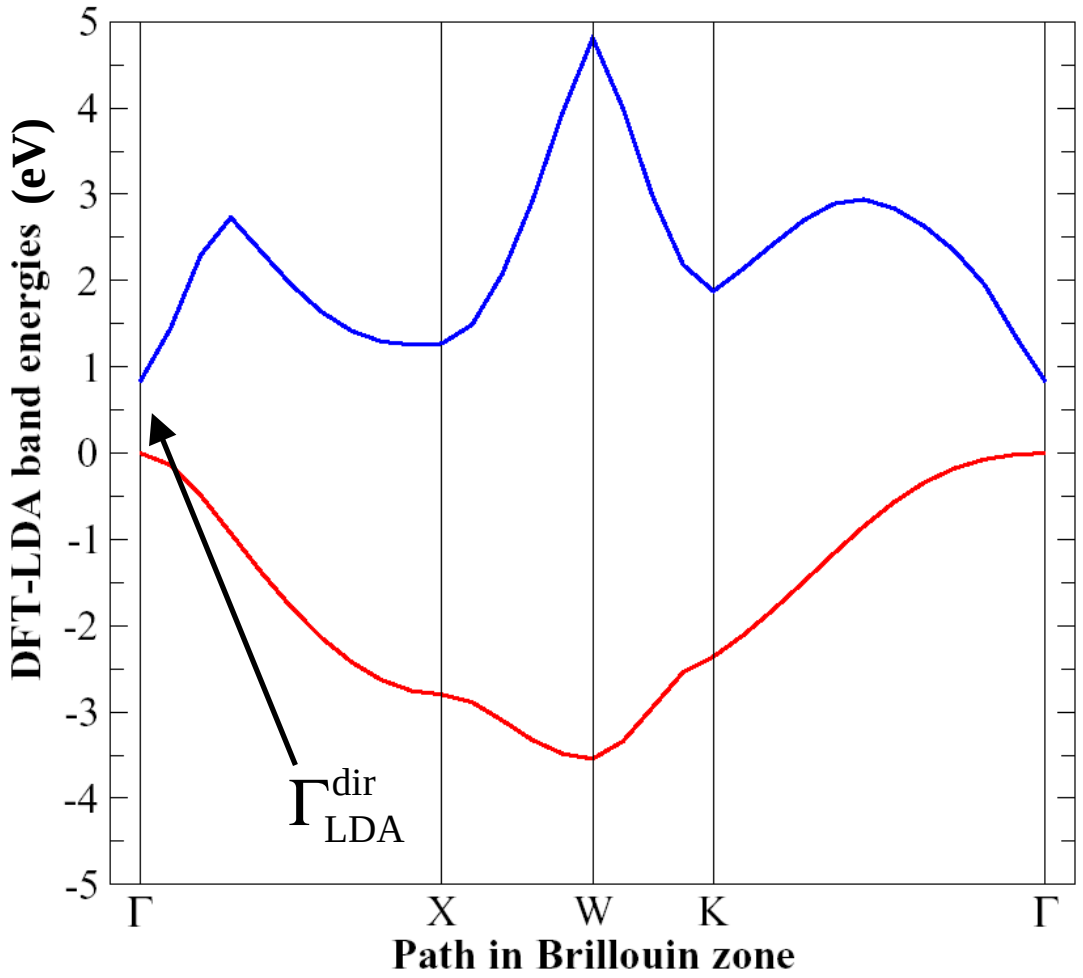
Quasiparticle band structure in the *GW*-approximation

Exercise 6.a

Philipp Eggert

DFT(LDA) band gap error 50%

Band structure DFT-LDA GaAs:



Experimental value:

$$\Gamma^{dir}_{exp} = 1.52 \text{ eV}$$

DFT-LDA:

$$\Gamma^{dir}_{LDA} \approx 0.80 \text{ eV}$$

$\Rightarrow$

underestimation of about 50 %

More sophisticated methods (EXX / GW)

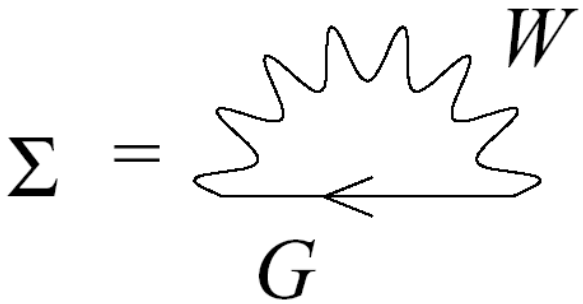
EXX ➔ Matthias Wahn (second part of this session)

GW ➔ this part of session

.....

What is GW?

➔an approximation for the self-energy



G = one particle Green‘s function,
W = screened Coulomb interaction

➔the self-energy contains exchange and dynamic correlation

➔through the self-energy the quasiparticle energies are accessible

➔quasiparticle energies are the one-particle excitation energies

➔**accurate description of band structure**

Numerical procedure to calculate QP energies

Kohn-Sham-equation ($\Rightarrow$ **underestimation of band gap**):

$$[h(\mathbf{r})+V_{\mathrm{H}}(\mathbf{r})]\varphi_{n\mathbf{k}}^{\mathrm{LDA}}(\mathbf{r})+V_{\mathrm{XC}}^{\mathrm{LDA}}(\mathbf{r})\varphi_{n\mathbf{k}}^{\mathrm{LDA}}(\mathbf{r})=\varepsilon_{n\mathbf{k}}^{\mathrm{LDA}}\varphi_{n\mathbf{k}}^{\mathrm{LDA}}(\mathbf{r})$$

SFHIngX-code

Quasiparticle equation (MBPT):

Nonlocal energy dependent self-energy contains correlation and exchange

$$[h(\mathbf{r})+V_{\mathrm{H}}(\mathbf{r})]\varphi_{n\mathbf{k}}^{\mathrm{QP}}(\mathbf{r})+\int\Sigma(\mathbf{r},\mathbf{r}',\varepsilon_{n\mathbf{k}}^{\mathrm{QP}})\varphi_{n\mathbf{k}}^{\mathrm{QP}}(\mathbf{r}')d^3r'=\varepsilon_{n\mathbf{k}}^{\mathrm{QP}}\varphi_{n\mathbf{k}}^{\mathrm{QP}}(\mathbf{r})$$

Quasiparticle correction ($\Rightarrow$ **accurate band structure**) :

$$\varepsilon_{n\mathbf{q}}^{\mathrm{QP}}-\varepsilon_{n\mathbf{q}}^{\mathrm{LDA}}=\langle\varphi_{n\mathbf{q}}^{\mathrm{LDA}}(\mathbf{r})\left|\Sigma\left(\mathbf{r},\mathbf{r}',\varepsilon_{n\mathbf{q}}^{\mathrm{QP}}\right)-V_{\mathrm{XC}}^{\mathrm{LDA}}(\mathbf{r})\right|\varphi_{n\mathbf{q}}^{\mathrm{LDA}}(\mathbf{r}')\rangle$$

gwst-code

***GW* real-space imaginary-time**

Convergence parameters *GW* => Σ

Construction of the Green's function in *gwst*:

$$G^{\mathrm{LDA}}(\mathbf{r},\mathbf{r}';\mathrm{i}\tau) = \begin{cases} +\sum_{n}^{\mathrm{occ}} \sum_{\mathbf{k}\in \mathrm{MP}} \varphi_{n\mathbf{k}}(\mathbf{r})\varphi_{n\mathbf{k}}^{*}(\mathbf{r}')\exp(\varepsilon_{n\mathbf{k}}\tau), \tau > 0 \\ -\sum_{n}^{\mathrm{unocc}} \sum_{\mathbf{k}\in \mathrm{MP}} \varphi_{n\mathbf{k}}(\mathbf{r})\varphi_{n\mathbf{k}}^{*}(\mathbf{r}')\exp(\varepsilon_{n\mathbf{k}}\tau), \tau < 0 \end{cases}$$

Wave functions are calculated with *SFHIngX* (via interface):

$$\varphi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{n,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

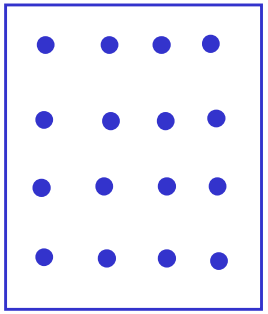
Convergence parameters:

1. **Number of plane waves in the Green's function: `ecutoff`**
2. **Number of bands in the Green's function: `bcutoff`**
3. **Number of k-points**
4. **Number of time-points**

} **not tested in this session**

Calculate quasiparticle band structure

Starting from the Green's function, self-energy is calculated at regular Monkhorst Pack **k-points**:

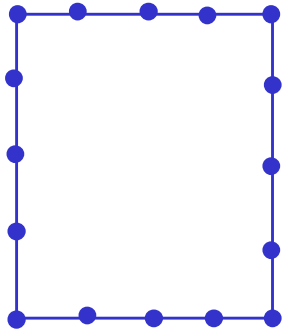


$$G \longrightarrow P \longrightarrow \varepsilon \longrightarrow \varepsilon^{-1} \longrightarrow W \longrightarrow \Sigma$$

Once self-energy is obtained

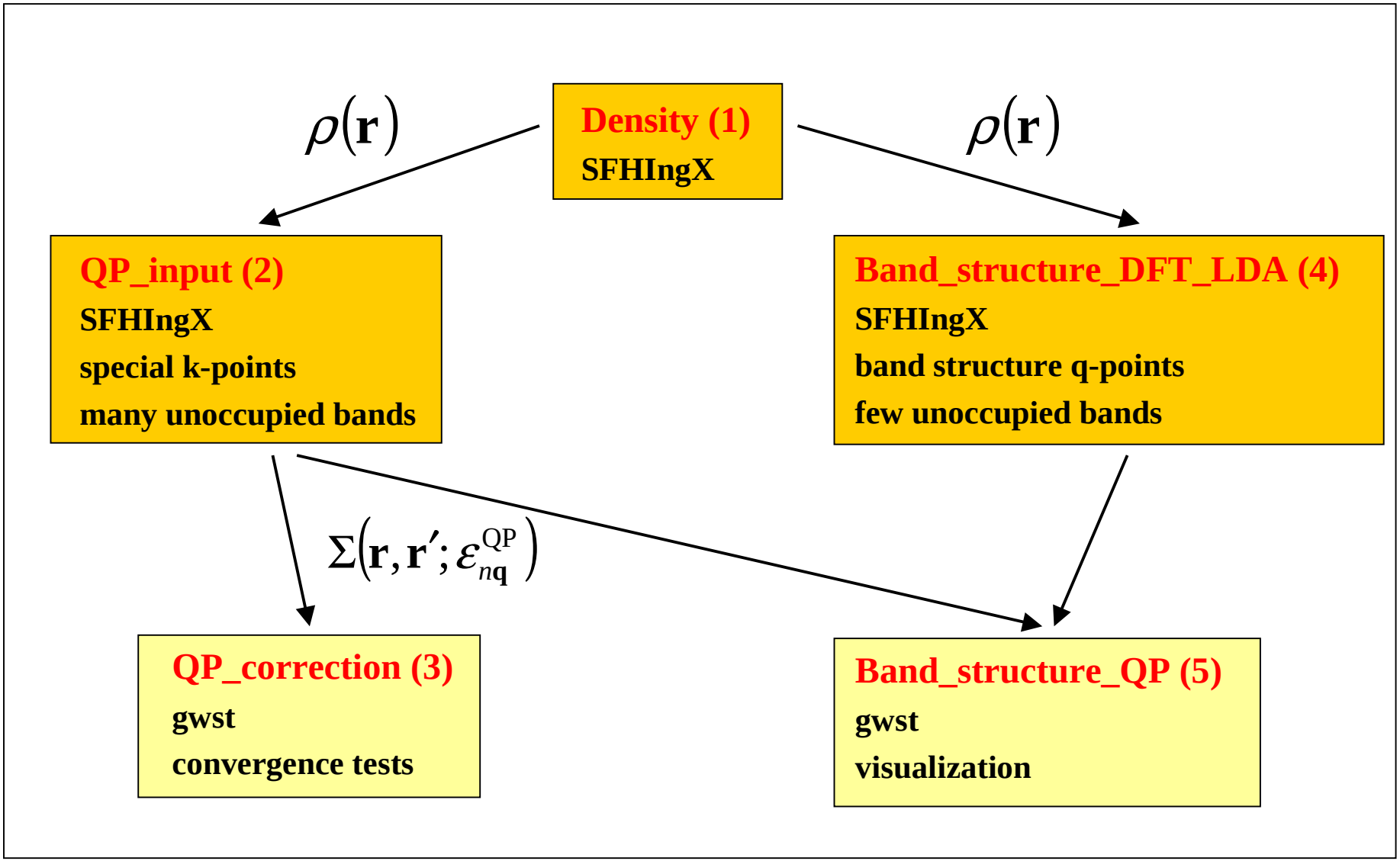
➔evaluation of quasiparticle energies at the band structure **q-points**

$$\varepsilon_{n\mathbf{q}}^{\mathrm{QP}} = \varepsilon_{n\mathbf{q}}^{\mathrm{LDA}} + \left\langle \varphi_{n\mathbf{q}}^{\mathrm{LDA}} \middle| \Sigma\left(\varepsilon_{n\mathbf{q}}^{\mathrm{QP}}\right) - V_{\mathrm{xc}}^{\mathrm{LDA}} \middle| \varphi_{n\mathbf{q}}^{\mathrm{LDA}} \right\rangle$$

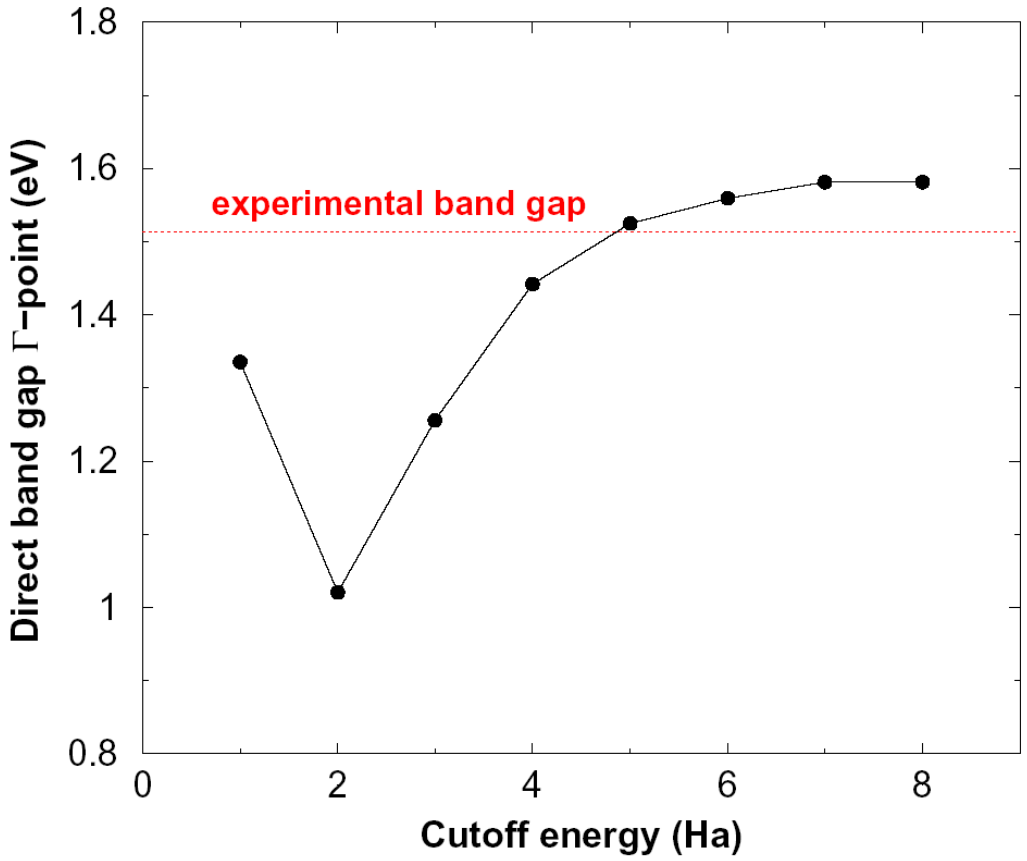


➔few number of unoccupied bands
(no convergence parameter)

Structure of a typical GW-calculation



Convergence test `ecutoff`

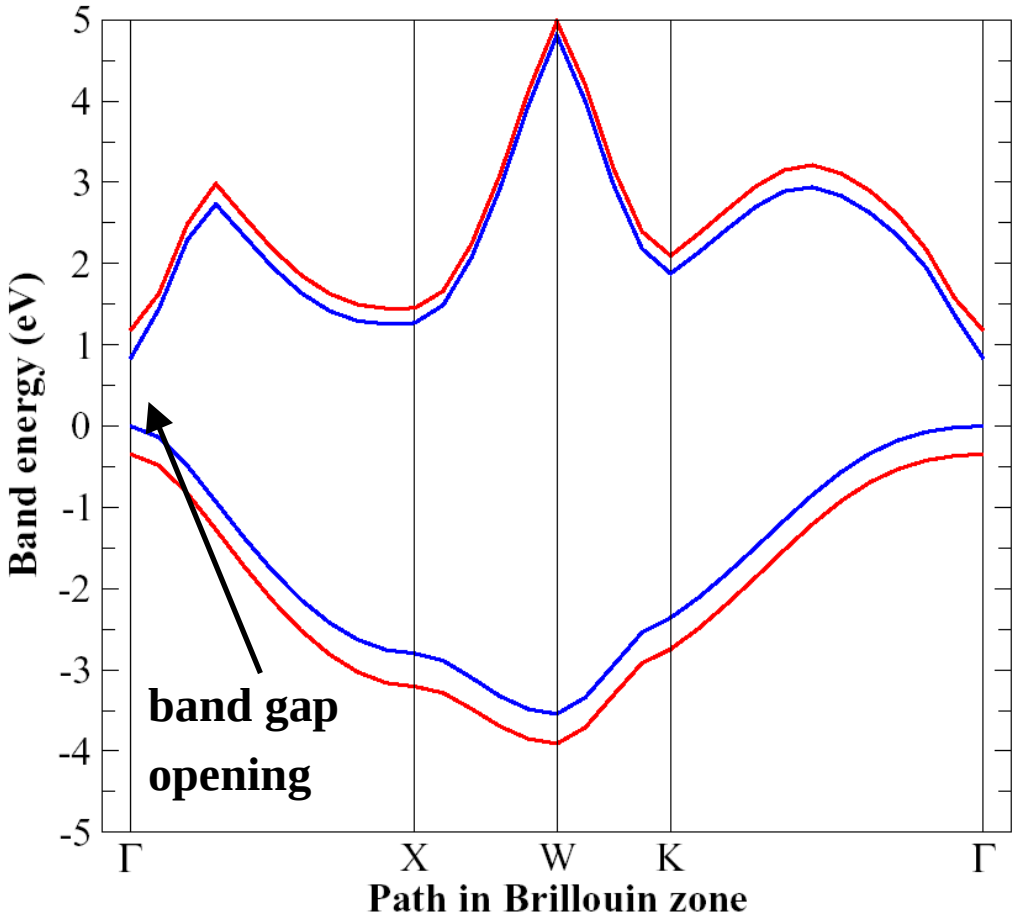


➔**LDA-pseudopotential**

➔**at the theoretical lattice constant**

➔**accurate description of direct band gap**

Comparison DFT-LDA and QP band structure



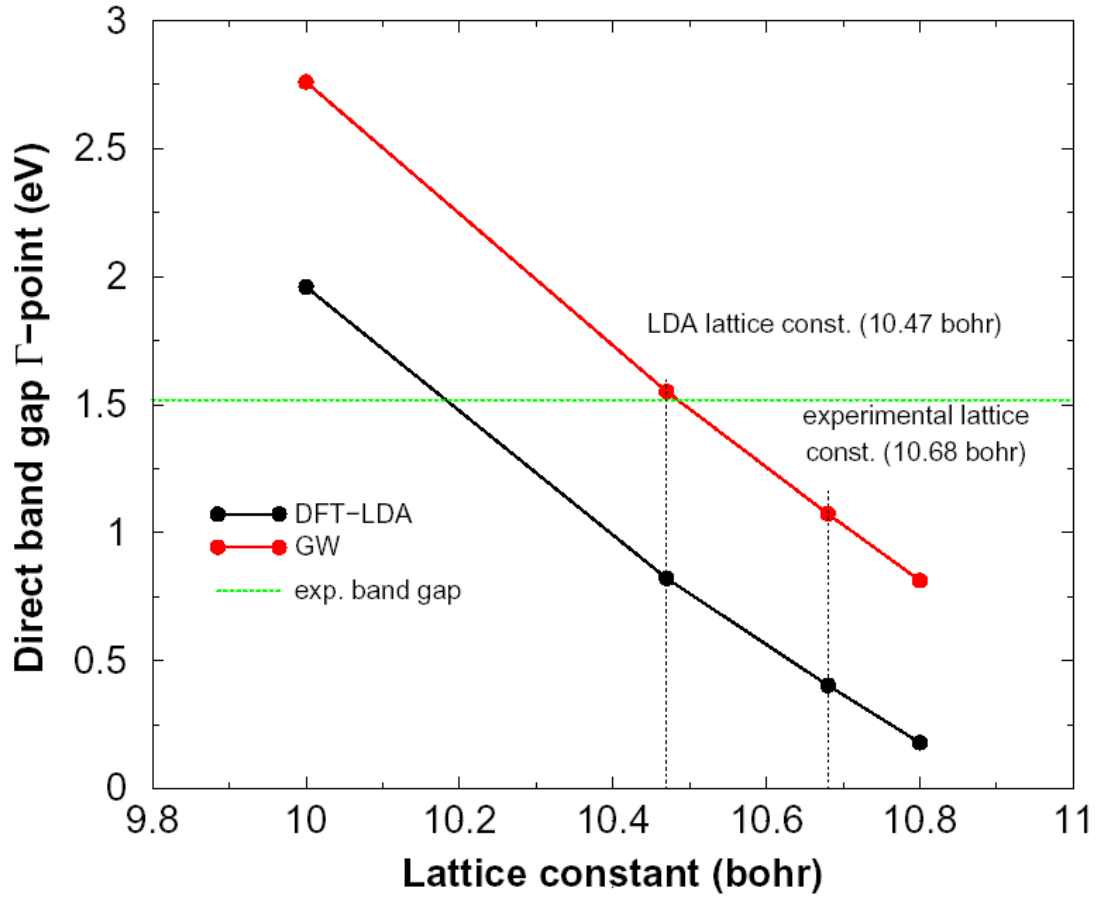
DFT-LDA

QP

➔valence bands are shifted to lower energies

➔Conduction bands are shifted to higher energies

Band gap depends strongly on the lattice constant



➔**LDA pseudopotential**

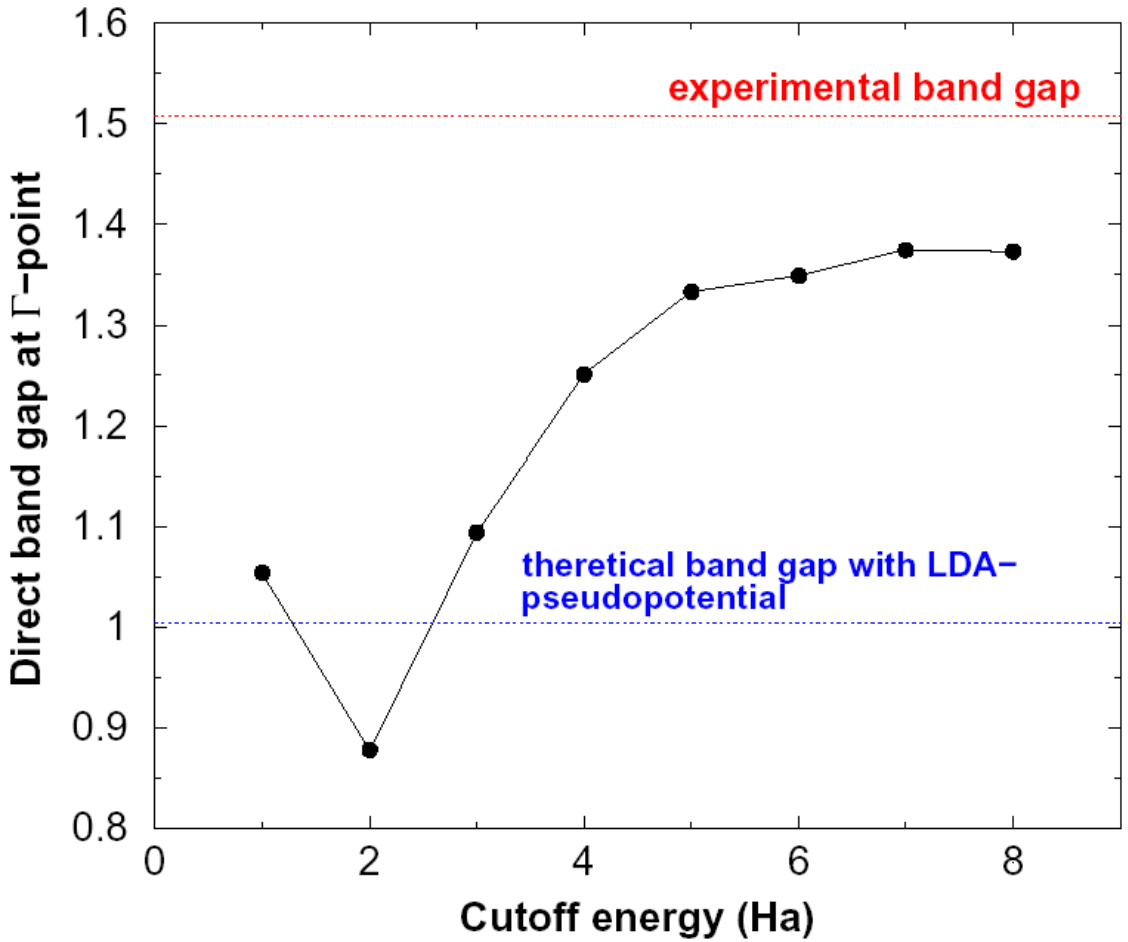
➔**wrong band gap at experimental lattice constant**

AND

➔**experimental lattice constant more accurately known**

KLI-pseudopotential gives the right band gap

experimental lattice constant: 10.68 bohr



➔Converged QP band gap: 1.37 eV

➔Error: 10%

Compare with error DFT-LDA: 50 %

GW-calculation:

➔Be careful with the lattice constant

➔The choice of pseudopotential is important