Tables from Chapter 4:

"Optical properties and electronic structure of wide band gap II-VI semiconductors"

by

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in

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TABLE LIST:

Notes:

1. This document is only for internal use of the NanoSem Laboratory at the Physics Department of Cinvestav.
2. The references were removed to avoid problems with the compilation of the document file, they can be found in the cited book.

Table 1. Crystal structural properties. Lattice parameters *a*, *c*, *c/a*, bond length *d*, and bond ratio γ. All dimensions in Å.

	Zincblende		***Wurzite***				
Space group:	$T_d^2 - F\bar{4}3m$		$C_{6v}^4 - P6_3mc$				
Compound	***a***	***d***	***a***	***c***	***c/a***	***γ***	***d***
BeS	4.864	2.106	-	-	-	-	-
BeSe	5.138	2.224	-	-	-	-	-
BeTe	5.617	2.432	-	-	-	-	-
CdS	5.835	2.527	4.137	6.714	1.623	1.005	2.528
CdSe	6.050	2.620	4.30	7.013	1.631	1.006	2.63
CdTe	6.478	2.805	4.572	7.484	1.637		2.802
HgS	5.872	2.543	-		-	-	-
HgSe	6.085	2.635	-	-	-	-	-
HgTe	6.460	2.797	-	-	-	-	-
MgS	5.620	2.434	-	-	-	-	-
MgSe	5.890	2.550	-	-	-	-	-
MgTe	6.280	2.719	-	-	-		-
ZnO	-	-	3.253	5.213	1.603	1.008	1.980
ZnS	5.406	2.341	3.811	6.235	1.636	-	2.335
ZnSe	5.668	2.454	4.003	6.540	1.634	-	2.453
ZnTe	6.103	2.643	4.310	7.090	1.645	-	2.646
Si	5.431	2.352	3.80	6.281	1.653		2.34
Ge	5.657	2.450	-	-	-	-	-
α-Sn	6.489	2.810	-	-	-	-	-
AlAs	5.639	2.442	-	-	-	-	-
GaAs	5.653	2.448	-	-	-	-	-
GaN	4.515	1.955	3.186	5.178	1.625	-	-
GaP	5.447	2.359	-	-	-	-	-
GaSb	6.094	2.638					
InAs	6.058	2.623	4.274	7.001	1.638	-	2.620
InN			3.562	5.899	1.656	-	2.192
InP	5.869	2.541	-	-	-	-	-
InSb	6.479	2.805	-	-	-	-	-

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 2. Varshni Parameters for the modeling of $E_g(T)$

Compound	$E_g(0)$ (eV)	α (meV/K)	β (K)	Ref.
h-CdS	2.588 ± .001	0.386	103	
c-CdSe	1.772±0.005	0.37±0.03	150±40	
c-CdSe	1.766 ± .003	0.696	281	
h-CdSe	1.834± .003	.424± .02	118± 40	
c-CdTe	1.602± .004	0.46± .07	160.1	
c-ZnS	3.8440	0.632	254	
c-ZnS	3.842±0.003	0.88±0.05	460±40	
c-ZnSe	2.8271	0.558	187	
c-ZnSe	2.825±0.002	0.67±0.05	270±90	
c-ZnSe	2.820 ± 0.005	0.73 ± 0.04	295 ± 35	
c-ZnTe	2.3960	0.549	159	
c-ZnTe	2.394	0.63	210	

c=cubic, h=hexagonal

Table 3. Parameters for the modeling of $E_g(T)$ following VLC

Compound	$E_g(0)$ (eV)	E_B (eV)	**Θ (K)**	**REF.**
h-CdSe	1.849 ± 0.003	0.036 ± 0.005	179 ± 40	
c-ZnS	3.8393	0.0733	272	
c-ZnSe	2.8243	0.0516	209	
c-ZnSe	2.800 ± 0.005	0.073 ± 0.004	260 ± 10	
c-ZnTe	2.3937	0.0375	163	

c=cubic, h=hexagonal.

Table 4. Parameters for the modeling of $E_g(T)$ following OC

COMPOUND	$E_g(0)$ (eV)	S	$\langle \hbar\omega \rangle$, **MEV**	**REF.**
c-CdSe	1.764	2.83	18.9	
c-CdTe	1.608	1.68	5.8	
c-ZnS	3.836	2.82	16.1	
c-ZnSe	2.818	3.12	15.1	
c-ZnTe	2.390	2.29	10.8	
h-CdS	2.568	1.54	13.9	
h-CdSe	1.849	2.94	25.4	
h-ZnS	3.929	4.3	17.1	

c=cubic, h=hexagonal

Tables from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 5. Data collection of the band gap of zincblende wide band gap II-VI semiconductors.

	Low temperature			Room temperature		
Compound	***Eg*** (eV)	**T** (K)	Ref.	***Eg*** (eV)	**T** (K)	Ref.
BeS	2.75i*, 5.51d*	0				
BeSe	2.39i*, 4.72d*	0		5.15d	300	
BeTe	1.80i*, 3.68d*	0		2.8i	300	
CdS				2.48	297	
				2.50	297	
				2.45	297	
				2.42	297	
CdSe	1.75	10		1.66	297	
	1.765	9		1.655 ± .005	297	
	1.78	5		1.692	300	
				1.74	297	
CdTe	1.6063	1.64		1.509± .005	297	
	1.598	5		1.509	300	
	1.608	0		1.511± .008	300	
				1.509 ± .002	300	
MgS				4.45± .02	297	
MgSe				3.59	297	
				4.0	300	
MgTe				3.5	300	
				3.49	300	
ZnS	3.841± .001	0		3.741± .004	300	
	3.78	19		3.68	295	
	3.85	19		3.74	295	
	3..84	4.2		3.723± .001	297	
ZnSe	2.8252± .0004	0		2.722± .003	300	
	2.821	9		2.70	295	
	2.8237 ± .0005	12		2.704± .001	297	
	2.820	5		2.730	300	
	2.82	10		2.69	297	
	2.8201± .0004	1.6		2.70	300	
ZnTe	2.3944±.0004	0		2.290± .002	300	
	2.3941± .0004	1.6		2.28	2.93	
	2.392	5		2.250	300	
	2.392 ± .001	12		2.271 ± .003	300	
α-Sn	0					
Ge	0.785	0		0.664	291	
Si	1.17i			1.1242i	300	
GaAs	1.52			1.415 ± .001	300	
InAs	0.418	4.2		0.354	295	
InP	1.4236	1.6		1.344	300	
InSb	0.2368	2		0.169	300	

*= theory, *i*=indirect gap, *d*=direct gap

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 6. E_A transitions of wurzite wide band gap II-VI semiconductors.

	Low temperature			Room temperature		
Compound	E_g (eV)	**T** (K)	Ref.	E_g (eV)	**T** (K)	Ref.
h-CdS	2.5827	1.2		2.485	300	
	2.596	0				
h-CdSe	1.849	0		1.756	300	
	1.829	80		1.751	293	
h-ZnO	3.4376	1.6		3.37	297	
h-ZnS	3.929	0		3.772	300	
	3.9107			3.76	300	
	3.903*	4.2				
h-ZnSe	2.874	4.2		2.834	300	

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 7. Reference values for the lattice constant (a, c), E_0 and Δ_0 values for wide band gap II-VI semiconductors. E_A $(= E_0)$, E_B, and E_C refer to wurzite crystals. All energy values in eV.

Zincblende	$\boldsymbol{a}$ (RT) (Å)	$\boldsymbol{E_0}$ (LT)	$\boldsymbol{E_0}$ (RT)	Δ_0^C	
BeS	4.864	2.75i*			
BeSe	5.137	2.39i*	5.1		
BeTe	5.617	1.80i*	2.8i		
CdS	5.835		2.48	0.07	
CdSe	6.050	1.77	1.66	0.42	
CdTe	6.478	1.60	1.51	0.91	
MgS	5.620		4.45		
MgSe	5.890		4.0		
MgTe	6.280		3.5		
ZnS	5.406	3.84	3.74	0.067	
ZnSe	5.668	2.82	2.70	0.42	
ZnTe	6.103	2.39	2.29	0.97	
Wurzite	$\boldsymbol{a}$(RT) $\boldsymbol{c}$(RT)	$\boldsymbol{E_0}$ (LT)	$\boldsymbol{E_0}$ (RT)	$\Delta_0^H = \boldsymbol{E_B}$-$\boldsymbol{E_C}$	$\boldsymbol{E_A}$-$\boldsymbol{E_B}$
h-CdS	4.137 6.714	2.59	2.49	0.063	0.016
h-CdSe	4.300 7.013	1.85	1.76	0.405	0.026
h-ZnO	3.253 5.213	3.44	3.37	0.039	0.003
h-ZnS	3.811 6.235	3.91	3.77	0.088	.029
h-ZnSe	4.003 6.540	2.87	2.83		

*= theory, *i*=indirect gap

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 8. Elastic stiffness constants and deformation potential of zincblende II-VI wide band gap semiconductors.

Compound	c_{11} (10^{10} Pa)	c_{12} (10^{10} Pa)	Ref.	a (eV)	b (eV)	Ref.
CdSe	6.67	4.63		-3.664	-0.8	
CdTe	5.351	3.681		-4.52[+]	-1.1[+]	
ZnS	1.067	0.666		-4.0	-0.62	
ZnSe	8.52	5.17		-4.53	-1.14	
ZnTe	7.13	4.07		-5.8	-1.8	
BeS	1.84[+]	0.75[+]				
BeSe	1.49[+]	0.59[+]				
BeTe	1.11[+]	0.43[+]				
GaAs	11.9	5.38		-8.93	-1.76	

*the elastic stiffness constants are the average of the values given in Refs. ___.
[+]theoretical calculations.

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 9. Calculated values for the shift of optical transitions at Γ of pseudomorphic heterostructures of II-VI semiconductors on GaAs(100).

System	$\varepsilon\,(10^{-2})$	ΔE_{HH} (meV)	ΔE_{LH} (meV)	ΔE_{SO} (meV)
CdSe/GaAs	6.6	21.7	325	94.5
CdTe/GaAs	12.7	38.8	8.6	213
ZnS/GaAs	- 4.6	- 73.7	-112.6	-225.8
ZnSe/GaAs	0.265	2.75	16.3	9.2
ZnTe/GaAs	7.37	82.8	769	249

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 10. Bowing parameters for $E_g(x)$ of II-VI wide band gap ternary zincblende alloys. b_{av} refers to the average of the given values.

Ternary	***b*** (eV)	**Ref.**	b_{av}
BeZnSe	$\approx 0^a$		
CdSeTe	0.755, 0.87		0.83
CdSSe	0.53, 0.54		0.54
CdSTe	1.84, 1.73, 1.74		1.77
CdZnS	0.6^b, 0.3		0.45
CdZnSe	0.30, 0.35, 0.35		0.33
CdZnTe	0.153^c, 0.33, 0.342, 0.463		0.32
MgZnSe	0.4, 0.47		0.44
MgZnTe	0.69		0.69
ZnSeTe	1.28, 1.7, 1.35, 1.23, 1.251		1.36
ZnSSe	0.56, 0.63, 0.456. 0.68, 0.510		0.57
ZnSTe	2.4, 2.7, 3.0		2.7

a: low berylium ($x < 0.4$) content, b: not a homogeneous cubic sample. c: average of 12 and 300 K values.

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 11. Experimental free exciton binding (E_1) and PL (X) transition energies, and calculated binding energies and modified Bohr radius of wide band gap II-VI semiconductors at the Γ point.

	Experimental		Theory			Material parameters		
	E_1 (meV)	Ref.	X (eV)	E_1 (meV)	a_H (Å)	m_e/m_0	m_{hh}/m_0	ε_0
CdS				16.9	45.3	0.14	0.51	9.4*
CdSe	15			13.0	57.5	0.11	0.45	9.6
CdTe	11		1.595 - 1.597	10.4	70.6	0.09	0.40	9.8
ZnS	38 ± 1		3.80 - 3.82	37.8	22.4	0.34	0.49*	8.5
ZnSe	20.0 ± 0.3		2.800 -2.804	20.1	41.1	0.145	0.49	8.7
ZnTe	12.8 ± 0.2		2.380 - 2.381	14.2	51.9	0.12	0.60	9.8
h-CdS	29 ± 1		2.551 - 2.553[A]	26.7	28.7	0.23	0.7	9.4
h-CdSe	15		1.824 - 1.827	14.9	51.9	0.12	0.45	9.3
h-ZnO	59		3.376 - 3.378[A]	42.5	21.7	0.28	0.59	7.8
h-ZnS	~ 40		3.79 - 3.81[A]	41.1	28.5	0.28	0.49	9.6

*parameter of the hexagonal structure. A: 1s exciton of A-band in hexagonal semiconductors.

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 12. Bound exciton binding energies and their optical transitions in zincblende wide band gap II-VI semiconductors. Most of the values based on data of Ref. __ and references therein.

	Donors		Acceptors	
Material	E_B^0 (meV)	(D^0, X) (eV)	E_B^0 (meV)	(A^0, X) (eV)
CdTe	0.6 - 2.9	1.593 - 1.596	6.1 - 7.8	1.588 - 1.591
ZnS	9 (I)	3.785 - 3.792	7 - 30	3.776 - 3.793
ZnSe	4.5 - 5.1 (Al)	2.797 - 2.798	9.4 -10.2 (Na)	2.788 - 2.793
	3.8 - 5 (Ga)	2.794 - 2.797	10.8 - 12 (Li)	2.790 - 2.792
	4.5 - 4.8 (Cl)	2.795 - 2.797	9 - 11 (N)	2.790 - 2.792
			4.9 - 5.2 (P)	2.796 - 2.798
			17 - 21 (Cu)	2.782 - 2.785
	5.5 (V_{Se})	2.7954	16.4 - 19.4 (V_{Zn})	2.780 - 2.784
ZnTe	3.4 - 6	2.372 - 2.376	4.5 - 12	2.367 - 2.374

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).

Table 13. Donor excitation energies in ZnSe from Refs. __ and references therein. Energies in meV.

	Al	Cl	Ga	In
1s - 2s	18.84 - 18.91	19.32 - 19.36	20.16 - 20.22	20.89 - 20.92
1s - 2p	18.96 - 19.16	19.64 - 19.71	20.71 - 21.1	21.65 - 21.75
1s - 3s	22.59		24.13 - 24.18	25.03
1s - 3p	22.75		24.33 - 24.7	25.32

Table from: I. Hernández.Calderón, "Optical properties and electronic structure of wide band gap II-VI semiconductors", in *II-VI Semiconductor Materials and their Applications*, Taylor and Francis New York, 113 –170 (2002).