

3. Realistic band structures

A successful approach for valence and conduction bands uses pseudopotential V_p

$$H = \frac{p^2}{2m} + V_p(\vec{r}) , \quad (3.1)$$

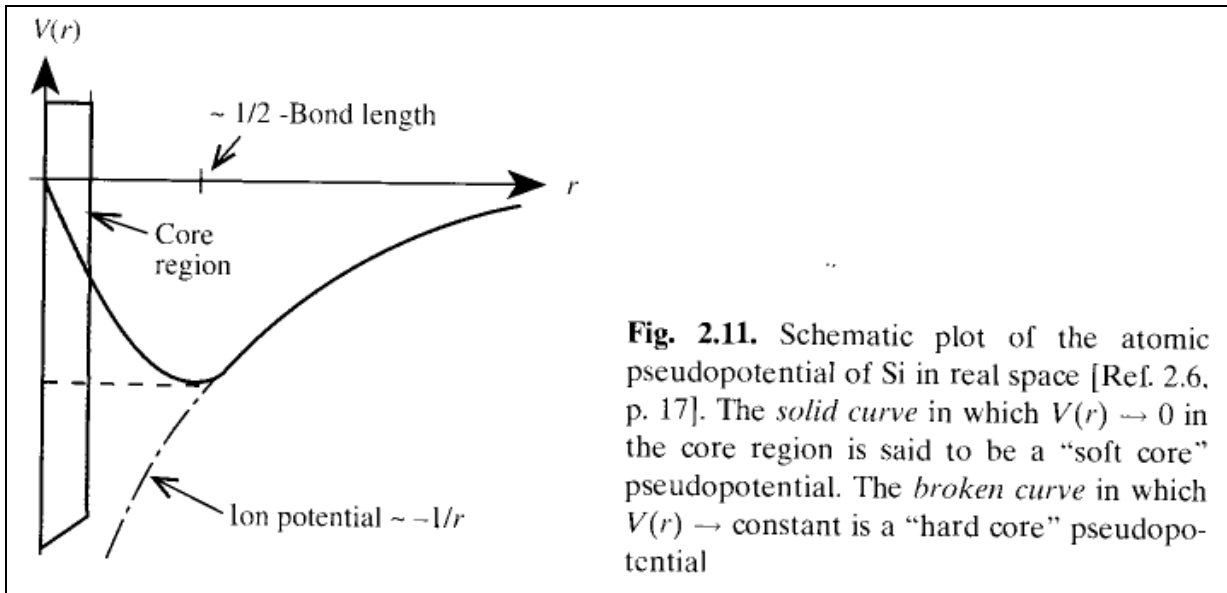
where

$$V_p(\vec{r}) = V(\vec{r}) + \sum_t (E_{\vec{k}} - E_t) |b_t\rangle \langle b_t| . \quad (3.2)$$

Here $|b_t\rangle$ are states of inner shells belonging to eigenenergies E_t . This potential leads to the same eigenenergies E_k of the valence and conduction bands as the actual potential V :

$$\left[\frac{p^2}{2m} + V_p(\vec{r}) \right] |\psi_{\vec{k}}\rangle = \left[\frac{p^2}{2m} + V(\vec{r}) + \sum_t (E_{\vec{k}} - E_t) |b_t\rangle \langle b_t| \right] |\psi_{\vec{k}}\rangle = E_{\vec{k}} |\psi_{\vec{k}}\rangle . \quad (3.3)$$

However, the corresponding eigenfunctions are smooth in the regions of inner atomic shells. The reason is the subtraction of pronounced variations of the actual potential in those regions, since the eigenstates $|b_t\rangle$ and $|\psi_{\vec{k}}\rangle$ are orthogonal.



„Successful“ calculations for Si, Ge, α -Sn, and several III-Vs and, II-VIs (Chellikowsky & Cohen) use:

$$V_p(\vec{r}) = \sum_{\vec{K}} V(\vec{K}) e^{i\vec{K}\vec{r}} , \quad (3.4)$$

where

$$V(\vec{K}) = \sum_{\alpha} S_{\alpha}(\vec{K}) V_{\alpha}(\vec{K}), \quad S_{\alpha}(\vec{K}) = \frac{1}{N\alpha} \sum_j e^{-i\vec{K}\vec{R}_j^{\alpha}}, \quad (3.5)$$

$$V_{\alpha}(\vec{K}) = \frac{1}{\Omega_a} \iiint e^{-i\vec{K}\vec{R}_j^{\alpha}} V_p^a(\vec{r}) d^3\vec{r}, \quad (3.6)$$

Choosing a (small) set of the “formfactors” ($V(\mathbf{K})$) might be based on “ab-initio” calculations, or also on empirical adjustment.

The work of Chellikowsky and Cohen (PRB 1976) includes also a few “nonlocal” terms.

TABLE I. Pseudopotential parameters for the diamond-structure semiconductors.

Compound	Form factors (Ry)			Lattice constant (\AA)	
	$V(\sqrt{3})$	$V(\sqrt{8})$	$V(\sqrt{11})$		
Si ^a	-0.224	0.055	0.072	5.43	
Si	-0.257	-0.040	0.033	5.43	
Ge	-0.221	0.019	0.056	5.65	
α -Sn	-0.190	-0.008	0.040	6.49	
Compound	Nonlocal parameters			Radii (\AA)	
	α_0 (Ry)	β_0	A_2 (Ry)	R_0	R_2
Si	0.55	0.32	0	1.06	0
Ge ^b	0	0	0.275	0	1.22
α -Sn	0	0.40	0.70	1.06	1.41

^a Purely local pseudopotential.

^b Gaussian nonlocal well.

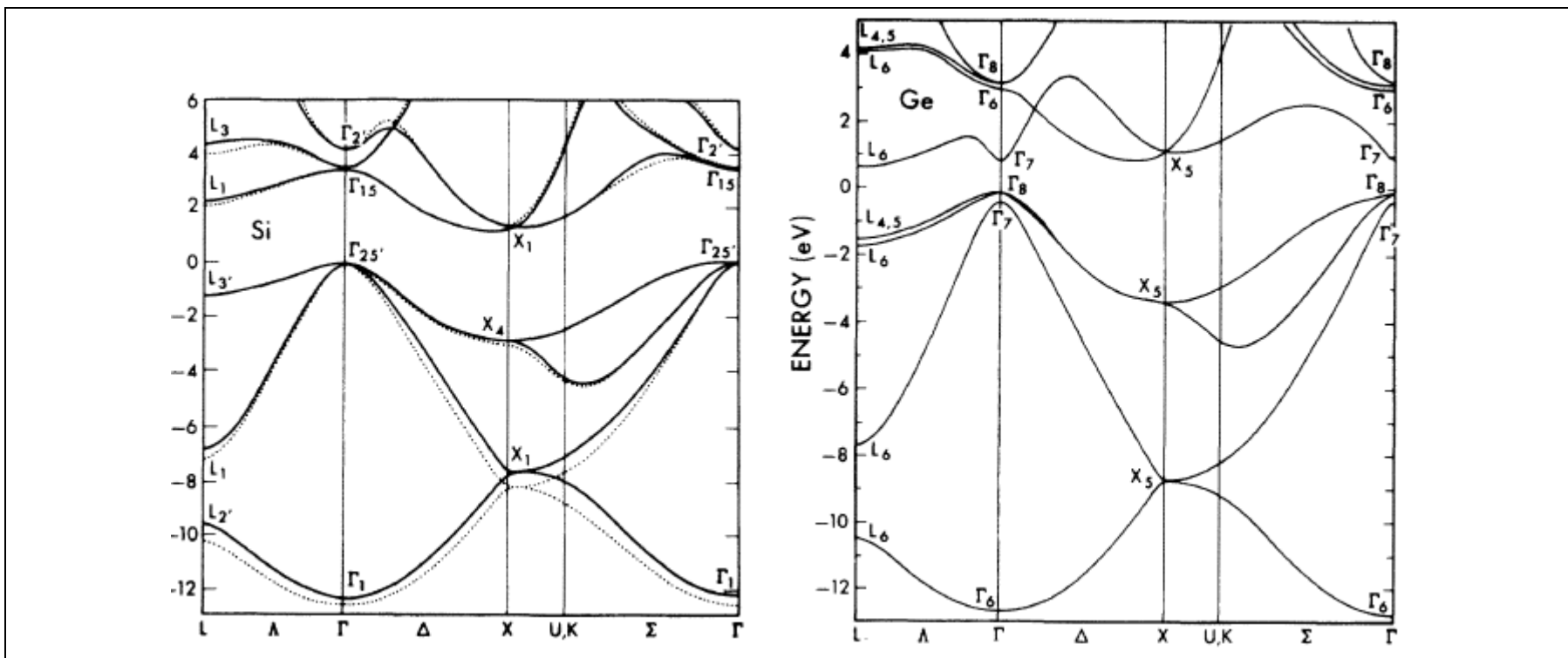
The resulting energies in high-symmetry points of the Brillouin zone are in fairly good agreement with experimental data (partly due to the empirical adjustment).

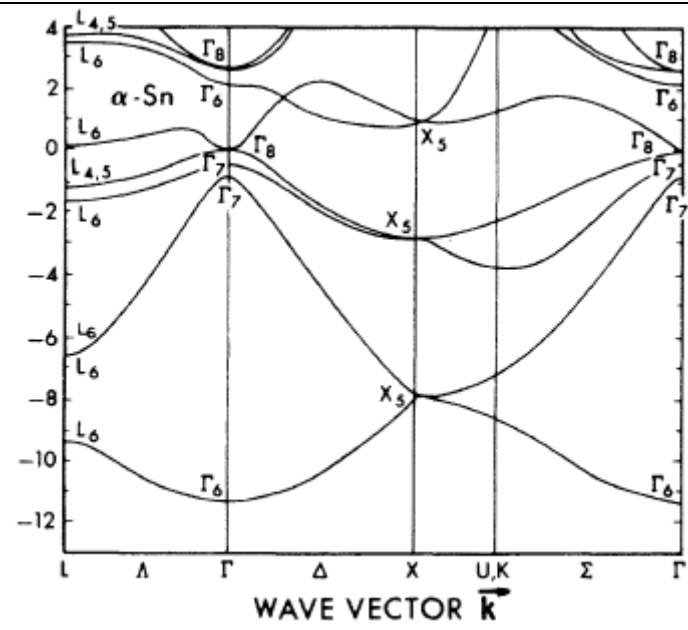
TABLE II. Eigenvalues for diamond-structure semi-conductors at Γ , X , and L . Energies are in eV.

Point	Level	Compound			
		Si ^a		Ge	α -Sn
		Local	Nonlocal		
Γ	Γ_6^v	-12.53	-12.36	-12.66	-11.34
	Γ_7^v			-0.29	-0.80
	Γ_8^v	0.00	0.00	0.00	0.00
	Γ_6^c	4.17	4.10	0.90	-0.42
	Γ_8^c			3.01	2.08
	Γ_8^c	3.43	3.43	3.22	2.66
X	X_5^v	-8.27	-7.69	-8.65	-7.88
	X_5^v	-2.99	-2.86	-3.29	-2.75
	X_5^c	1.22	1.17	1.16	0.90
L	L_6^v	-10.17	-9.55	-10.39	-9.44
	L_6^v	-7.24	-6.96	-7.61	-6.60
	L_6^v			-1.63	-1.68
	$L_{4,5}^v$	-1.22	-1.23	-1.43	-1.20
	L_6^c	2.15	2.23	0.76	0.14
	L_6^c			4.16	3.48
	$L_{4,5}^c$	4.00	4.34	4.25	3.77

^a Spin-orbit corrections not included.

The resulting bandstructures along several high-symmetry directions for elemental semiconductors:





Formfactors and electron energies for several III-V compounds:

TABLE VIII. Pseudopotential parameters for the III-V zinc-blende semiconductors. α_0 and A_2 are in Ry.

Compound	Form factors (Ry)						Lattice constant (Å)
	$V^S(\sqrt{3})$	$V^S(\sqrt{8})$	$V^S(\sqrt{11})$	$V^A(\sqrt{3})$	$V^A(\sqrt{4})$	$V^A(\sqrt{11})$	
GaP	-0.230	0.020	0.057	0.100	0.070	0.025	5.45
GaAs	-0.214	0.014	0.067	0.055	0.038	0.001	5.65
GaSb	-0.220	0.005	0.045	0.040	0.030	0.000	6.10
InP	-0.235	0.000	0.053	0.080	0.060	0.030	5.86
InAs	-0.230	0.000	0.045	0.055	0.045	0.010	6.05
InSb	-0.200	-0.010	0.044	0.044	0.030	0.015	6.47

Compound	Nonlocal parameters					Spin orbit μ
	Cation		α_0	Anion		
	β_0	A_2			β_0	A_2
GaP	0.30	0.40	0.32	0.05	0.45	...
GaAs ^a	0	0.125	0	0	0.625	0.000 80
GaSb	0.20	0.20	0	0.30	0.60	0.0011
InP	0.25	0.55	0.30	0.05	0.35	0.0020
InAs	0.35	0.50	0	0.25	1.00	0.0012
InSb	0.45	0.55	0	0.48	0.70	0.0018

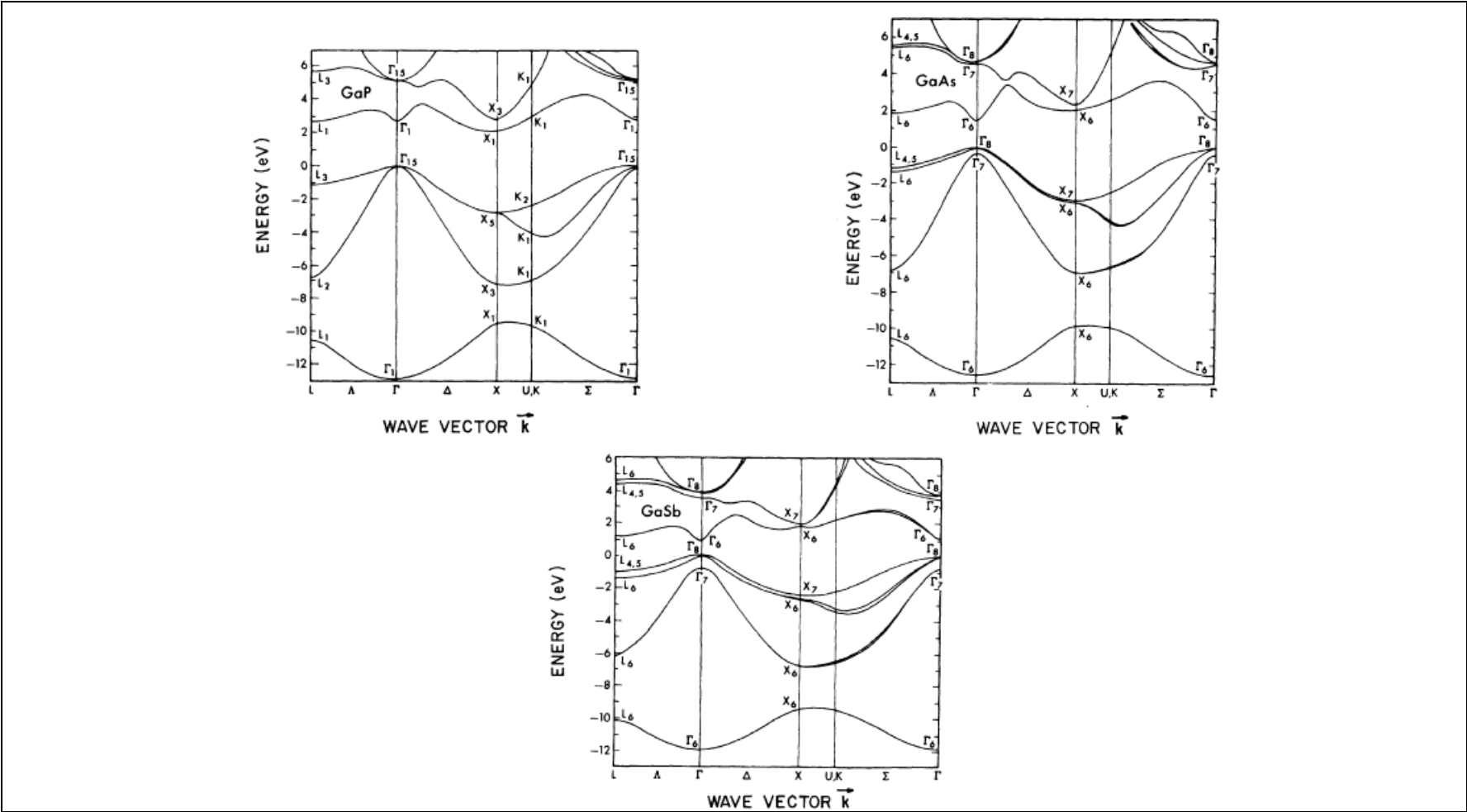
^a Gaussian nonlocal well.

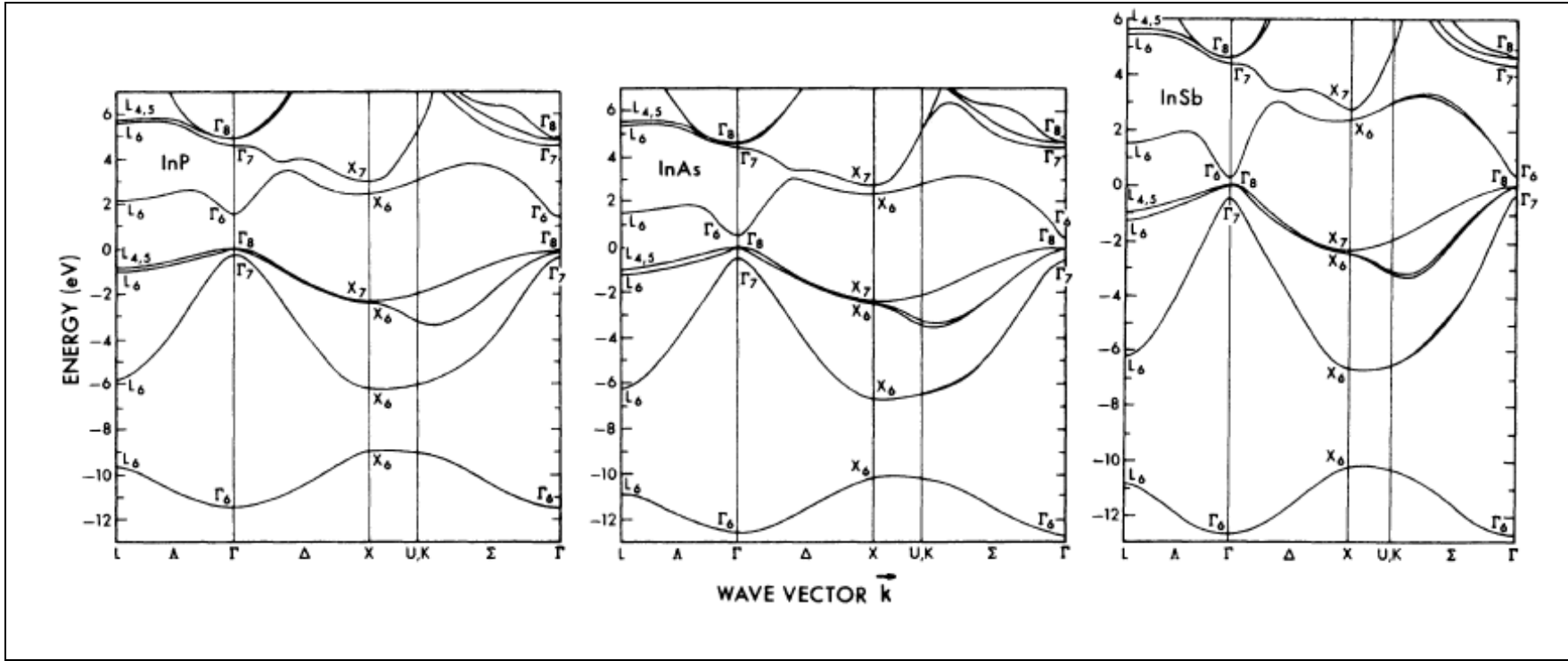
TABLE IX. Eigenvalues at Γ , X , and L for III-V zinc-blende semiconductors. Energies are in eV.

Point	Level	Compound					
		GaP ^a	GaAs	GaSb	InP	InAs	InSb
Γ	Γ_6^v	-12.99	-12.55	-12.00	-11.42	-12.69	-11.71
	Γ_7^v		-0.35	-0.76	-0.21	-0.43	-0.82
	Γ_8^v	0.00	0.00	0.00	0.00	0.00	0.00
	Γ_6^c	2.88	1.51	0.86	1.50	0.37	0.25
	Γ_7^c		4.55	3.44	4.64	4.39	3.16
	Γ_8^c	5.24	4.71	3.77	4.92	4.63	3.59
X	X_6^v	-9.46	-9.83	-9.33	-8.91	-10.20	-9.20
	X_6^v	-7.07	-6.88	-6.76	-6.01	-6.64	-6.43
	X_6^v		-2.99	-2.61	-2.09	-2.47	-2.45
	X_7^v	-2.73	-2.89	-2.37	-2.06	-2.37	-2.24
	X_6^c	2.16	2.03	1.72	2.44	2.28	1.71
	X_7^c	2.71	2.38	1.79	2.97	2.66	1.83
L	L_6^v	-10.60	-10.60	-10.17	-9.67	-10.92	-9.95
	L_6^v	-6.84	-6.83	-6.25	-5.84	-6.23	-5.92
	L_6^v		-1.42	-1.45	-1.09	-1.26	-1.44
	$L_{4,5}^v$	-1.10	-1.20	-1.00	-0.94	-1.00	-0.96
	L_6^c	2.79	1.82	1.22	2.19	1.53	1.03
	L_6^c		5.47	4.43	5.58	5.42	4.30
	$L_{4,5}^c$	5.74	5.52	4.59	5.70	5.55	4.53

^a Spin-orbit interactions not included.

Bandstructures along high-symmetry directions:

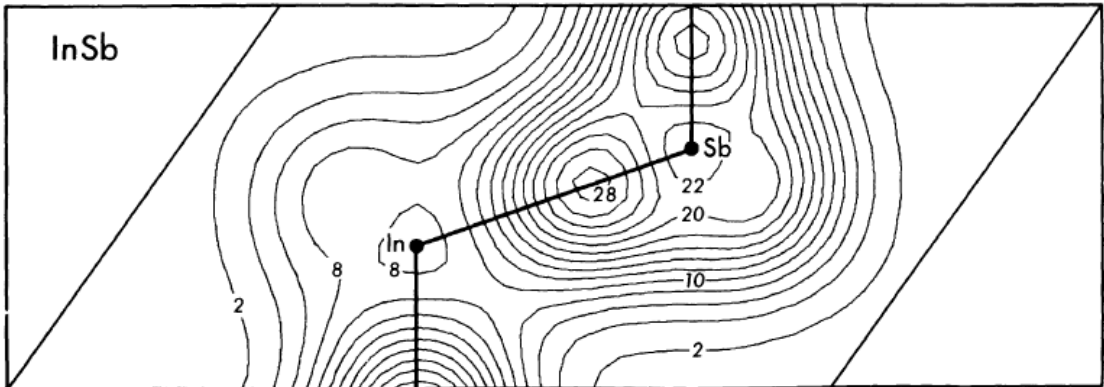
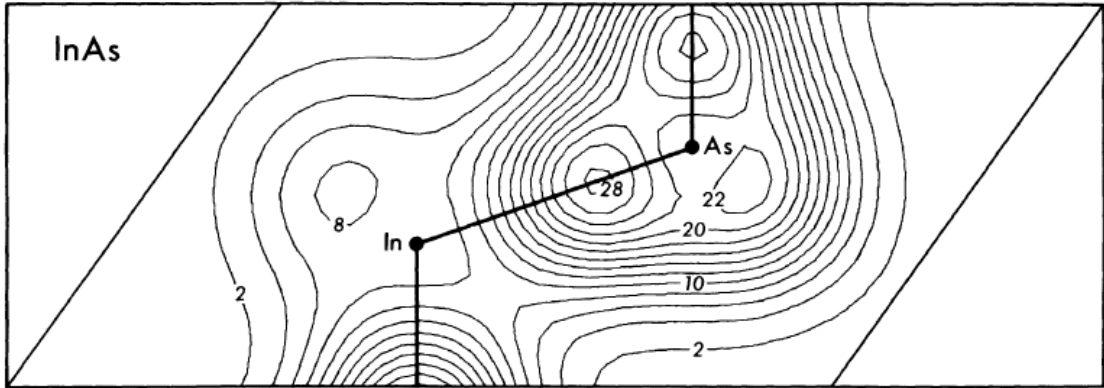
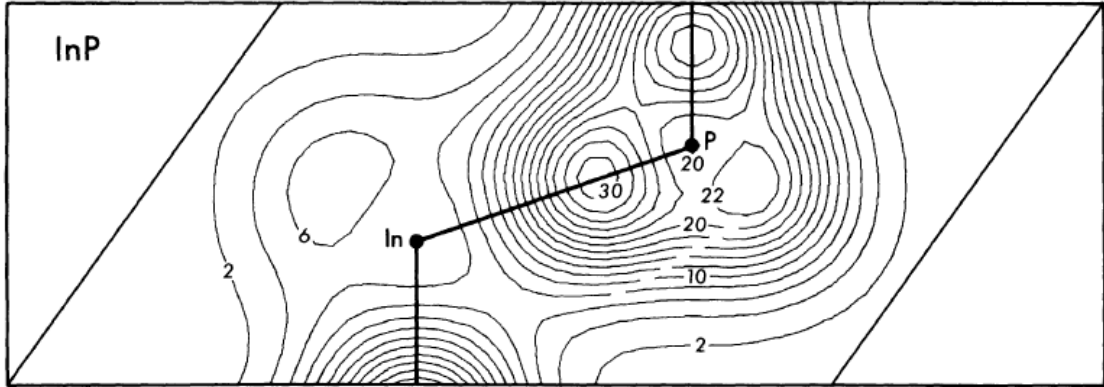




Valence charge densities of In compounds (covalent and ionic contribution to bonding)

TABLE XIX. Fourier coefficients of the valence charge densities for the In zinc blends. The real part of the coefficient is listed first. The origin for this calculation is at the cation site.

$\vec{G}(\mathbf{a}/2\pi)$	Fourier coefficients (e/Ω_c)					
	InP		InAs		InSb	
(000)	8.000	0.000	8.000	0.000	8.000	0.000
(111)	0.801	-2.067	0.885	-1.998	0.994	-1.915
(200)	-1.013	0.000	-0.860	0.000	-0.718	0.000
(220)	0.097	0.000	0.135	0.000	0.144	0.000
(311)	-0.255	-0.160	-0.200	-0.151	-0.223	-0.161
(222)	0.048	-0.439	0.030	-0.437	0.020	-0.409
(400)	-0.237	0.000	-0.215	0.000	-0.245	0.000
(331)	0.071	0.063	0.040	0.047	0.045	0.038
(420)	0.069	0.000	0.055	0.000	0.048	0.000
(422)	-0.046	0.043	-0.042	0.020	-0.043	0.024



II-VI compounds (ZnSe and CdTe)

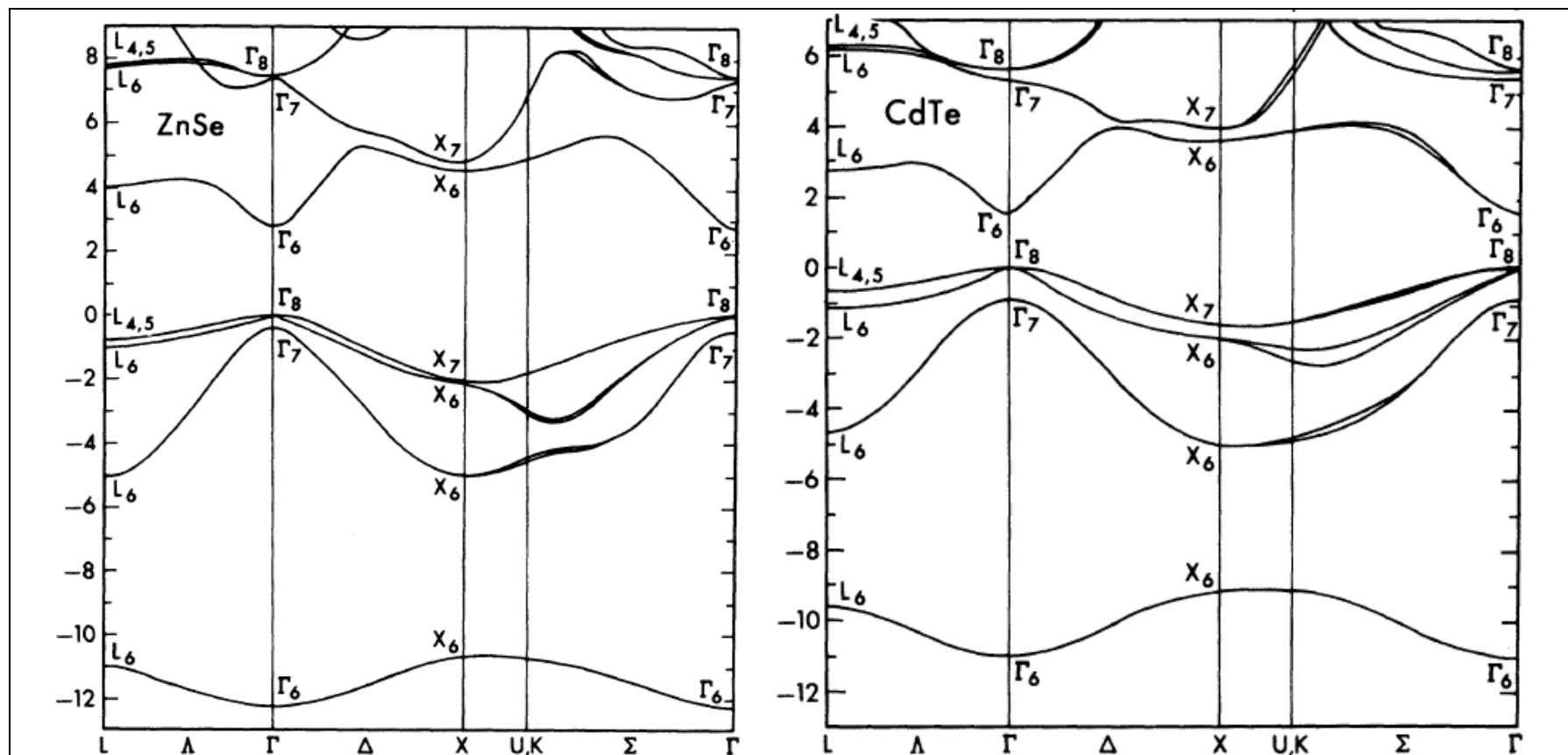
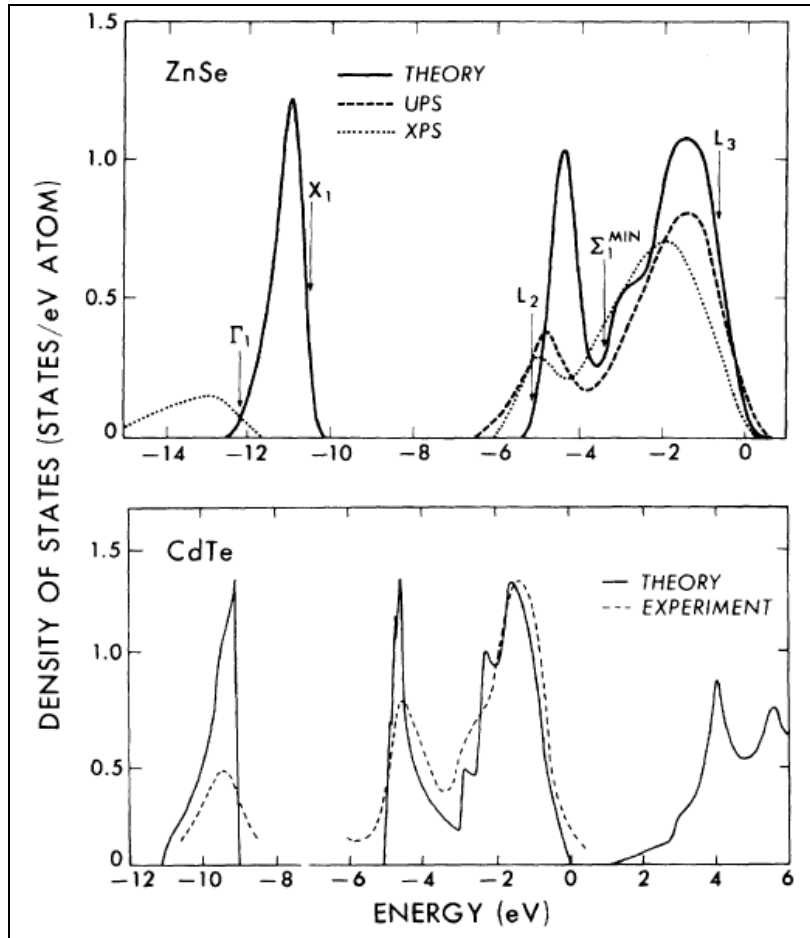


TABLE XXI. Eigenvalues for the II-VI zinc-blende semiconductors at Γ , X , and L . Energies are in eV.

Point	Level	Compound	
		ZnSe	CdTe
Γ	Γ_6^v	-12.25	-11.07
	Γ_7^v	- 0.45	- 0.89
	Γ_8^v	0.00	0.00
	Γ_6^c	2.76	1.59
	Γ_7^c	7.33	5.36
	Γ_8^c	7.42	5.61
X	X_6^v	-10.72	- 9.12
	X_6^v	- 4.96	- 5.05
	X_6^v	- 2.17	- 1.98
	X_7^v	- 1.96	- 1.60
	X_6^c	4.54	3.48
	X_7^c	5.17	3.95
L	L_6^v	-11.08	- 9.64
	L_6^v	- 5.08	- 4.73
	L_6^v	- 1.04	- 1.18
	$L_{4,5}^v$	- 0.76	- 0.65
	L_6^c	3.96	2.82
	L_6^c	7.68	6.18
	$L_{4,5}^c$	7.72	6.35

Density of states



Compare DOS with the calculated bandstructures for ZnSe and CdTe.