Study of Electronic and Structural properties of Cadmium Sulfide (CdS) in Zinc-Blend and Wurtizite phase using DFT and DFT+U.

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Introduction:

Cadmium Chalcogenides are monochalcogenides have the formula CdX (X = S, Se, and Te). They typically crystallize in one of three motifs, ZB, WZ, and rock-salt (cubic) structures [1], and the experimentally stable crystal phase of CdS is WZ structure [2]. Farther more, the CdS can crystallize in either ZB crystal structure with space group F-43m or WZ crystal structure with P6$_3$mc space group under ambient conditions [3]. The rock-salt structure is only observed under high pressure [4, 5]. Cadmium chalcogenides CdX (X= S, Se and Te) and their combinations are widely studied members of II-VI semiconductor family [6]. CdS is one of CdX and CdX compounds are the archetypal systems of the II-VI semiconductor [7]. Thin films are most auspicious for occupation in solar cells, photo electrochemical cells out of which axenic CdX have received intensive attention. Because their optical band gaps lies close to the range of optimum theoretically achievable energy conversion efficiency [8]. They can also be used in hetero-junctions, IR detectors, Lux meters, switching devices and Schottky barriers etc. Due to their potential applications, the II-VI compounds peculiarly are attracting a lot of attention in producing hetero-junction, photo-electrochemical, solar cells, optoelectronic devices, light emitting diodes and field effect transistor etc [9].

Objectives

- To study Electronic and structural properties of CdS in zinc-blend phase and wurtizite phase within computational methods particularly using DFT and DFT+U.

Computational Methods

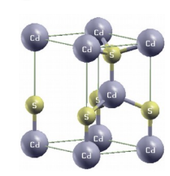
The physical (structural) and Electronic properties of CdS in both phase was calculated using QUANTUM-ESPRESSO code in the frame work of the density functional theory. The interaction between core and valance electrons described using norm-conserving pseudopotentials and Projector augmented-wave pseudopotential . The exchange-correlation effect in Kohn-Sham will treated by local density approximation (LDA) and generalized gradient approximation (GGA) as parameterized by Perdew, Burke and Ernzerhof (PBE) for Structural properties and hybrid functional approximation (PBE0 or HSE06) and Hubbard-correction(GGA+U) for Electronic properties calculation. Because evaluated band gap values using GGA were far away from the experimental value. This problem was improved by using norm-conserving pseudopotential method within the hybrid functional approximation (PBE0 or HSE06).

Results and Discussion

Structural properties of CdS

Figure 1 and table 1 Shows kinetic energy at which Minimum energy achieved when k-points held at 3x3x3 in both phase.
Figure 2 and table 2 shows that k-point convergence for the fixed lattice constant and fixed cutoff energy

Table 1 : Convergence points



Phase	K-point convergence	Energy cutoff converged (Ry).	Methods
zb	6x6x6	60	LDA
	6x6x6	55	PBE
	5x5x5	60	DFT+U
	6x6x6	60	PBE0
wz	6x6x6	55	LDA
	5x5x5	55	PBE
	5x5x5	60	DFT+U
	5x5x5	60	PBE0

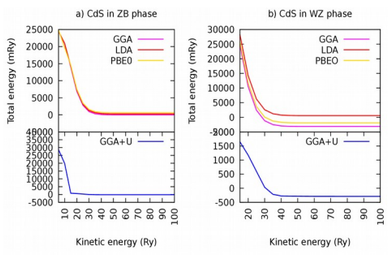


Figure 1 : Cutoff energy convergence a) ZB b) WZ

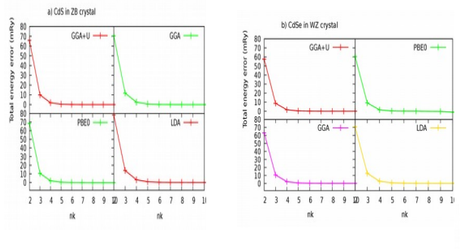


Figure 2 : k-point Convergence a) ZB b) WZ

Methods		LDA	PBE	DFT+U	PBE0
Phase					
zb	Present	a = 5.819	a =5.979	a = 5.983	a = 5.847
	Theory	a=5.81[10], 5.85[11], 5.80[12]			
	Experiment	a=5.82[13]			
wz	Present	a=4.158	a = 4.226	a = 4.37	a = 4.160
		c=6.752	c = 6.863	c = 7.10	c = 6.756
	Theory	a=4.097[10], a=4.160[11]			
		c=6.752, c=6.70			
	Experiment	a=4.136[13]			
		c=6.756			

Table 2 : Calculated equilibrium Lattice constant of CdS by using Quantum-espresso 6.5

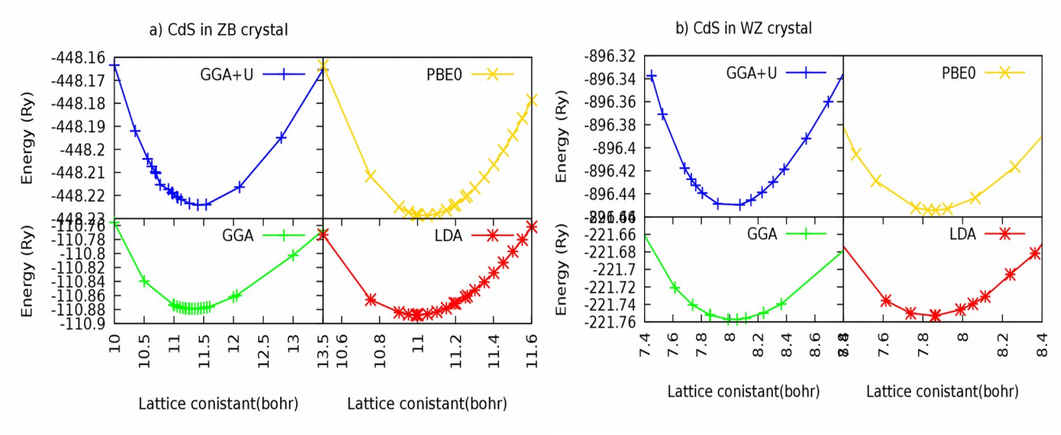


Figure 3: Total energy of CdS versus lattice constant a) in ZB phase b) in WZ phase.

Electronic properties CdS

Table 3 : Calculated band gap of CdS by using QE and Experimental value.

Method	LDA	PBE	PBE+U	PBE0	Experiment
Phase					
ZB	0.741	1.030	2.45	2.48	2.37 [14]
WZ	0.701	1.04	2.41	2.47	2.48 [15]

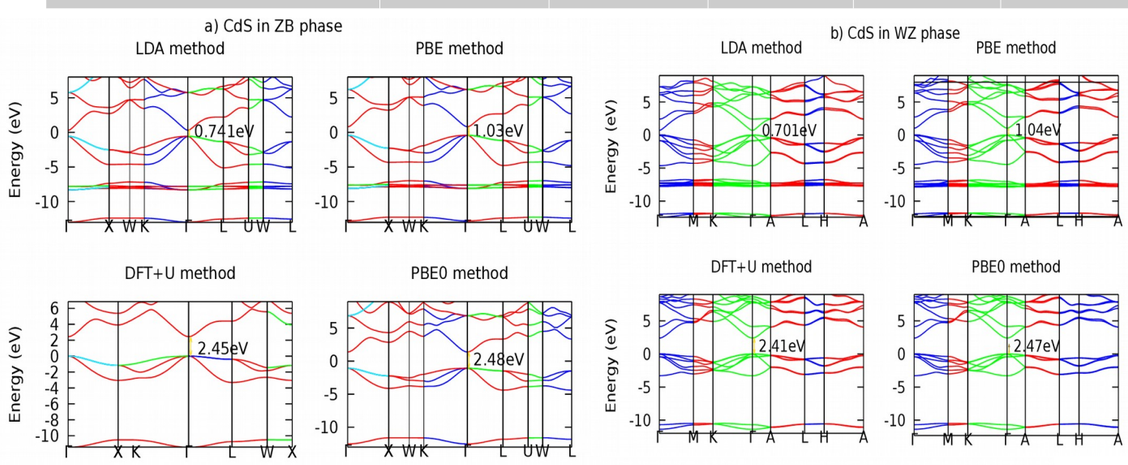


Figure 4: Plotted Band structure of CdS along high symmetry point a) ZB phase b) WZ phase.

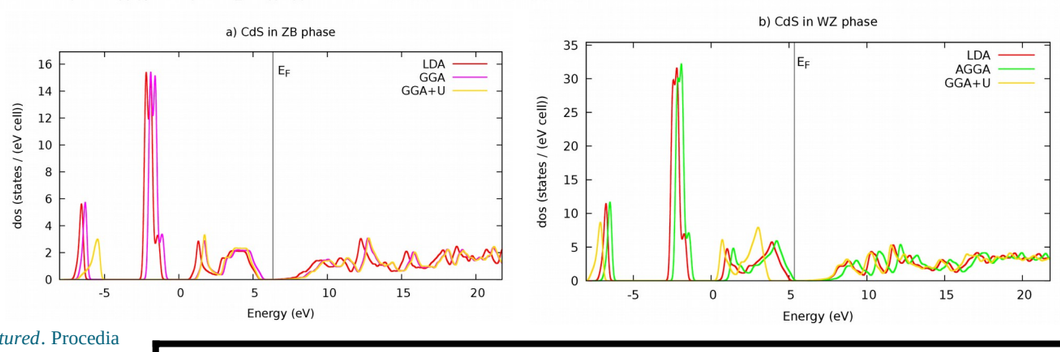


Figure 5: Plotted dos of CdS a) ZB phase b) WZ phase

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Conclusion

The structural and electronic properties of zb- and wz-CdS are studied using DFT and DFT+U. The exchange correlation functional is approximated using LDA, GGA/PBE, GGA+U and PBE0. The lattice constants optimization was performed using LDA, PBE, DFT+U and PBE0 approximations and the obtained results are in good agreement with experimental. The band structure calculation was performed using LDA, PBE, DFT+U and PBE0 approximations. The results reveal that LDA and GGA under estimate the band gap due to their poor approximation of exchange-correlation functional. However, the Hubbard correction (DFT+U) and the hybrid functional approximation (PBE0) give a band gap value which is consistent with the experimental results.

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