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Empirical Model for Accurate Bandgap Prediction in Cubic Solids

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Authors' contributions

This work was carried out in collaboration between both authors. Author AIP designed the study, wrote the protocol and wrote the first draft of the manuscript. Author BSF managed the analyses of the study. Both authors read and approved the final manuscript.

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ABSTRACT

An empirical model is developed and tested on cubic solids for the calculation of bandgaps. The dataset for the model is derived from a semi-local approximation in which the local density approximation (LDA) treats the exchange-correlation energy and potential. The agreement between obtained result and experimental data is very good and is of the same order as the more expensive methods.

Keywords: Semi-local approximation; exchange-correlation energy; bandgap; cubic solids.

1. INTRODUCTION

Materials play important roles in our quality of live and survival. Human existence had witnessed progressive development from the Stone Age, till this present silicon age. The capacity to make available different material types has helped to shape the different level of developments witnessed at these times. In the early years, material investigation and development was majorly through the traditional 'trial by error' approach. Over time, the adoption of multidisciplinary approach to materials investigation and synthesis had proved a

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productive route. The role of statistical and quantum mechanics at describing any material composition down to the atomic level can't be overemphasized. One of the most successful statistical and quantum mechanics based tool used by material scientist today is the Density Functional Theory (DFT). It has demonstrated acceptable role in complementing new materials development efforts.

Most DFT calculations use semi-local approximation such as the local-density approximation (LDA) [1,2] or the generalized gradient approximation (GGA) [3]. The semi-local approximations are computationally cheap compared to the more sophisticated methods. They have shown capacity for results that are accurate enough for predictions and have in some cases helped to interpret experimental data better. Their application to solids has not yield acceptable results in all cases. As an example, the LDA and GGA will accurately predict structural as well as the energetic properties of molecular species and periodic solids but will severely underestimate the band gap of semiconductors and insulators.

A large share of today's technological advancement is semiconductor dependent. Semiconductors are materials with band gap, which needs to be properly characterized prior to synthesis and fabrication. The LDA-DFT will underestimate bandgap by as much as 37.90% while its GGA-DFT counterpart will underestimate bandgap by a whopping 47.09%. In pursuit of better band gap estimation/prediction, other methods had been developed. The first among these alternative methods is the optimized effective potential (OEP) method. Its performance had showed mixed results, with better band gap prediction in some instances and strong underestimation or overestimation in others [4,5]. Another better method is the LDA + U, which is a variant of DFT with on-site Coulomb self-interaction potentials [6]. The method (LDA + U) is as cheap as the semi-local approximations, but only applies to localized electrons. A much more improved method is the hybrid functionals (HSE), which have shown success in many classes of solids. It is however computationally expensive [7,8]. The DFT plus Dynamic Mean Field Theory (DFT + DMFT) method is known to give accurate results but it is a more significantly expensive calculations [9]. The *GW* is a method known to yield very accurate band gaps, but with highly expensive calculations [10–15]. The modified Becke and Johnson (mBJ) exchange potential [16] is capable of yielding band gaps with accuracies comparable to those from more expensive schemes.

The need for necessary platforms (hardware and software) for electronic structure calculations can't be overemphasized. The deployment of expensive platforms for individuals or institution with meager resources can hamper, if not totally make the conduct of qualitative research a mirage. With the availability of fast personal computers (PC's) and open source ab initio DFT codes, the need to contribute creditably to ongoing research efforts in the materials science community shouldn't become jeopardized on the account of lack of affordable tools. It is in this light that a much less expensive way of calculating more precisely the fundamental bandgap of cubic semiconductors and insulators using an empirical model and LDA-DFT generated data are discussed.

2. METHODOLOGY

A multiple regression method is chosen for developing the model. Multiple regression, refer to set of techniques for studying the straight-line relationships among two or more variables [17]. The equation to be evaluated is of the form:

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \ldots + \beta_p X_{pi} + \epsilon_i \qquad (1.1)$$

where X_i is the independent variables and Y_i is the dependent variable. The subscript i represents the observation (row) number. The β_S are the unknown regression coefficients while ϵ_i is the error/residual of observation for the ith dataset. To obtain the unknown regression coefficients, the least squares analysis method is used, where the relationship between a dependent variable and p independent variables can be written as:

$$\hat{y}_j = b_0 + b_1 x_{1i} + b_2 x_{2i} + \ldots + b_p x_{pi} \qquad (1.2)$$

with the $b's$ selected to minimize the sum of the squared residuals.

In matrix form, (1.1) can be written as:

$$\begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_i \end{pmatrix} = \begin{bmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1p} \\ 1 & X_{21} & X_{22} & \cdots & X_{2p} \\ 1 & X_{31} & X_{23} & \cdots & X_{3p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{i1} & X_{i2} & \cdots & X_{ip} \end{bmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \vdots \\ \epsilon_i \end{pmatrix} \qquad (1.3)$$

The values of b as an estimate of β can be obtained by solving the normal equations as follows;

$$X'Xb = X'Y \tag{1.4}$$

Where

$$b = \left(X'X\right)^{-1}\left(X'Y\right) \tag{1.5}$$

and $X'X$ is:

$$\begin{bmatrix} n & \sum X_{i1} & \sum X_{i2} & \cdots & \sum X_{ip} \\ \sum X_{i1} & \sum X_{i1}^2 & \sum X_{i1}X_{i2} & \cdots & \sum X_{i1}X_{ip} \\ \sum X_{i2} & \sum X_{i1}X_{i2} & \sum X_{i2}^2 & \cdots & \sum X_{i2}X_{ip} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum X_{ip} & \sum X_{i1}X_{ip} & \sum X_{i2}X_{ip} & \cdots & \sum X_{ip}^2 \end{bmatrix} \tag{1.6}$$

With

$$X'Y = \begin{pmatrix} \sum Y_i \\ \sum X_{i1}Y_i \\ \sum X_{i2}Y_i \\ \vdots \\ \sum X_{ip}Y_i \end{pmatrix} \tag{1.7}$$

thus,

$$b = \begin{bmatrix} n & \sum X_{i1} & \sum X_{i2} & \cdots & \sum X_{ip} \\ \sum X_{i1} & \sum X_{i1}^2 & \sum X_{i1}X_{i2} & \cdots & \sum X_{i1}X_{ip} \\ \sum X_{i2} & \sum X_{i1}X_{i2} & \sum X_{i2}^2 & \cdots & \sum X_{i2}X_{ip} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum X_{ip} & \sum X_{i1}X_{ip} & \sum X_{i2}X_{ihp} & \cdots & \sum X_{ip}^2 \end{bmatrix}^{-1} \begin{pmatrix} \sum Y_i \\ \sum X_{i1}Y_i \\ \sum X_{i2}Y_i \\ \vdots \\ \sum X_{ip}Y_i \end{pmatrix} \tag{1.8}$$

After solving (1.8), the values of $b's$ are substituted into (1.2).

The input datasets needed to develop the model are given in Table 1.

These datasets (LP (X_{i2}) and LDA E_g (X_{i3})) are obtained using the Quantum Espresso (QE) DFT code [18]. Based on the input datasets, all other statistical data needed to evaluate the $b's$ as an estimate of $\beta's$ are given in Table 2.

From Table 2, $\sum X_{i2} = 146.0897$, $\sum X_{i3} = 22.1757$, $\sum Y_i = 36.767$, $\sum X_{i2}^2 = 1561.6174$, $\sum X_{i3}^2 = 69.498$, $\sum X_{i2}X_{i3} = 201.6091$, $\sum X_{i2}Y_i = 338.3608$, $\sum X_{i3}Y_i = 109.7854$.

Inserting these values into (1.8), it becomes:

$$\begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 14 & 146.0897 & 22.1757 \\ 146.0897 & 1561.6174 & 201.6091 \\ 22.1757 & 201.6091 & 69.4985 \end{bmatrix}^{-1} \begin{bmatrix} 36.767 \\ 338.3608 \\ 109.7854 \end{bmatrix} \tag{1.9}$$

$$\begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 12.42933 & -1.04039 & -0.94788 \\ -1.04039 & 0.088109 & 0.076372 \\ -0.94788 & 0.076372 & 0.095292 \end{bmatrix} \begin{bmatrix} 36.767 \\ 338.3608 \\ 109.7854 \end{bmatrix} \tag{1.10}$$

$$\begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 0.897341 \\ -0.05476 \\ 1.452197 \end{bmatrix} \tag{1.11}$$

The estimated regression equation is obtained by substituting b_0, b_1 and $b_2$into (1.2), leading to:

$$\hat{y}_i = 0.897341 - 0.05476X_{i2} + 1.452197X_{i3} \tag{1.12}$$

Table 1. QE derived Lattice Parameter (LP (X_{i2})) and Bandgap (LDA E_g (X_{i3})) alongside experimental bandgap data (Expt. E_g (Y_i)

S/N	Materials	LP (X_{i2})	LDA E_g (X_{i3})	Expt. E_g (Y_i)
1	AlSb	11.5991	1.2238	1.686
2	GaAs	10.6068	0.9173	1.519
3	InAs	11.4011	0.3483	0.414
4	InP	11.0078	0.8886	1.424
5	GaSb	11.4038	0.4207	0.811
6	MgO	7.8051	5.4092	7.83
7	ZnSe	10.5792	1.4286	2.825
8	$SrTiO_3$	7.203	2.0214	3.3
9	GaP	10.2038	1.5133	2.339
10	CdS	10.9949	1.0554	2.583
11	CdSe	11.3971	0.6797	1.846
12	InSb	12.1998	0.3465	0.234
13	CdTe	12.2001	0.8215	1.606
14	CsCl	7.4881	5.1014	8.35

Table 2. Estimated linear multiple regression for the Lattice Parameter (LP (X_{i2})), Bandgap (LDA E_g (X_{i3})) and the experimental bandgap (Expt. E_g (Y_i)

S/N	X_{i2}	X_{i3}	Y_i	X_{i2}^2	X_{i3}^2	$X_{i2}X_{i3}$	$X_{i2}Y_i$	$X_{i3}Y_i$
1	11.5991	1.2238	1.686	134.5391	1.497686	14.19498	19.5560826	2.0633268
2	10.6068	0.9173	1.519	112.5042	0.841439	9.729618	16.1117292	1.3933787
3	11.4011	0.3483	0.414	129.9851	0.121313	3.971003	4.7200554	0.1441962
4	11.0078	0.8886	1.424	121.1717	0.78961	9.781531	15.6751072	1.2653664
5	11.4038	0.4207	0.811	130.0467	0.176988	4.797579	9.2484818	0.3411877
6	7.8051	5.4092	7.83	60.91959	29.25944	42.21935	61.113933	42.354036
7	10.5792	1.4286	2.825	111.9195	2.040898	15.11345	29.88624	4.035795
8	7.203	2.0214	3.3	51.88321	4.086058	14.56014	23.7699	6.67062
9	10.2038	1.5133	2.339	104.1175	2.290077	15.44141	23.8666882	3.5396087
10	10.9949	1.0554	2.583	120.8878	1.113869	11.60402	28.3998267	2.7260982
11	11.3971	0.6797	1.846	129.8939	0.461992	7.746609	21.0390466	1.2547262
12	12.1998	0.3465	0.234	148.8351	0.120062	4.227231	2.8547532	0.081081
13	12.2001	0.8215	1.606	148.8424	0.674862	10.02238	19.5933606	1.319329
14	7.4881	5. 5.1014	8.35	56.07164	26.02428	38.19979	62.5256	42.59669
Total	146.0897	22.1757	36.767	1561.6174	69.4985	201.6091	338.3608	109.7854

where $\hat{y}_i$ is the predicted bandgap, X_{i2} is the calculated lattice parameter and X_{i3} is the calculated bandgap. On a general note, (1.12) can be expressed as:

$$\hat{y}_i = 0.897341 - 0.05476X_{i2} + 1.452197X_{i3} + \epsilon_i \quad (1.13)$$

where the residual (ϵ_i) of the model is determined as:

$$\epsilon_i = y_i - \hat{y}_i \quad (1.14)$$

The residual and other indices calculated for each input dataset are given in Table 3.

The reliability (R^2), of (1.13) can be evaluated using:

$$R = \sqrt{\frac{S_t - S_r}{S_t}} = \sqrt{1 - \frac{S_r}{S_t}} \quad (1.15)$$

with $S_t = \sum_{i=1}^{n}\left(Y_i - \acute{Y}\right)^2$, $S_r = \sum_{i=1}^{n} e_i^2$ and

$$\acute{Y} = \frac{\sum Y_i}{n} = \frac{36.767}{14} = 2.626214 \quad (1.16)$$

$$R^2 = 1 - \frac{2.198\ 124}{79.5\ 35\ 37} = 0.972363 \quad (1.17)$$

The result in (1.17) indicates that the regression model has ~97% fit with the data used.

Table 3. Estimated residual and other values for the lattice parameters, LDA bandgap and experimental bandgaps

S/N	LDA E_g (X_{i3})	Expt. E_g (Y_i)	Predicted E_g $(\hat{y}_j)$	Residuals (ϵ_i)	ϵ_i^2	$Y_i - \acute{Y}$	$\left(Y_i - \acute{Y}\right)^2$
1	1.2238	1.686	2.0393	0.3533840	0.12488029	-0.940214	0.884002366
2	0.9173	1.519	1.6486	0.1296249	0.01680262	-1.107214	1.225922842
3	0.3483	0.414	0.7788	0.3648306	0.13310143	-2.212214	4.893890782
4	0.8886	1.424	1.5849	0.1609882	0.02591720	-1.202214	1.445318502
5	0.4207	0.811	0.8838	0.0728216	0.00530299	-1.815214	3.295001866
6	5.4092	7.83	8.3251	0.4951562	0.24517972	5.203786	27.07938873
7	1.4286	2.825	2.3926	-0.4323568	0.18693248	0.198786	0.039515874
8	2.0214	3.3	3.4383	0.1383844	0.01915024	0.673786	0.453987574
9	1.5133	2.339	2.5362	0.1972008	0.03888817	-0.287214	0.082491882
10	1.0554	2.583	1.8279	-0.7550794	0.57014493	-0.043214	0.00186745
11	0.6797	1.846	1.2603	-0.5856931	0.34303650	-0.780214	0.608733886
12	0.3465	0.234	0.7324	0.4984799	0.24848223	-2.392214	5.722687822
13	0.8215	1.606	1.4222	-0.1837443	0.03376198	-1.020214	1.040836606
14	5.1014	8.35	7.8955	-0.4544701	0.20654310	5.723786	32.76172617
Total		**36.767**			**2.198124**		**79.53537**

Table 4. Theoretical and experimental band gaps (in eV). The structure is indicated in parenthesis. For comparison, results from the literature which were obtained by other methods (mBJ, HSE03, HSE06, G_0W_0, and *GW*) are also shown. The experimental values were taken from Refs. [7,8,11,15,19–21]

Solid	LDA	mBJ	HSE	*GW*	G_0W_0	Expt.	This Work
Si (A4)	0.569	1.17[a]	1.28[b]	1.41[d]	1.12[e]	1.17	1.17
Ge (A4)	0.164	0.85[a]	0.83[b]	0.95[d]	0.66[f]	0.74	0.55
AlP (B3)	1.509	2.32[a]	2.51[b]	2.90[d]	2.44[e]	2.45	2.53
MgO (B1)	5.409	7.17[a]	6.67[b]	9.16[d]	7.25[e]	7.83	8.33
ZnS (B3)	2.287	3.66[a]	3.49[b]	4.15[d]	3.29[e]	3.91	3.67
ZnO (B1)	1.294	2.68[a]	2.49[c]	3.80[d]	2.51[f]	3.44	2.34
CdS (B3)	1.055	2.66[a]	2.25[b]	2.87[d]	2.06[e]	2.42	1.83
GaAs (B3)	0.917	1.64[a]	1.12[b]	1.85[d]	1.30[e]	1.52	1.65
GaP (B3)	1.513	-	-	-	-	2.32	2.54
GaSb (B3)	0.421	-	-	-	-	0.81	0.88
CdSe (B3)	0.680	-	-	-	-	1.84	1.26
CdTe (B3)	0.822	-	-	-	-	1.61	1.42

[a]mBJ Ref. [16]. [b]HSE03 [7]. [c]HSE06 [22]. [d]Reference [15]. [e]Reference [14]. [f]Reference [12]

3. RESULTS AND DISCUSSION

The results obtained using the model, alongside data from other sophisticated calculations are given in Table 4. For Si (A4 structure), the percentage difference between experimental data and the traditional LDA is 51.4%. It is 9.4% for HSE, 20.5% (*GW*), 4.27% (G_0W_0), 0% (mBJ) and also 0% for the newly developed model. The result for Ge (also A4 structure) shows percentage difference of 77.8% between experimental data and LDA while it is 12.2% (HSE), 28.4% (*GW*), 10.8% (G_0W_0), 14.9% (mBJ) and the model 25.7%. The compound AlP (B3) belongs to the zinc blende cubic structure. The difference between its experimental data and LDA is 38.4%. It is 2.4% for HSE, 18.44% (*GW*), 0.4% (G_0W_0), 5.3% (mBJ) and 3.3% for the developed model. GaAs is another compound with the B3 structure. The percentage difference between its experimental bandgap and the theoretical predicted LDA is 39.7%. It is 26.3% (HSE), 21.7% (*GW*), 14.5% (G_0W_0), 7.9% (mBJ) and 8.6% for the developed model. The experimental bandgap for MgO is 7.83 eV. It is an insulator with the B1 structure. The predicted bandgap using the model is 8.33 eV (difference = 6.38%). The difference is 14.8% (HSE), 17% (*GW*), 7.4% (G_0W_0), 8.4% (mBJ) and 30.9% (LDA). ZnO is another compound with the B1 structure. Its experimental bandgap is 3.44 eV. The percentage difference between this experimental bandgap and LDA derived bandgap for ZnO is 62.4%. It is 32% for the newly developed model, 22.1% (mBJ), 27.6% (HSE), 10.5% (*GW*) and 27% for G_0W_0.

4. CONCLUSION

The calculation of the electronic structure requires the use of exchange-correlation potential within the Kohn-Sham equation. An exchange-correlation potential that depends solely on semi-local quantities is found to give poor band gaps in semiconductors and insulators. While the majority of ab initio DFT codes available to material scientist rely on semi-local dependent exchange-correlation potential, the more accurate methods/codes are very expensive. The summary is that accurate band gaps can be obtained in semiconductors and insulators with an exchange-correlation potential that depends solely on semilocal quantities. The accuracy of the obtained result compared with the expensive hybrid and *GW* methods shows that the proposed model can lead to calculations that are cheap (requires no additional investment on hardware and software) and thus can be applied to cubic systems in an efficient manner. Although, the present work had focused on cubic lattices, its extension to other material systems remains an interesting adventure.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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