TABLES

TABLE I. LDA calculated (cal) equilibrium zinc-blendelattice constants a (in Å), bulk moduli B (in kbar), and the pressure derivative B' of the bulk modulus. Results are compared with available experimental (exp) data (Ref. [1]). Compounds denoted by an asterisk exist in wurtzite structure, while HgS exist in the cinnabar structure. For these compounds a_{exp} and B_{exp} are estimated from the properties of their wurtzite countpart or from LDA calculations.

Compound	a_{cal}	a_{exp}	B_{cal}	B_{exp}	B'_{cal}
C	3.5393	3.5668	4692	4420	3.8
Si	5.4069	5.4307	966	979	4.4
Ge	5.6540	5.6579	708	689	4.5
Sn	6.5029	6.4890	443	456	4.6
AlN*	4.3641	4.3600	2158	2158	4.2
AlP	5.4461	5.4635	903	860	4.4
AlAs	5.6435	5.6600	754	781	4.4
AlSb	6.1234	6.1355	560	551	4.4
GaN*	4.4881	4.5000	2063	2054	4.6
GaP	5.4374	5.4505	896	882	4.7
GaAs	5.6490	5.6533	742	756	4.8
GaSb	6.0917	6.0959	556	563	4.9
InN*	4.9753	4.9800	1498	1480	4.7
InP	5.8615	5.8687	716	710	4.8
InAs	6.0512	6.0583	603	579	4.9
InSb	6.4763	6.4794	468	483	4.9
ZnS	5.3476	5.4102	906	771	5.0
ZnSe	5.6079	5.6676	740	624	5.0
ZnTe	6.0295	6.0890	559	509	5.1
CdS*	5.7958	5.8180	703	620	4.8
CdSe*	6.0412	6.0520	592	530	4.8
CdTe	6.4400	6.4820	466	445	4.9
HgS	5.8476	5.8500	689	685	5.0
HgSe	6.0950	6.0850	589	500	5.0
HgTe	6.4677	6.4603	477	423	5.1

TABLE II. LDA Calculated band gap volume deformation potentials [Eq. (2)] (in eV) and pressure coefficient [Eq. (1)] (in meV/kbar) of the three main transitions $\Gamma_{8v} \rightarrow X_{6c}$, $\Gamma_{8v} \rightarrow L_{6c}$, and $\Gamma_{8v} \rightarrow \Gamma_{6c}$ for group IV, III-V and II-VI semiconductors. Results for $a_p^{\Gamma-\Gamma}$ are compared with available experimental (exp) data (Ref. [1], unless specified otherwise).

Compound	$a_v^{\Gamma-X}$	$a_p^{\Gamma-X}$	$a_v^{\Gamma-L}$	$a_p^{\Gamma-L}$	$a_v^{\Gamma-\Gamma}$	$a_p^{\Gamma-\Gamma}$	$a_p^{\Gamma-\Gamma}(exp)$
C	-2.31	0.49	-13.65	2.91	-23.08	4.9	
Si	1.84	-1.90	-3.60	3.73	-11.39	11.8	
Ge	1.16	-1.64	-3.07	4.34	-9.10	12.9	
Sn	0.97	-2.19	-1.96	4.42	-6.97	15.7	
AlN	-0.42	0.19	-9.04	4.11	-9.04	4.2	
AlP	1.86	-2.06	-3.77	4.17	-8.50	9.4	
AlAs	1.63	-2.16	-3.77	5.00	-7.86	10.4	10.2
AlSb	1.71	-3.05	-2.90	5.18	-7.85	14.0	
GaN	-0.35	0.17	-6.72	3.26	-6.40	3.1	4.0[a]
GaP	1.97	-2.20	-2.96	3.30	-7.99	8.9	9.7
GaAs	1.81	-2.44	-2.66	3.58	-7.25	9.8	8.5−12.6
GaSb	1.80	-3.24	-2.04	3.67	-7.01	12.6	14.0
InN	-0.45	0.30	-3.97	2.65	-2.75	1.8	
InP	1.62	-2.26	-2.25	3.14	-5.30	7.4	8.0; 7.5−9.3[b]
InAs	1.58	-2.62	-1.98	3.28	-4.93	8.2	11.4; 9.6−11.4[b]
InSb	1.66	-3.55	-1.65	3.53	-5.60	12.0	12.8-15.5
ZnS	2.10	-2.32	-1.97	2.17	-4.28	4.7	5.8;6.4[c];6.7[d]
ZnSe	2.16	-2.92	-1.74	2.35	-3.96	5.4	7.2−7.5;7.0[c]
ZnTe	2.42	-4.33	-1.31	2.34	-4.67	8.4	11.5;10.5[e]
CdS	1.62	-2.30	-1.38	1.96	-2.08	3.0	4.4;4.6[c]
CdSe	1.81	-3.05	-1.17	1.98	-1.96	3.3	5.8
CdTe	2.09	-4.48	-0.98	2.10	-2.95	6.3	7.6[e];6.5−8.6[f]
HgS	1.91	-2.77	-0.34	0.49	-1.23	1.8	
HgSe	2.20	-3.74	-0.06	0.10	-1.15	2.0	
HgTe	2.49	-5.22	-0.01	0.02	-2.34	4.9	

[a] Ref. [2]; [b] Ref. [3]; [c] Ref. [4]; [d] Ref. [5]; [e] Ref. [6]; [f] Ref. [7];

TABLE III. LDA Calculated "absolute" volume deformation potentials (in eV) of the VBM (Γ_{8v}) and the CBM (Γ_{6c}) states at Γ for group IV, III-V and II-VI semiconductors.

Compound	a_v^{VBM}	a_v^{CBM}
C	2.55	-20.53
Si	2.05	-9.34
Ge	-0.35	-9.45
Sn	-0.92	-7.89
AlN	4.94	-4.10
AlP	2.64	-5.86
AlAs	1.53	-6.33
AlSb	0.73	-7.12
GaN	0.69	-5.71
GaP	-0.58	-8.57
GaAs	-1.21	-8.46
GaSb	-1.32	-8.33
InN	0.73	-2.02
InP	-0.41	-5.71
InAs	-1.00	-5.93
InSb	-1.24	-6.84
ZnS	-1.74	-6.02
ZnSe	-1.97	-5.93
ZnTe	-2.28	-6.95
CdS	-1.51	-3.59
CdSe	-1.81	-3.77
CdTe	-2.14	-5.09
HgS	-3.06	-4.29
HgSe	-3.20	-4.35
HgTe	-3.45	-5.79

TABLE IV. LDA corrected band gap volume deformation potentials (in eV) and pressure coefficient (in meV/kbar) of the three main transitions $\Gamma_{8v} \rightarrow X_{6c}$, $\Gamma_{8v} \rightarrow L_{6c}$, and $\Gamma_{8v} \rightarrow \Gamma_{6c}$ for group IV, III-V and II-VI semiconductors. The pressure coefficients are obtained using Eq. (1) and experimental bulk moduli of Table II.

Compound	$a_v^{\Gamma-X}$	$a_p^{\Gamma-X}$	$a_v^{\Gamma-L}$	$a_p^{\Gamma-L}$	$a_v^{\Gamma-\Gamma}$	$a_p^{\Gamma-\Gamma}$
C	-3.12	0.7	-14.77	3.3	-24.77	5.6
Si	1.35	-1.4	-4.07	4.2	-12.44	12.7
Ge	0.49	-0.7	-4.00	5.8	-10.06	14.6
Sn	0.46	-1.0	-2.71	5.9	-7.58	16.6
AlN	-1.13	0.5	-9.89	4.6	-10.16	4.7
AlP	1.34	-1.6	-4.38	5.1	-9.52	11.1
AlAs	1.01	-1.3	-4.60	5.9	-8.93	11.4
AlSb	1.18	-2.1	-3.64	6.6	-8.85	16.1
GaN	-1.21	0.6	-8.15	4.0	-7.37	3.6
GaP	1.27	-1.4	-3.83	4.3	-8.83	10.0
GaAs	1.05	-1.4	-3.70	4.9	-8.15	10.8
GaSb	1.12	-2.0	-3.06	5.4	-8.01	14.2
InN	-1.35	0.9	-5.23	3.5	-3.66	2.5
InP	1.00	-1.4	-3.00	4.2	-5.93	8.4
InAs	0.92	-1.6	-2.89	5.0	-5.66	9.8
InSb	1.10	-2.3	-2.51	5.2	-6.35	13.1
ZnS	1.09	-1.4	-3.09	4.0	-5.16	6.7
ZnSe	1.36	-2.2	-2.92	4.7	-4.99	8.0
ZnTe	1.72	-3.4	-2.40	4.7	-5.60	11.0
CdS	0.88	-1.4	-2.23	3.6	-2.94	4.7
CdSe	1.03	-1.9	-2.19	4.1	-2.90	5.5
CdTe	1.44	-3.2	-1.88	4.2	-3.70	8.3
HgS	1.32	-1.9	-1.10	1.6	-2.16	3.2
HgSe	1.56	-3.1	-0.90	1.8	-2.15	4.3
HgTe	1.97	-4.7	-0.74	1.8	-3.19	7.5

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