# 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.

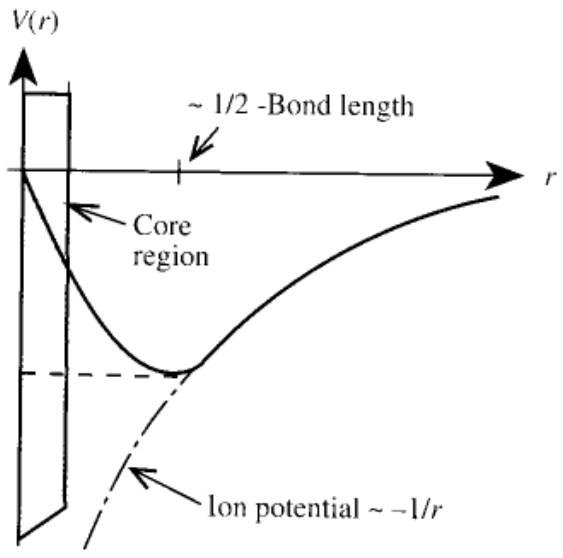



**Fig. 2.11.** Schematic plot of the atomic pseudopotential of Si in real space [Ref. 2.6, p. 17]. The *solid curve* in which $V(r) \to 0$ in the core region is said to be a "soft core" pseudopotential. The *broken curve* in which $V(r) \to$ constant is a "hard core" pseudopotential

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 |
| $\alpha$-Sn | −0.190 | −0.008 | 0.040 | 6.49 |

| Compound | Nonlocal parameters $\alpha_0$ (Ry) | $\beta_0$ | $A_2$ (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 |
| $\alpha$-Sn | 0 | 0.40 | 0.70 | 1.06 | 1.41 |

[a] Purely local pseudopotential.
[b] Gaussian nonlocal well.

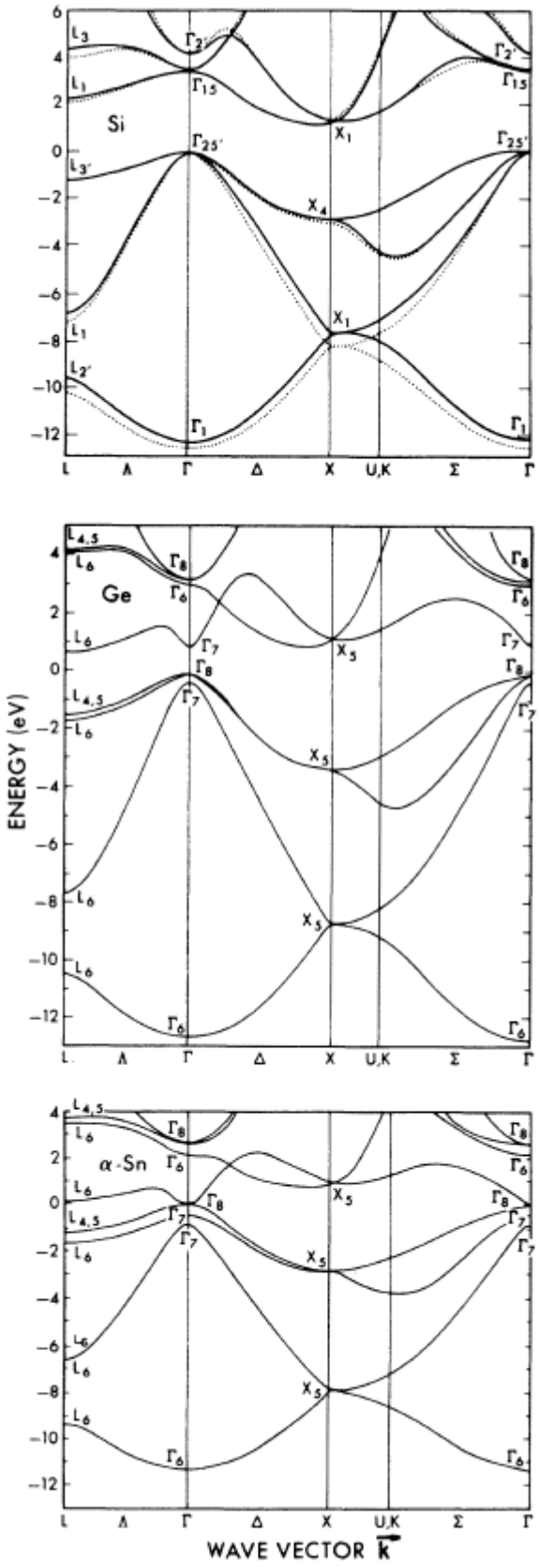
Formfaktory pseudopotenciálu, Chelikowsky and Cohen, PRB (1976).

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

| Point | Level | Si [a] | | Compound Ge | Compound $\alpha$-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 |
| $X$ | $X_5^v$ | −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 $\Gamma$, $X$, $L$. 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. $\alpha_0$ 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 $\beta_0$ | Cation $A_2$ | Cation $\alpha_0$ | Anion $\beta_0$ | Anion $A_2$ | Spin orbit $\mu$ |
|---|---|---|---|---|---|---|
| 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.

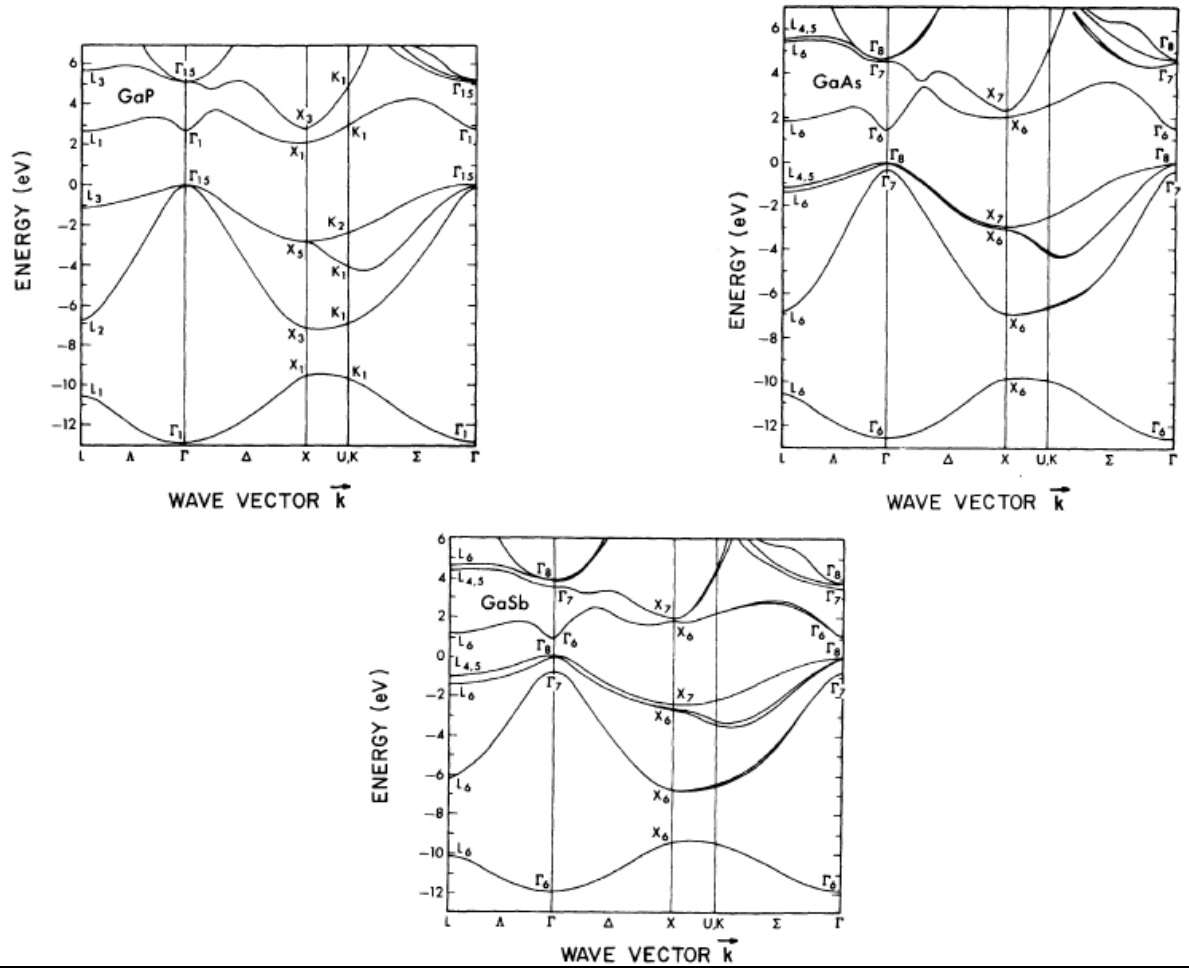
Formfaktory pseudopotenciálu, Chelikowsky and Cohen, PRB (1976).

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

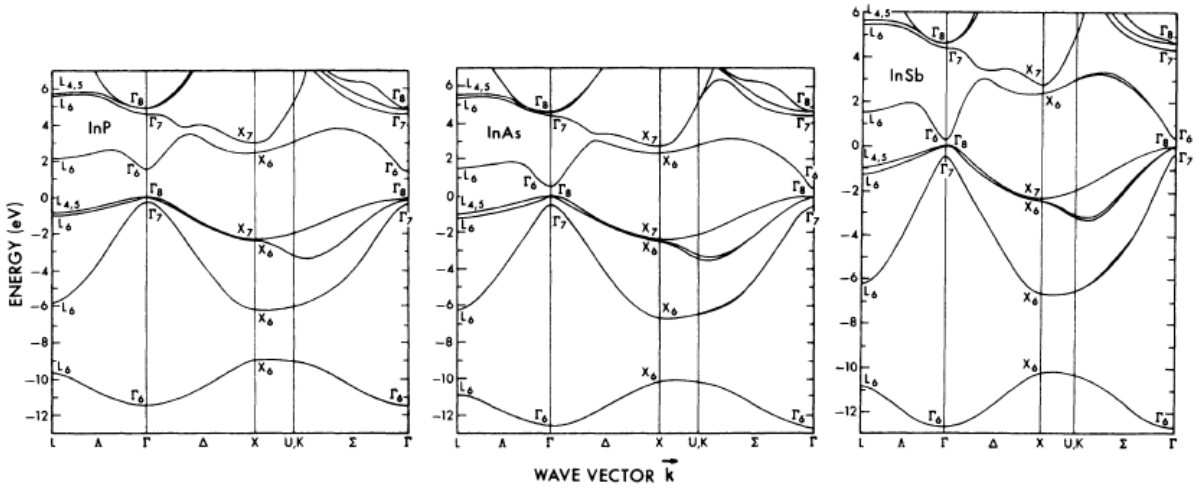
| Point | Level | Compound GaP [a] | GaAs | GaSb | InP | InAs | InSb |
|---|---|---|---|---|---|---|---|
| Γ | $\Gamma_6^v$ | −12.99 | −12.55 | −12.00 | −11.42 | −12.69 | −11.71 |
| | $\Gamma_7^v$ | | −0.35 | −0.76 | −0.21 | −0.43 | −0.82 |
| | $\Gamma_8^v$ | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | $\Gamma_6^v$ | 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 |
| | $X_6^v$ | −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

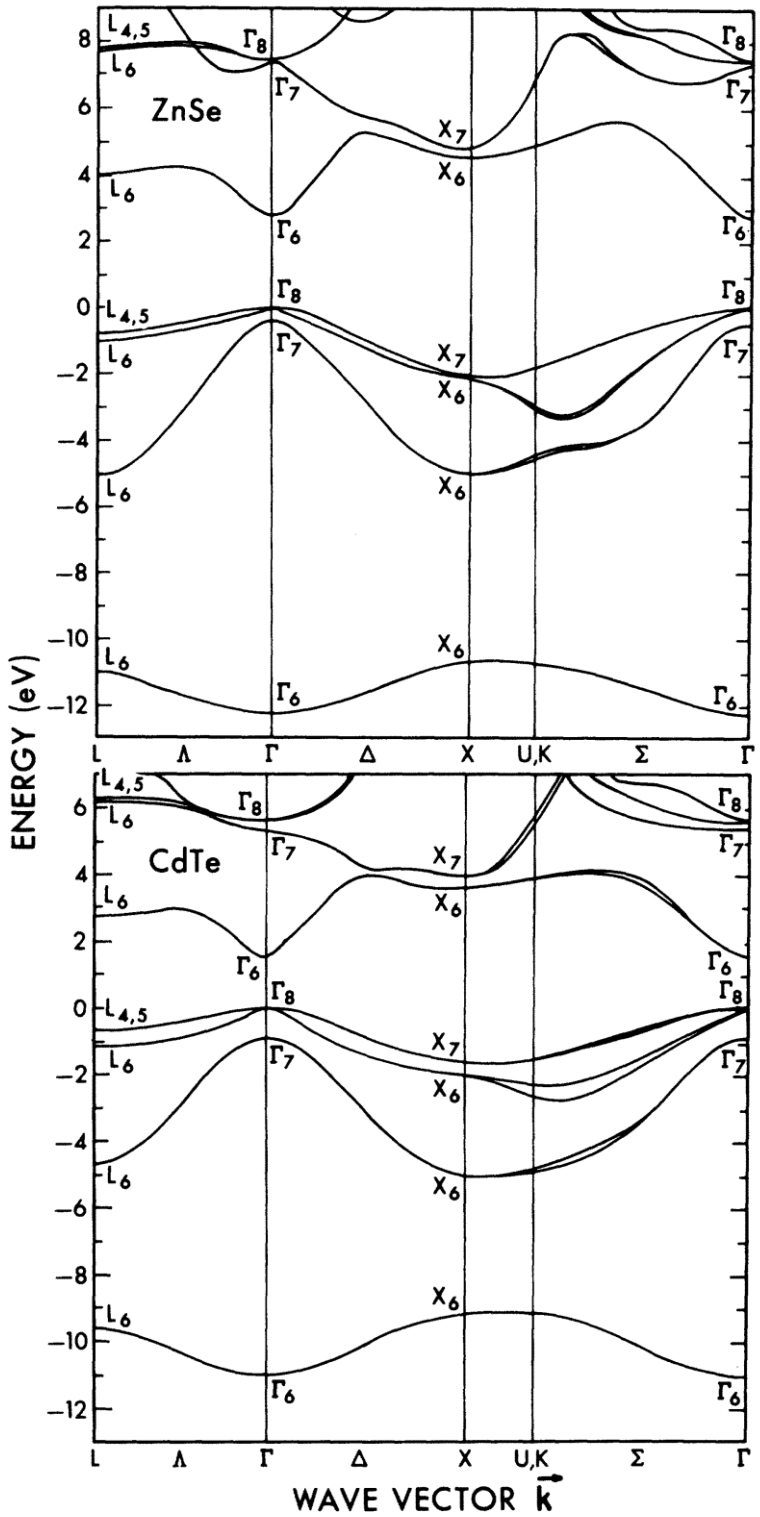



FIG. 17. Band structures for ZnSe and CdTe.

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 ($e/\Omega_c$) 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 $\Gamma$, $X$, 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).

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