75         | 0.919        | 0.910         | 0.04  | 0.0016  |
| 15  | SrS   | 4.10         | 0.914        | 0.857         | 0.03  | 0.0009  |
| 16  | ZnS   | 3.68         | 0.764        | 0.828         | 0.02  | 0.0004  |
| 17  | ZnSe  | 2.70         | 0.740        | 0.776         | 0.03  | 0.0009  |
| 18  | KF    | 10.0         | 0.955        | 0.948         | 1.13  | 0.01    |
| 19  | KBr   | 6.840        | 0.952        | 0.911         | 0.02  | 0.000004|
| 20  | KCl   | 7.834        | 0.953        | 0.925         | 1.07  | 0.0049  |
| 21  | KI    | 5.890        | 0.950        | 0.893         | 0.01  | 0.0001  |
| 22  | LiF   | 13.09        | 0.915        | 0.970         | 1.30  | 0.09    |
| 23  | LiCl  | 9.40         | 0.903        | 0.943         | 1.10  | 0.01    |
| 24  | LiBr  | 7.65         | 0.899        | 0.922         | 1.01  | 0.0064  |
| 25  | LiI   | 5.89         | 0.890        | 0.891         | 0.03  | 0.0001  |
| 26  | NaF   | 10.70        | 0.946        | 0.954         | 1.17  | 0.04    |
| 27  | NaCl  | 8.025        | 0.935        | 0.928         | 1.03  | 0.09    |
| 28  | NaBr  | 7.10         | 0.934        | 0.928         | 0.99  | 0.0025  |
| 29  | NaI   | 5.666        | 0.927        | 0.888         | 0.93  | 0.00009 |
| 30  | RbF   | 10.3         | 0.960        | 0.958         | 1.15  | 0.1     |
| 31  | CsS   | 2.485        | 0.794        | 0.762         | 0.80  | 0.00036 |

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.](image)

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 mathematical models, 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.

References

[1] Pisani, C., Dovesi, R., & Roetti, C. (1988). Different Approaches to the Study of the Electronic Properties of Periodic Systems. In Hartree - Fock ab initio treatment of crystalline systems (pp. 1-33). Springer Berlin Heidelberg
[2] Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). Principles of instrumental analysis. Cengage learning.
[3] Wold, S., Ruhe, A., Wold, H., & Dunn, III, W. J. (1984). The collinearity problem in linear regression. The partial least squares (PLS) approach to generalized inverses. SIAM Journal on Scientific and Statistical Computing, 5(3), 735-743.
[4] Arif, G. E., Abdullah, F. A., & Al-Douri, Y. (2014). Modeling of the Electronic Properties of Hexagonal Semiconductors. Advanced Materials Research Vol. 925, pp. 364-368.
[5] William L. Oberkampf, Christopher J. Roy. “Verification and Validation in Scientific Computing”. Cambridge University Press. 2010.
[6] Arif, G. E., Al-Douri, Y. “Mathematical Modeling of Physical Properties for Hexagonal Binaries”. Scholar’s Press, Germany. 2016.
Sastry S. (2012). PHI Learning Pvt. I. td., "Introductory Methods of Numerical Analysis "

[8] أميل صبيحي سعد شكر الله (2001), التحليل العددي التطبيقي, النظرية – القيادات والطرق التقريرية, المطبعة مؤسسة بيتر للطباعة والتوريدات - القاهرة- مصر

[9] Grundmann, M. (2010). The physics of semiconductors: an introduction including nanophysics and applications (2nd ed.). New York: Springer-Verlag.

[10] Senthil, J K., Tak, Y., Seol, M., & Yong, K. (2009). Synthesis and Characterization of ZnO Nanowire – CdO Composite Nanostructures, Nanoscale Research Letters 4, 1329-1334.

[11] Palik, E. D. (1991). Handbook of optical constants of solids II. New York: Academic Press.

[12] Schröer, P., Krüger, P., & Pollmann, J. (1993). First-principles calculation of the electronic structure of the wurtzite semiconductors ZnO and ZnS. Physical Review B, 47(12), 6971-6980.

[13] Niesert, M. (2011). Ab initio calculations of spin-wave excitation spectra from time-dependent density - functional theory (Vol.38). Forschungszentrum Jülich.

[14] Reshak, A. H. (2013). Crystals structure, linear and nonlinear optical susceptibilities. Malaysia: Universiti Malaysia Perlis.

[15] Nelles, O. (2013). Nonlinear system identification: from classical approaches to neural networks and fuzzy models. Springer Science & Business Media.

[16] Douglas C. Montgomery, (2012) ,by John Wiley, and Sons, Inc " Introduction to Linear Regression analysis.

[17] أموري هادي كاظم الحسناوي (2002)، طرق القياس الاقتصادي , دار وائل للنشر - عمان – الأردن.

استخدام طرق المربعات الصغرى وطرق الانحدار الغير خطية لحساب القيمة التقديرية للتأين بدالة فجوة الطاقة

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الملخص

الهدف من البحث إيجاد أفضل النماذج الرياضية لحساب القيمة التقديرية لمقدار التأين للمركبات الفيزيائية لأشباه الموصلات بالاعتماد على فجوة الطاقة باستخدام بعض طرق التحليل العددي كطريقة المربعات الصغرى وحصولنا على أحسن فروعها طريقة معادلة معقدة الحدود اللاخطية من الدرجة الثانية وقارنا النتائج الجديدة مع الطرق الأخرى وحصلنا على طرق أخرى أكثر كفاءة ومن جهة أخرى استخدمنا بعض طرق التحليل الإحصائي كطريقة الإنحدار وحصلنا على أحسن فروعها نموذج الإنحدار اللاخطي التربيعي.