3. Realistické pásové struktury

Pseudopotenciál V_p

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

kde

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

Zde je $|b_t\rangle$ stav vnitřní slupky příslušný k energii E_t. Tento potenciál dává stejné vlastní energie E_k, ale vlastní funkce jsou hladké v oblasti vnitřních slupek (skutečný rychle se měnící potenciál zde byl odečten):

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

neboť vlastní stavy $|b_t\rangle$ a $|\psi_{\vec{k}}\rangle$ jsou ortogonální.

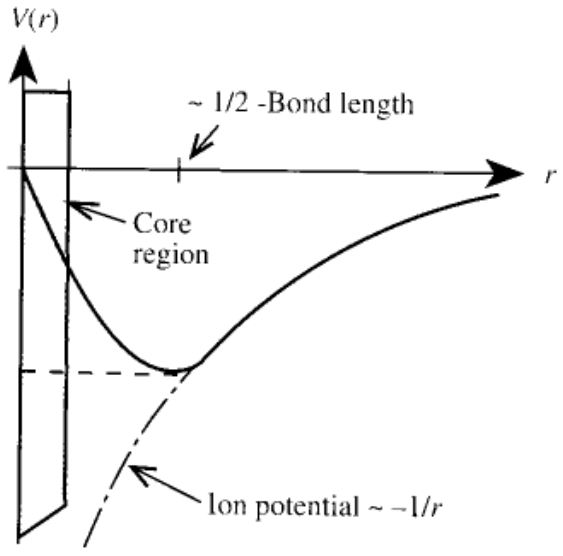


Fig. 2.11. Schematic plot of the atomic pseudopotential of Si in real space [Ref. 2.6, p. 17]. The *solid curve* in which $V(r) \to 0$ in the core region is said to be a "soft core" pseudopotential. The *broken curve* in which $V(r) \to$ constant is a "hard core" pseudopotential

Atomový pseudopotenciál Si schematicky.

„Úspěšné“ výpočty pro Si, Ge, α-Sn, III-V, II-VI, Chellikowsky & Cohen:

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

kde

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

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

Empirická adjustace, případně „ab-initio“ pseudopotenciály.

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

Compound	Form factors (Ry) $V(\sqrt{3})$	$V(\sqrt{8})$	$V(\sqrt{11})$	Lattice constant (Å)
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 α_0 (Ry)	β_0	A_2 (Ry)	Radii (Å) 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.

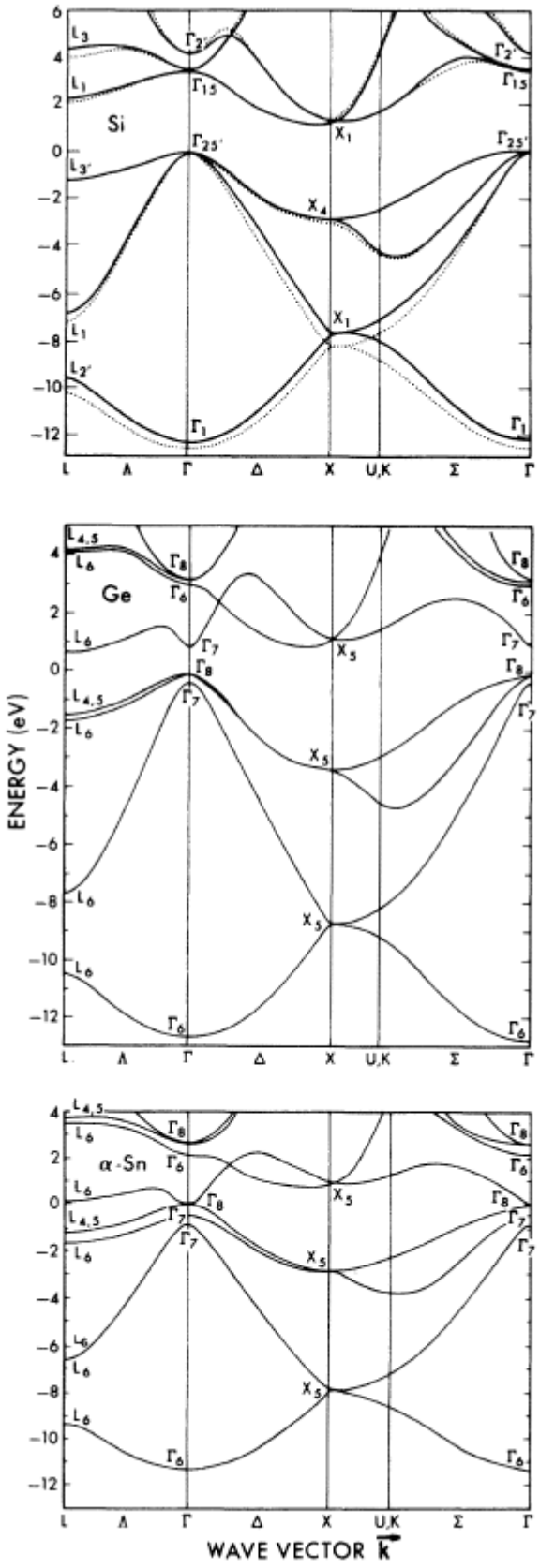
Formfaktory pseudopotenciálu, Chelikowsky and Cohen, PRB (1976).

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

Point	Level	Si [a]		Compound Ge	Compound 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_7^c	4.17	4.10	0.90	−0.42
	Γ_6^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.

Energie stavů v Γ, X, L. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).



Pásová struktura Si, Ge a α-Sn. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).

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

Compound	Form factors (Ry) $V^S(\sqrt{3})$	$V^S(\sqrt{8})$	$V^S(\sqrt{11})$	$V^A(\sqrt{3})$	$V^A(\sqrt{4})$	$V^A(\sqrt{11})$	Lattice constant (Å)
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 Cation β_0	Cation A_2	Cation α_0	Anion β_0	Anion A_2	Spin orbit μ
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.

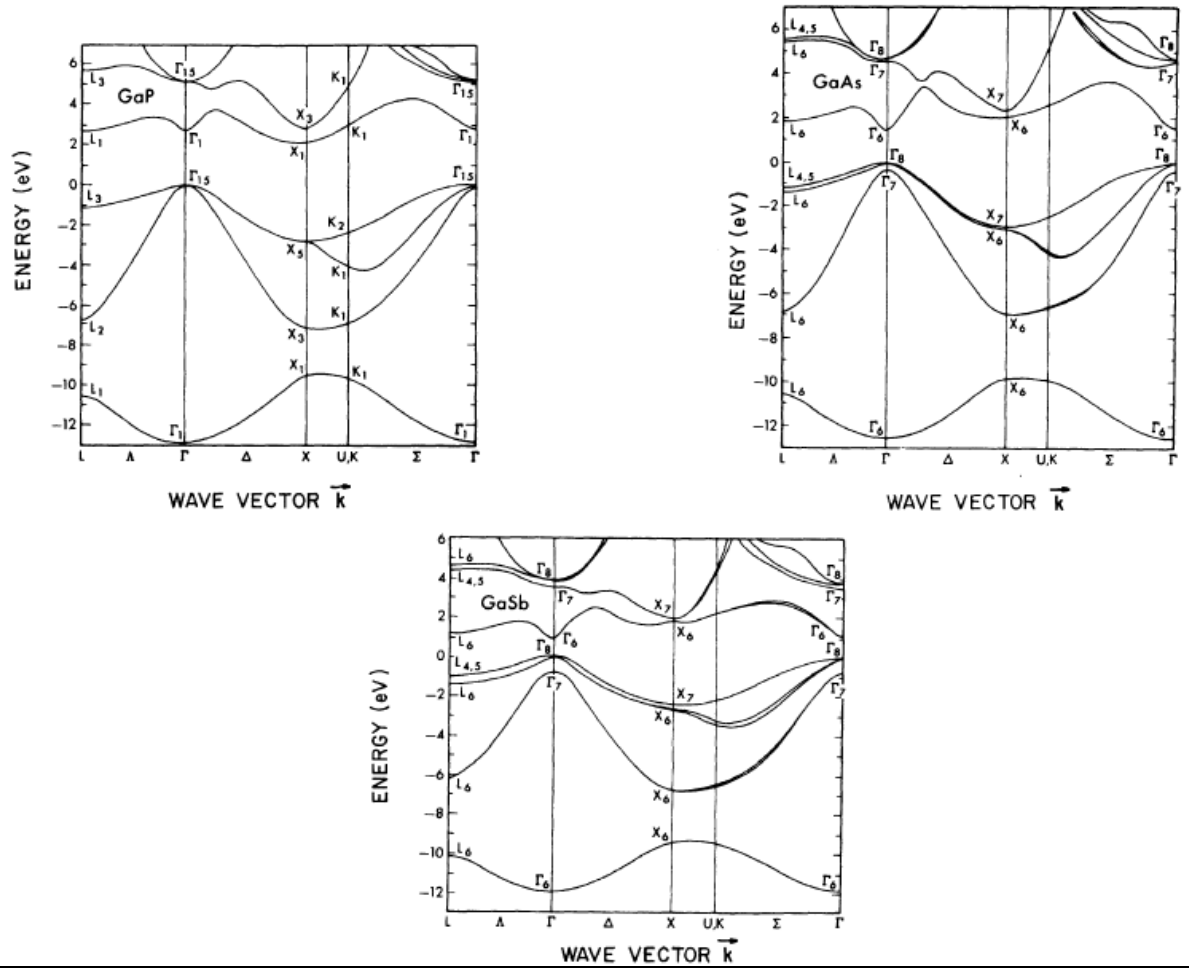
Formfaktory pseudopotenciálu, Chelikowsky and Cohen, PRB (1976).

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

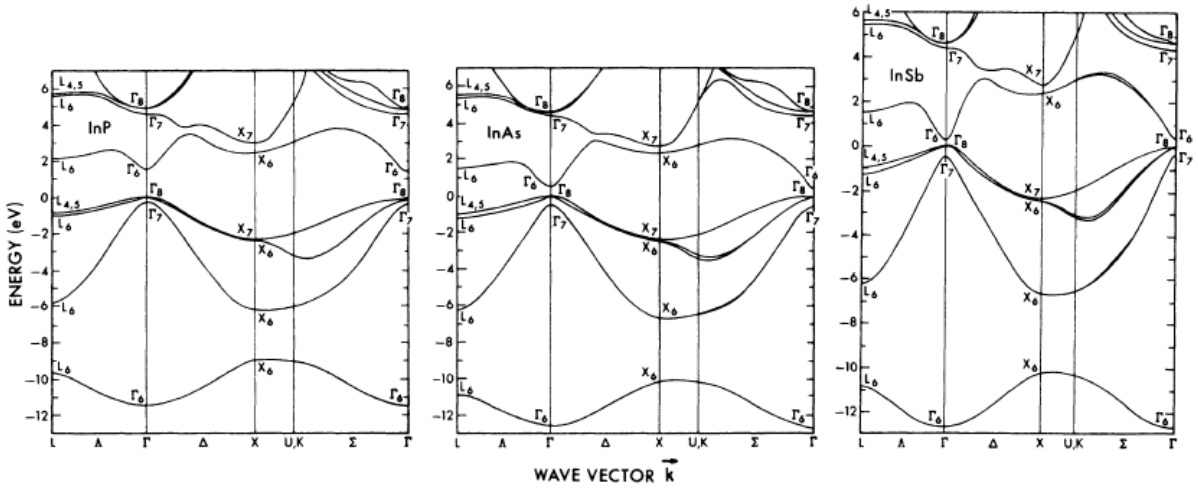
Point	Level	Compound GaP [a]	GaAs	GaSb	InP	InAs	InSb
Γ	Γ_6^v	−12.99	−12.55	−12.00	−11.42	−12.69	−11.71
	Γ_7^v		−0.35	−0.76	−0.21	−0.43	−0.82
	Γ_8^v	0.00	0.00	0.00	0.00	0.00	0.00
	Γ_6^v	2.88	1.51	0.86	1.50	0.37	0.25
	Γ_7^c		4.55	3.44	4.64	4.39	3.16
	Γ_8^c	5.24	4.71	3.77	4.92	4.63	3.59
X	X_6^v	−9.46	−9.83	−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.

Energie stavů v Γ, X, L. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).



Pásová struktura. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).



Pásová struktura. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).

2 vybrané II-VI

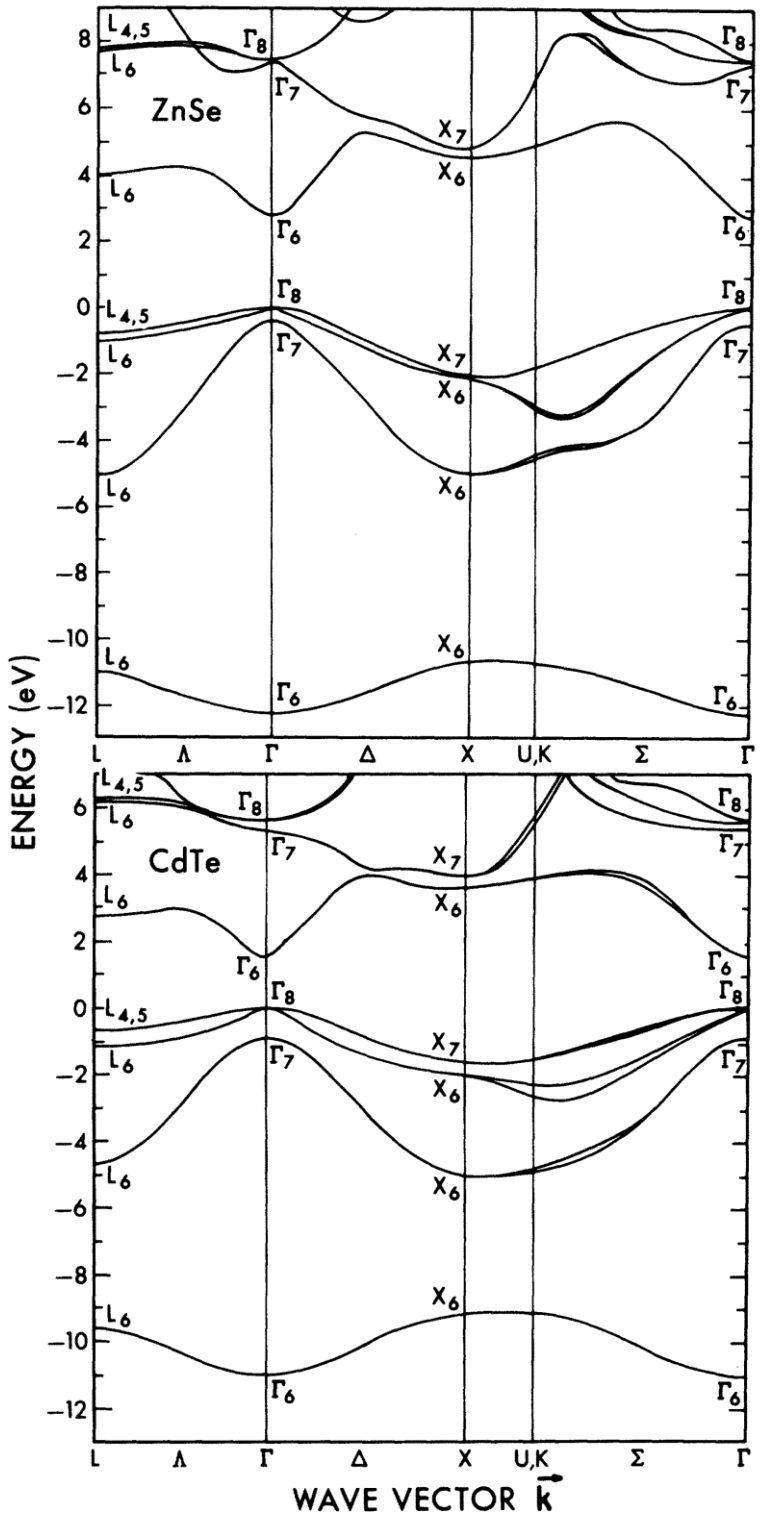


FIG. 17. Band structures for ZnSe and CdTe.

Pásová struktura. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).

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

$\vec{G}(a/2\pi)$	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

Formfaktory pseudopotenciálu, Chelikowsky and Cohen, PRB (1976).

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

Energie stavů v Γ, X, L. Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).