

Chapter 3

Estimation of Lattice Constant and Bulk Modulus of Materials: III-V (III-N, III-P), II-VI (BeX, MgX, CdX: X= O, S, Se, Te)

3.1 Introduction

In solids, all the electronic and optical properties depend primarily on lattice parameters. Thus an efficient determination of the lattice constant is necessary for an exact determination of the other properties. For computing the properties of a material the following three approaches are generally used by the researchers:

- (i) Calculating properties with experimentally determined lattice parameters and atomic positions.
- (ii) Performing the computation with experimental lattice constant and theoretically optimized atomic positions.
- (iii) Calculating the properties at optimized atomic position and lattice constants.

Among these the last one is considered to be the most suitable for theoretical prediction of properties as being ab-initio approach in real sense without using experimental results. In DFT based computational methods, as the accuracy in results obtained depends primarily upon the exchange correlation functional chosen. As already discussed in first chapter, there exist no universal functional which is optimum for all types of materials. Therefore, we have to make the testing of the various functionals in order to describe the desired behavior of a give class of materials. Hybrid functionals [1,2] are known for a better description of solids, however the high computational cost make them difficult to be used for large systems. Thus local and semilocal functionals are still considered to be the better choice for calculating the ground state properties of solids. In this chapter we report the calculated equilibrium lattice constants and bulk modulus of all the materials under study using the five different functionals i.e. LDA, PBE, WC, PBEsol and SCAN. This chapter contains four sections. In the first section the general introduction is given, the second section contains the method adopted and computational details. In third section all calculated lattice parameter and bulk modulus are presented along with the various statistical quantities used to test the performance of functionals. In addition the comparison with

other reported results are also discussed. In the last the conclusions are made in the fourth section.

3.2 Computational details

WIEN2k [3] code was used for calculating the lattice constants and bulk properties of all the materials under study. However, In order to get the good converged lattice constants, the calculations were tested for different k-meshes in Brillouin zone and size of the basis set given by Rk_{\max} , where R is the radius of the smallest muffin tin sphere and K_{\max} is largest K vector. The exchange correlation functional used are XC functionals used are LDA [4], PBE [5,6], WC[7], PBEsol [8], SCAN [9]. For CdX (X=O, S, Se, Te), in order to minimize the linearization error and to make the equilibrium lattice constant to be independent of the radius of the muffin tin sphere we included the local orbital depending upon the second order energy derivative of radial wave function, as suggested by Tran[10].

For optimization of lattice constants, we started with an assumed starting guess of the volume of the unit cell (experimental reported). Then the total energy was calculated as a function of the unit cell and was fitted to Murnaghan equation of state to find the ground state parameters [11].

$$E(V) = E_0 + \frac{B_0}{B_0'(B_0-1)} \left[B_0' \left(1 - \frac{V_0}{V} \right) + \left(\frac{V_0}{V} \right)^{B_0'} - 1 \right] \quad (3.1)$$

Here E_0 , B_0 , B_0' , V_0 are the fitted such that $E(V)$ from above equation (3.1) matches the calculated total energy at different volumes. From the fitted curve the volume corresponding to minimum value of total energy was obtained. The optimized volume so obtained was then used to get the optimized lattice constant. For assessing the performance of functionals, the following statistical quantities have been used: mean error (ME), mean absolute error (MAE), mean relative errors (MRE in %), mean absolute relative error (MARE in %).

3.3 Results and discussion

The optimized lattice parameters obtained with different approximations are shown in table 3.1 with respective errors ME, MAE, MRE and MARE in various calculations written at the bottom of the table. The calculated results are also shown

graphically in fig 3.1 in which the inclined straight line represents the experimental values while calculated parameters by different symbols.

Table 3.1: Equilibrium lattice parameters (in Å) of semiconductors included in our study, calculated with LDA, PBE, WC and PBEsol along with Experimental values.

Material		LDA	PBE	WC	PBEsol	SCAN	Expt.	optB88vdWc [17]
WZInN	a	3.5073	3.5852	3.5421	3.5408		3.545 ¹²	
	c	5.6689	5.7916	5.7226	5.7191		5.703 ¹²	
ZBInN	a	4.9461	5.0545	4.9942	4.9921		4.98 ¹²	
WZAlN	a	3.0908	3.132	3.1142	3.1151		3.112 ¹²	
	c	4.9478	5.0219	4.9874	4.987		4.982 ¹²	
ZBAlN	a	4.3467	4.4064	4.38	4.3809		4.38 ¹²	
WZGaN	a	3.1593,3.154*	3.2219	3.1893	3.1884		3.189 ¹²	
	c	5.1497,5.118*	5.248	5.1964	5.1939		5.185 ¹²	
ZBGaN	a	4.4619,4.489*	4.5512	4.5073	4.5058		4.5 ¹²	
ZBGaP		5.4105	5.5221	5.4564	5.4558	5.4493	5.451 ¹³	5.499
ZBAlP		5.4434	5.5171	5.4778	5.479	5.4749	5.463 ¹³	5.514
ZBInP		5.8445	5.9749	5.8955	5.8951	5.8939	5.869 ¹³	5.955
ZBBP		4.4954	4.5528	4.5255	4.5245	4.5256	4.538 ¹³	4.554
ZBBeS		4.8023	4.882	4.846	4.843	4.867	4.862 ¹⁴	4.871
ZBBeSe		5.082	5.178	5.133	5.129	5.152	5.14 ¹⁴	5.168
ZBBeTe		5.556	5.665	5.61	5.605	5.641	5.56 ¹⁴	5.659
WZBeO	a	2.666	2.713	2.694	2.693	2.688	2.698 ¹⁴	2.713
	c	4.331	4.44	4.372	4.376	4.361	4.277 ¹⁴	4.406
RSMgO		4.164	4.259	4.22	4.219	4.194	4.218 ¹³	4.228
RSMgS		5.131	5.231	5.189	5.183	5.19	5.203 ¹⁵	5.211
RSMgSe		5.392	5.509	5.457	5.45	5.465	5.47 ¹⁵	5.478
WZMgTe	a	4.509	4.608	4.562	4.56	4.567	4.55 ¹⁵	4.574
RSCdO		4.636	4.77	4.694	4.692	4.698	4.696 ¹⁶	4.756
ZBCdS		5.758	5.928	5.828	5.826	5.864	5.82 ¹⁶	5.906
ZBCdSe		6.009	6.198	6.085	6.083	6.115	6.084 ¹⁶	6.168
ZBCdTe		6.411	6.621	6.493	6.491	6.528	6.48 ¹⁶	6.583
	ME	-0.01876	0.0671	0.009	0.007	0.024		
	MAE	0.04668	0.067	0.015	0.015	0.026		
	MRE%	-0.744	1.268	0.173	0.1426	0.3285		
	MARE%	0.934875	1.268	0.299	0.309	0.49		

*calculated with TBLMTO(code).

The last column in the table 3.1 contains the lattice constants calculated with optB88vdWc taken from the reference [17].

Table 3.2: Statistical quantities i.e. ME, MAE, MRE (%) and MARE (%) in the optimized lattice constants for different series of materials studied as produced by various functionals tested.

		LDA	PBE	WC	PBEsol	SCAN
	ME	-0.0341	0.048	0.00639	0.00513	
III-N	MAE	0.0341	0.048	0.00703	0.0063	
	MRE(%)	-0.799	1.069	0.124	0.101	
	MARE(%)	0.799	1.069	0.142	0.131	
	ME	-0.0318	0.0614	0.0085	0.0084	0.0057
III-P	MAE	0.0318	0.0614	0.0148	0.0151	0.0127
	MRE%	-0.161	1.105	0.135	0.13	0.09
	MARE%	0.61	1.105	0.275	0.28	0.24
	ME	-0.0199	0.0612	0.0236	0.0218	0.0344
BeX	MAE	0.0415	0.0612	0.0344	0.0358	0.0384
	MRE%	-0.47	1.318	0.5	0.47	0.68
	MARE%	0.975	1.318	0.748	0.783	0.82
	ME	0.059	0.055	0.002	-0.001	0.025
MgX	MAE	0.059	0.055	0.013	0.015	0.022
	MRE%	-1.13	0.98	0.026	-0.032	0.034
	MARE%	1.13	0.98	0.23	0.26	0.39
	ME	-0.067	0.11	0.005	0.003	0.031
CdX	MAE	0.067	0.109	0.006	0.005	0.031
	MRE%	-1.16	1.87	0.079	0.044	0.51
	MARE%	1.16	1.87	0.098	0.092	0.051

We start our discussion with assessing the performance of different functionals in calculating the lattice constants of all materials studied. For sake of simplicity, the discussion about the results for III-V and II-VI has been taken one by one for each of six series (i.e. III-N, III-P, BeX, MgX, CdX).

For III-Nitrides, the equilibrium LDA lattice constant underestimate while PBE overestimate the experimental values with ME of -0.0341 Å and 0.048 Å respectively as reported earlier [18]. The functional WC and PBEsol yields the lattice constants

much closer to experimental values as suggested by the lowest values of statistical quantities written in Table 3.2. With small differences in ME, MAE, MRE and MARE for WC and PBEsol approximations, both of these functional are equally applicable for optimization of lattice constant for group-III nitrides.

Table 3.3: Comparison of WC and PBEsol optimized lattice constants (Å) of III-N with hybrid and OPT functional results.

		WC	PBEsol	Hybrid	OptB88-vdW ^c	Expt. [*]
WZInN	a	3.5421	3.5408	3.542 ^b	3.572	3.545
	c	5.7226	5.7191	5.711 ^b	5.784	5.703
ZBInN	a	4.9942	4.9921	4.956 ^a , 4.988 ^b	5.039	4.98
WZAlN	a	3.1142	3.1151	3.103 ^b , 3.064 ^d	3.13	3.112
	c	4.9874	4.987	4.970 ^b , 4.908 ^d	5.021	4.982
ZBAlN	a	4.38	4.3809	4.367 ^a , 4.363 ^b	4.404	4.38
WZGaN	a	3.1893	3.1884	3.180 ^b , 3.232 ^d	3.211	3.189
	c	5.1964	5.1939	5.172 ^b , 5.268 ^d	5.24	5.185
ZBGaN	a	4.5073	4.5058	4.483 ^a , 4.489 ^b	4.541	4.5

*All the experimental values are taken from ref. [12].

^afrom ref. [19].

^b from ref. [20].

^c from ref. [17].

^d from ref. [21].

Table 3.3 shows a comparison of our calculated WC and PBEsol optimized lattice constants with hybrid density functional results [19, 20] and lattice parameters optimized with OPT functional as given in recently proposed database [17]. The comparison concludes that PBEsol reproduces the experimental values in better way, supported by minimum values of ME and MAE of 0.0063 Å and 0.0073 Å when compared with present WC, hybrid functional used in reference [20] with ME, MAE of -0.0073 Å, 0.0091 Å and OPT functional used in reference [17] with ME and MAE of 0.041 for InN, AlN, GaN in wurtzite and zinc blende structures respectively. The hybrid functional with optimized α parameter used in reference [19] underestimate the lattice constants for III-N semiconductors in zinc blende phase with ME of -0.018 Å while the present PBEsol results overestimate with ME of 0.0063 Å.

For group III-P, SCAN outperforms all other studied functionals in calculating the lattice constants with ME, MAE, MRE (%) and MARE (%) having the values of 0.0057, 0.0127, 0.09, and 0.24 for respectively. WC and PBEsol are equally accurate for III-P, with almost similar error values as shown in Table 3.2. Both of these functionals also provide rather good lattice constants with slightly higher ME of 0.0085 Å and 0.0084 Å respectively in addition to SCAN. WC yields almost identical lattice constant for BP as obtained with SCAN, however PBEsol has been found to underestimate with a mean error of -0.0135 Å. LDA underestimates the lattice constants systematically for all the III-P with ME and MRE of -0.0318 Å and -0.61 respectively, while PBE overestimates with a mean error of 0.0614 Å. Among the phosphides studied, all the tested functionals give the largest deviations from experimental lattice constant in case of InP. The results for bulk modulus show an opposite trend as compared to that shown by lattice constants. The functionals which lead to the underestimate the lattice constants overestimate the bulk modulus. These observations are in agreement with the recent similar type of study with extended set of elements studied [22].

Table 3.4: Comparison of calculated lattice constants (in Å) of III-P in zinc blende structure using PBEsol, SCAN with those reported hybrid and optB88-vdW functionals for III-P.

Material	PBEsol	SCAN	Expt.	optB88-vdW[17]	Hybrid[19]
ZBGaP	5.4558	5.4493	5.451	5.499	5.449
ZBAIP	5.479	5.4749	5.463	5.514	5.487
ZBInP	5.8951	5.8939	5.869	5.955	5.885
ZBBP	4.5245	4.5256	4.538	4.554	
ME	0.0084	0.0057		0.05	
MAE	0.0151	0.0127		0.05	
MRE(%)	0.13	0.09		0.89	
MARE(%)	0.28	0.24		0.89	

In the table 3.4, a comparison of present results for lattice constants of III-P along with those calculated using optB88-vdW[17] functional and hybrid functional [25] using optimized α is also made. This comparison shows a better agreement for our

calculated SCAN, PBEsol and WC results with experimental values as compared to optB88-vdW and hybrid functionals, suggested by much lower values of statistical quantities, as shown in bottom of the table 3.4. The calculated bulk moduli of all the materials studied are presented in table 3.5 with various errors written at the bottom of the table. In addition, the errors in the predicted bulk moduli using different functionals for different series of materials are given in table 3.6.

Table 3.5: Calculated bulk modulus (in GPa) of all the III-V and II-VI binary semiconductors included in the study with different functionals used.

	LDA	PBE	WC	PBEsol	SCAN	Expt.	OPT
ZBGaP	90.61	77.47	85.54	85.4	88.17	89.6	77.43
ZBAIP	90.03	81.58	87.22	86.9	90.52	87.4	83.37
ZBInP	71.7	59.19	66.89	67.18	68.79	72	59.7
ZBBP	175.92	161.94	169.33	169.41	171.78	168	161.63
ZBBeS	102.14	92.95	97.22	97.24	98.49	105	95.57
ZBBeSe	83.41	74.55	78.98	79.09	79.53	92.2	78.4
ZBBeTe	63.3	56.03	60	60.03	59.13	67	58.67
WZBeO	231.61	208.56	216.8	217.05	232.85		215.74
RSMgO	172.45	147.57	155.8	156.5	170.77	169.8	160.67
RSMgS	82.91	73.52	77.52	77.96	81.45	79.8	78.3
RSMgSe	68.84	60.1	63.93	64.28	66.36	62.8	65
WZMgTe	38.51	33.69	35.99	36.15	37.25	34	36.33
RSCdO	161.85	124.3	145.52	144.47	149.81	147	136.67
ZBCdS	67.96	52.86	61.2	61.09	61.52	55	57.1
ZBCdSe	57.97	44.24	52.01	51.87	52.76	45.1	48.23
ZBCdTe	45.88	34.74	41.29	41.14	41.17	42	37.83
ME(GPa)	3.225	-5.822	-2.97	-2.955	-0.5337		
MAE(GPa)	5.826	9.778	4.785	5.19	4.66		
MRE(%)	5.278	-4.992	-2.073	-2.066	0.272		
MARE(%)	8.29	9.857	6.475	6.515	6.517		

The results show that for AlP and InP the bulk modulus calculated with LDA have the minimum deviation of 1.01 GPa and -0.3 GPa respectively, from the experiments. The bulk modulus of GaP and BP have been found to be better predicted

by WC and PBEsol. Overall MAE values (2.67 GPa and 2.73 GPa) with WC and PBEsol suggest these functionals to be efficient for III-P semiconductors. PBE systematically underestimates the bulk modulus with a ME of -9.21 GPa. The minimum value of ME (0.565 GPa) and MRE (-0.06%) in bulk modulus of III-P is obtained with SCAN. However, minimum value of MAE (2.67GPa) is obtained with WC. LDA also performs well in calculating the bulk modulus of phosphides studied with error values within a small range around that for others GGA and meta GGA functionals used.

Table 3.6: Various error values in bulk modulus of the different series of the materials studied.

		LDA	PBE	WC	PBEsol	SCAN
	ME	2.8	-9.21	-2.01	-2.03	0.565
III-P	MAE	2.965	9.21	2.67	2.73	2.89
	MRE%	2.11	-10.4	-2.76	-2.78	-0.06
	MARE%	2.32	10.4	3.15	3.2	2.97
	ME	-5.12	-13.6	-9.33	-9.28	-9.02
BeX	MAE	5.12	13.6	9.33	9.28	9.02
	MRE%	-5.92	-15.7	-10.7	-10.7	-10.5
	MARE%	5.92	15.7	10.7	10.7	10.5
	ME	4.08	-7.91	-3.29	-2.88	2.28
MgX	MAE	4.08	7.91	3.29	2.88	2.28
	MRE%	7.07	-3.6	-0.862	-0.364	4.46
	MARE%	7.07	3.6	4.69	4.7	4.42
	ME	11.14	-8.39	2.75	2.37	4.04
CdX	MAE	11.14	8.39	3.85	4.06	4.45
	MRE%	17.85	9.73	6.03	5.58	7.19
	MARE%	17.85	9.73	7.36	7.46	8.18

Concerning the lattice constants of beryllium chalcogenides (BeS, BeSe, BeTe) and beryllium oxide (BeO), in terms of ME and MRE, PBEsol performs better while WC have better performance in terms of MAE and MARE. WC and PBEsol leads to the almost identical results for this class of materials and on average are good for BeX materials with smaller errors relative to the experimental values. However, in case of

BeTe, LDA optimized lattice constant has the minimum error (-0.004 Å). Regarding the bulk modulus, LDA outperforms all other functionals with minimum values of MAE (5.12GPa) and MARE (5.92%) for the phosphides.

MgO and magnesium chalcogenides which usually crystallize in the rock salt phase except MgTe which prefers wurtzite structure, under ambient conditions. For all the RS magnesium chalcogenides, SCAN underestimates the lattice constants for MgO, MgS and MgSe while overestimates for WZ-MgTe. WC and SCAN yield almost similar lattice constants for RS MgS while in other cases WC resembles the PBEsol results. In case of MgO, PBEsol has been found to be the best functional with an error of 0.001 Å, however SCAN predicts the lattice constant of MgSe with minimum deviation (-0.0048 Å) from the experiment. On average WC and PBEsol are found to be more suitable functionals for chalcogenides and oxide of magnesium as shown by the minimum error values given in table 3.2. Turning towards the bulk modulus, it is observed that SCAN yields the best results with small overestimation (ME of 2.28 Å and MRE of 4.46%) relative to the experimental values. PBE underestimates the bulk modulus which decreases as we move from lighter to heavier elements resulting in a decrease in relative errors with the maximum relative error of 13.1% for MgO to minimum relative error of 0.91% for MgTe. On moving in the direction of increasing mass number, the bulk modulus and hence rigidity reduces. This suggests that PBE is more stable for soft magnesium compounds. Like SCAN, LDA also overestimate the bulk modulus of magnesium oxide and chalcogenides.

In CdX (X=O, S, Se, Te) Compounds, the presence of 4d orbital in its valence shell needs a larger muffin tin sphere and hence leads to the linearization errors. In order to tackle such problem, we included the so called higher derivative local orbital which depends upon the second order energy derivative [10]. These local orbitals are known as higher derivative local orbitals (HDLO). For this class of materials, SCAN and PBE both overestimate the lattice constants in a systematic manner. However, SCAN results, with a ME of 0.031 Å are much better than those with PBE which leads to a ME of 0.109 Å. WC also competes in accuracy of lattice constants of CdX compounds, to PBEsol with a slightly greater value of MARE (0.098%) as compared to 0.092% with PBEsol. As for other materials studied LDA underestimates the lattice constants of CdX compounds also with almost identical errors (ranging between 0.6 Å to 0.7 Å) for all these compounds. On analyzing the results for bulk modulus, a

reduction in the error values has been observed as we move along series of the XC functionals used i.e. LDA, PBE, PBEsol, WC with largest MARE (17.85%) with LDA to minimum MARE (7.36%) with WC. SCAN yields the bulk modulus cadmium compounds almost identical to PBE, however with a slight improvement shown by a decrease in the MARE from 9.73% by PBE to 8.18%. On average PBEsol provides both the lattice constants and bulk modulus of CdX series of II-VI compounds studied, more closely to experiments as compared to the studied functionals.

The comparison of our present results for lattice constants of all the III-V and II-VI compound semiconductors studied with those calculated using optB88-vdW functionals as reported in reference [17] shows that our WC and PBEsol optimized lattice constants have smaller deviations from experimental results as compared to OPT optimized lattice parameters. In fact OPT yields results of the order of our reported PBE results, however with a slight improvement. An exception has been observed in case of MgX (X=O, S, Se, Te) compounds where OPT results match more to the SCAN optimized lattice constants, much better as compared to PBE results. This statement is based on the results as given in the table 3.1. Considering the performance over the whole set of the compounds studied, SCAN provides a slightly greater MARE (0.49%) as compared to that for WC (0.30%) and PBEsol (0.309). A similar type of observations had been observed recently [22] for semiconductor compounds out of a relatively larger set (64 solids) of the bulk solids. For semiconductors, the authors have reported in ref. [22] MARE of 0.5% in estimating lattice constants with SCAN which is almost same as reported in this present study (0.049%). However, their PBEsol lattice constants of semiconductors included in their study, have a slightly larger value of MARE (0.4%) as compared to MARE (0.3%) reported in this thesis. Further in calculation of lattice constants of the semiconductors studied in our present work with PBEsol functional is smaller than those reported in [22]. The lattice constants of III-V (AlN, GaN, InN, GaP, InP, AlP) calculated with hybrid functional as reported in ref. [19] has been found to have larger errors as compared to our present WC and PBEsol results as shown in the tables 3.3 and 3.4. On comparing the present WC and PBEsol optimized lattice constants of CdX (X=O, S, Se, Te) with those calculated using ACBN0 [23] functional as reported in ref. [16], WC and PBEsol have been found to perform better.

3.4 Conclusions

The lattice constants and bulk modulus of the III-V (III-N, III-P) and II-VI (BeX, MgX, CdX; X=O, S, Se, Te) binary bulk solids in their ground states have been calculated using various local and semi local functionals. The results show that LDA underestimate while PBE overestimate the experimental lattice constants for all the materials studied with a MARE of the order of 1%. Such trend in LDA and PBE results are in agreement with earlier reported results [18, 24, 22]. WC and PBEsol improve over the standard functional (LDA, PBE) for all classes of materials studied except in case of BeX where the results are of the same order as obtained with LDA. SCAN reproduces the experimental lattice constants for III-P with minimum deviation as compared to other functionals studied, however leads to larger deviations in case of CdX series. WC, PBEsol and SCAN produced the lattice constants in better agreement with experiment as compared to optB88vdW functional [17]. On average WC and PBEsol functional have been found to be better approximations in estimating the lattice constants and bulk modulus of III-V and II-VI binary compounds studied with small values of MARE (~0.3% and 6.5 %) for lattice constants and bulk modulus respectively. SCAN which is supposed to be the best functional in estimating the ground state properties of the solids [9, 14] shows a rather larger MARE (0.49%) for lattice constants of the materials studied, however it leads to almost same MARE (6.517%) for bulk modulus as that obtained with WC and PBEsol.

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