

### 3. Realistické pásové struktury

Pseudopotenciál  $V_p$

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

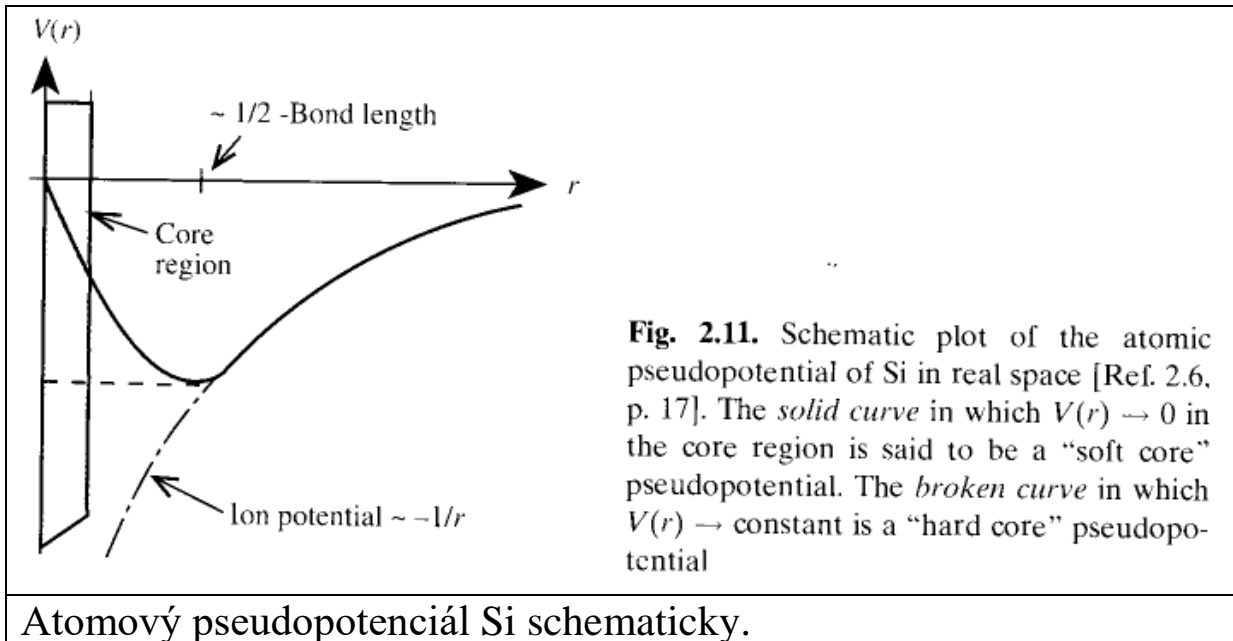
kde

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

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

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

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



Atomový pseudopotenciál Si schematicky.

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

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

kde

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

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

Empirická adjustace, případně „ab-initio“ pseudopotenciály.

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

Compound	Form factors (Ry)			Lattice constant ( $\text{\AA}$ )	
	$V(\sqrt{3})$	$V(\sqrt{8})$	$V(\sqrt{11})$		
Si <sup>a</sup>	-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	
$\alpha$ -Sn	-0.190	-0.008	0.040	6.49	
Compound	Nonlocal parameters			Radii ( $\text{\AA}$ )	
	$\alpha_0$ (Ry)	$\beta_0$	$A_2$ (Ry)	$R_0$	$R_2$
Si	0.55	0.32	0	1.06	0
Ge <sup>b</sup>	0	0	0.275	0	1.22
$\alpha$ -Sn	0	0.40	0.70	1.06	1.41

<sup>a</sup> Purely local pseudopotential.

<sup>b</sup> Gaussian nonlocal well.

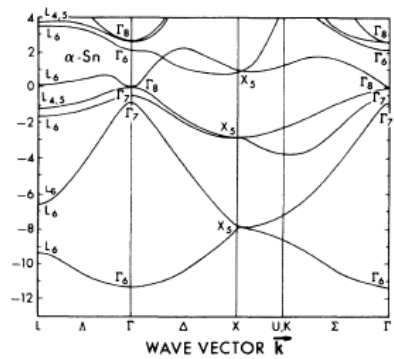
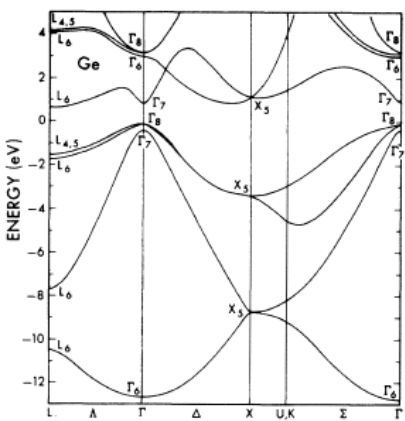
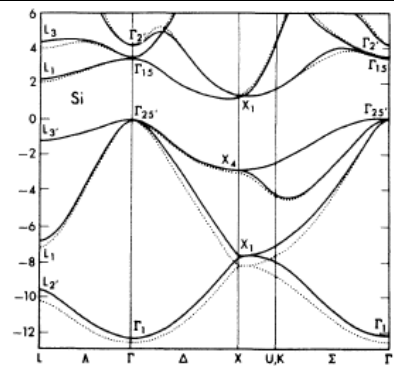
Formfaktory pseudopotenciálu, Chelikowsky and Cohen, PRB (1976).

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

Point	Level	Compound			
		Si <sup>a</sup>		Ge	$\alpha$ -Sn
		Local	Nonlocal		
$\Gamma$	$\Gamma_6^v$	-12.53	-12.36	-12.66	-11.34
	$\Gamma_7^v$			-0.29	-0.80
	$\Gamma_8^v$	0.00	0.00	0.00	0.00
	$\Gamma_7^c$	4.17	4.10	0.90	-0.42
	$\Gamma_6^c$			3.01	2.08
	$\Gamma_8^c$	3.43	3.43	3.22	2.66
$X$	$X_5^p$	-8.27	-7.69	-8.65	-7.88
	$X_5^p$	-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

<sup>a</sup> Spin-orbit corrections not included.

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



Pásová struktura Si, Ge a  $\alpha$ -Sn.

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

TABLE VIII. Pseudopotential parameters for the III-V zinc-blende semiconductors.  $\alpha_0$  and  $A_2$  are in Ry.

Compound	$V^S(\sqrt{3})$	$V^S(\sqrt{8})$	Form factors (Ry)				Lattice constant ( $\text{\AA}$ )
			$V^S(\sqrt{11})$	$V^A(\sqrt{3})$	$V^A(\sqrt{4})$	$V^A(\sqrt{11})$	
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 $\mu$
	Cation		$\alpha_0$	Anion		
	$\beta_0$	$A_2$			$\beta_0$	$A_2$
GaP	0.30	0.40	0.32	0.05	0.45	...
GaAs <sup>a</sup>	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

<sup>a</sup> Gaussian nonlocal well.

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

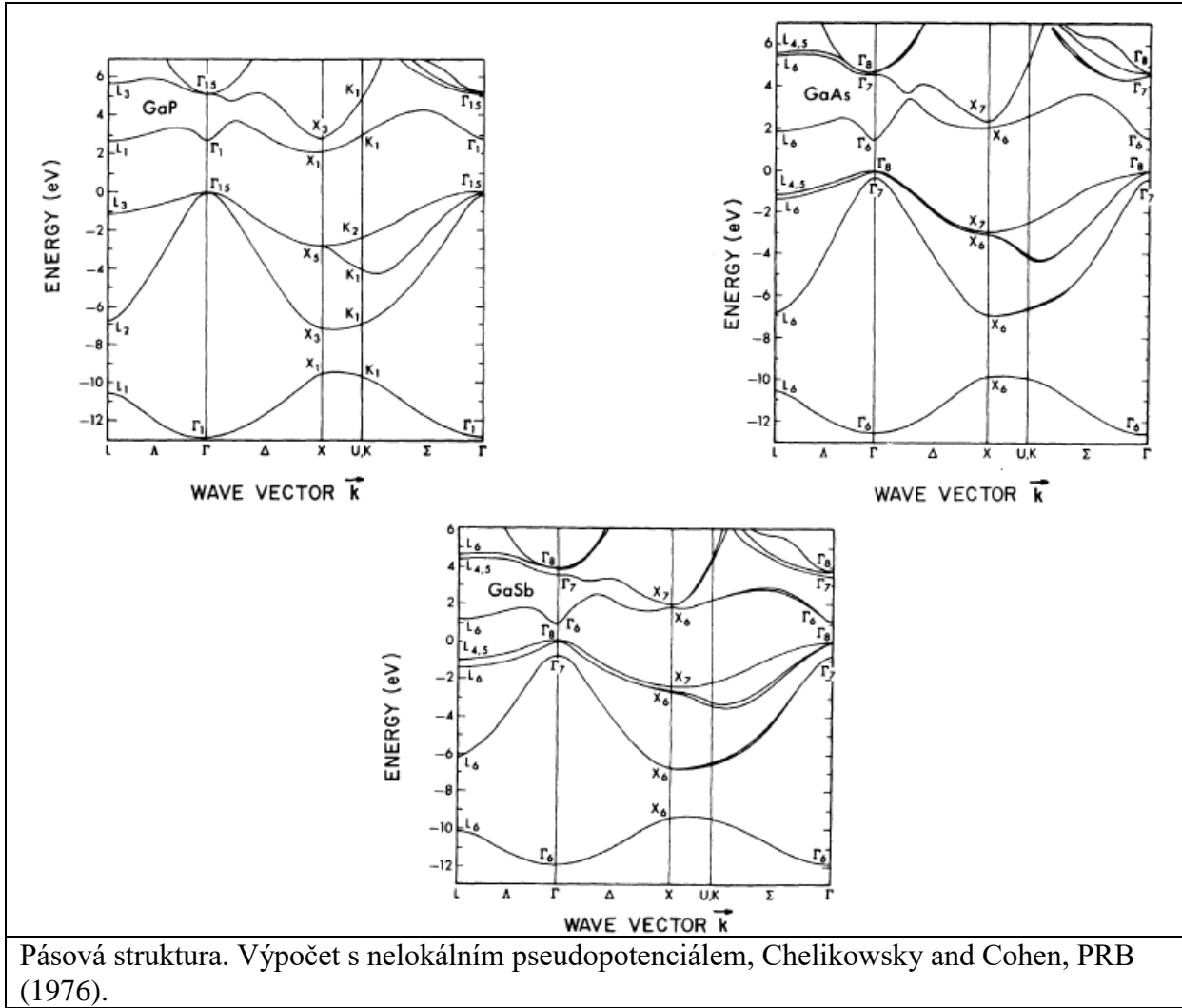
TABLE IX. Eigenvalues at  $\Gamma$ ,  $X$ , and  $L$  for III-V zinc-blende semiconductors. Energies are in eV.

Point	Level	Compound					
		GaP <sup>a</sup>	GaAs	GaSb	InP	InAs	InSb
$\Gamma$	$\Gamma_6^v$	-12.99	-12.55	-12.00	-11.42	-12.69	-11.71
	$\Gamma_7^v$		-0.35	-0.76	-0.21	-0.43	-0.82
	$\Gamma_8^v$	0.00	0.00	0.00	0.00	0.00	0.00
	$\Gamma_6^c$	2.88	1.51	0.86	1.50	0.37	0.25
	$\Gamma_7^c$		4.55	3.44	4.64	4.39	3.16
	$\Gamma_8^c$	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
	$X_7^v$	-7.07	-6.88	-6.76	-6.01	-6.64	-6.43
	$X_8^v$		-2.99	-2.61	-2.09	-2.47	-2.45
	$X_7^c$	-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
	$L_7^v$	-6.84	-6.83	-6.25	-5.84	-6.23	-5.92
	$L_8^v$		-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
	$L_7^c$		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

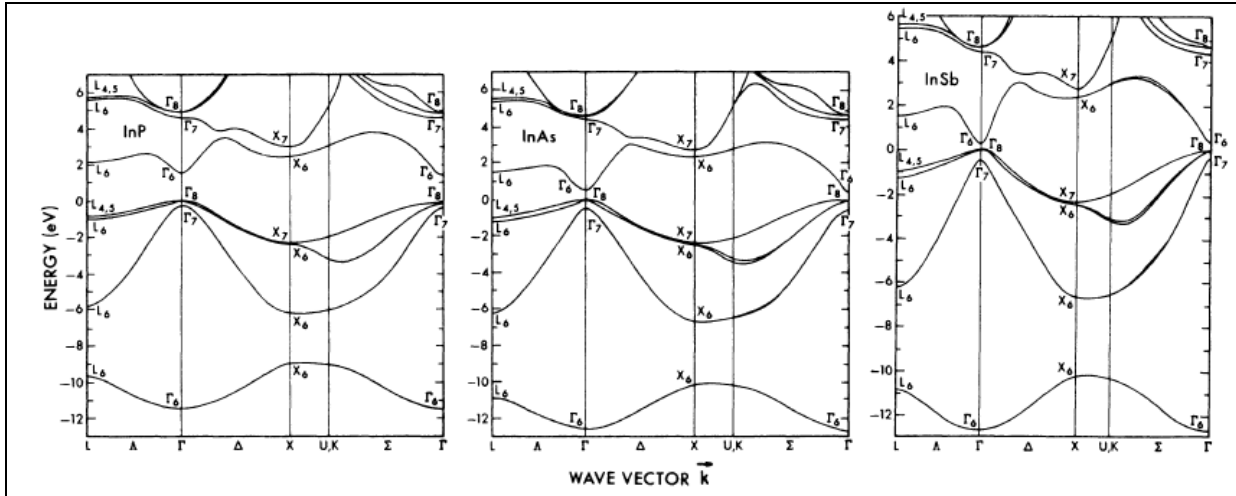
<sup>a</sup> Spin-orbit interactions not included.

Energie stavů v  $\Gamma$ ,  $X$ ,  $L$ . 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).



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

Point	Level	Compound	
		ZnSe	CdTe
$\Gamma$	$\Gamma_6^v$	-12.25	-11.07
	$\Gamma_7^v$	- 0.45	- 0.89
	$\Gamma_8^v$	0.00	0.00
	$\Gamma_6^c$	2.76	1.59
	$\Gamma_7^c$	7.33	5.36
	$\Gamma_8^c$	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  $\Gamma$ ,  $X$ ,  $L$ . Výpočet s nelokálním pseudopotenciálem, Chelikowsky and Cohen, PRB (1976).

Podarí se najít pseudopotenciálové výpočty pásové struktury diamantu? Pokud ano, jak se od sebe liší vypočtená pásová struktura diamantu a křemíku?