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The *GW* approximation in less than 60 minutes

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Outline

I. Standard DFT suffers from the band gap problem

II. Introduction of the Green's function

III. The *GW* approximation

IV. The *GW* code in ABINIT and the G_0W_0 method

V. Some applications

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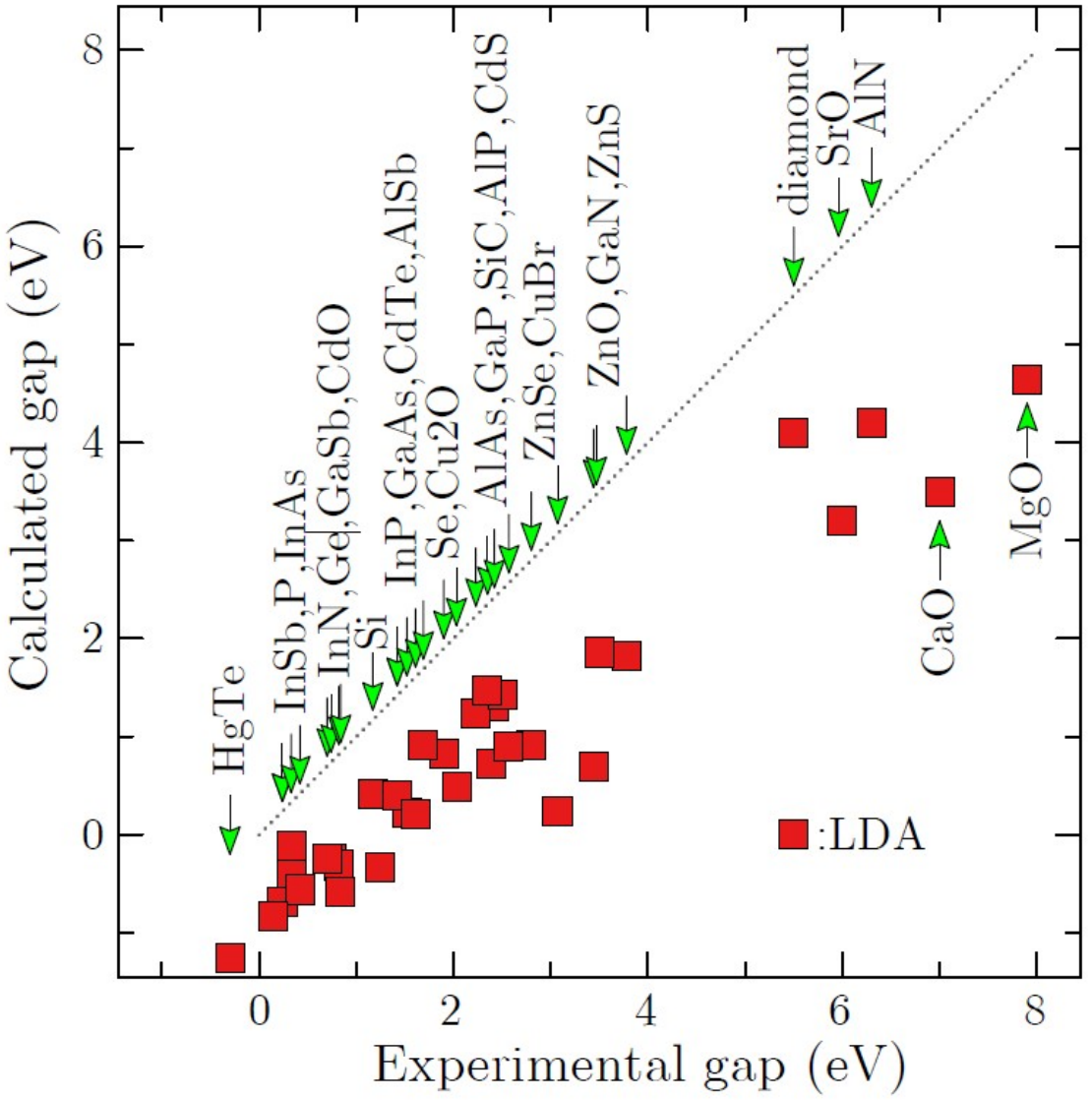
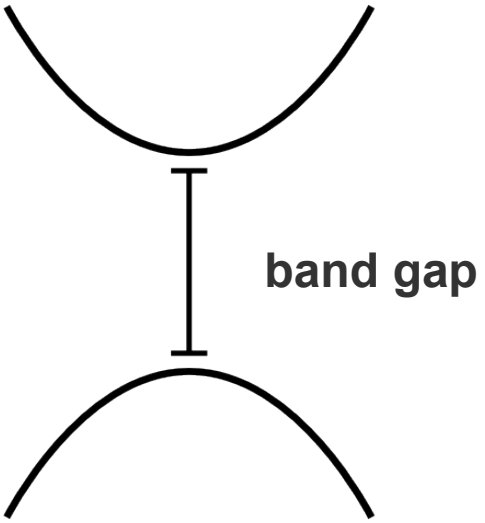
Standard DFT has unfortunately some shortcomings



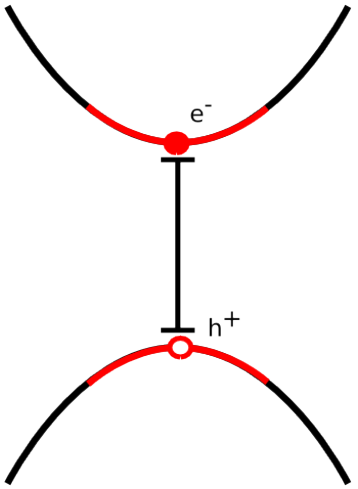
after van Schilfgaarde *et al* PRL **96** 226402 (2008)



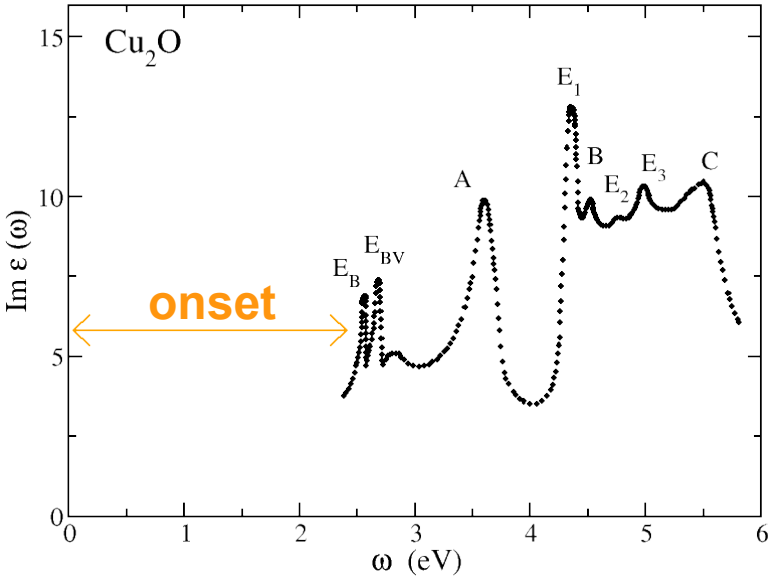
Band gap problem!

A pervasive problem

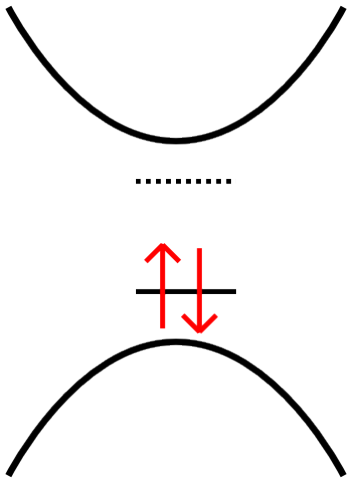
Effective masses
for transport in semiconductors



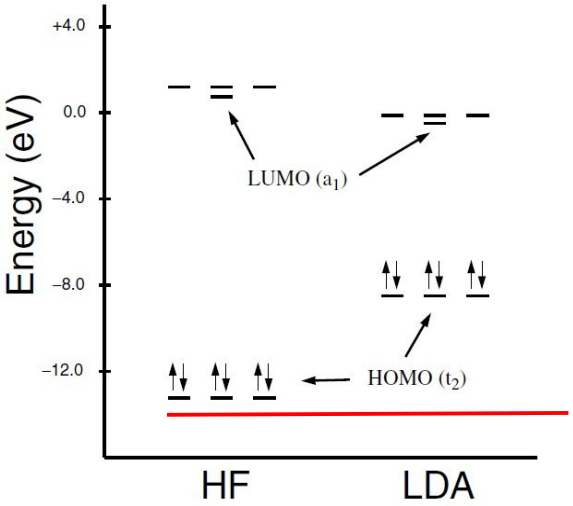
Optical absorption



Defect formation energy,
dopant solubility



Photoemission

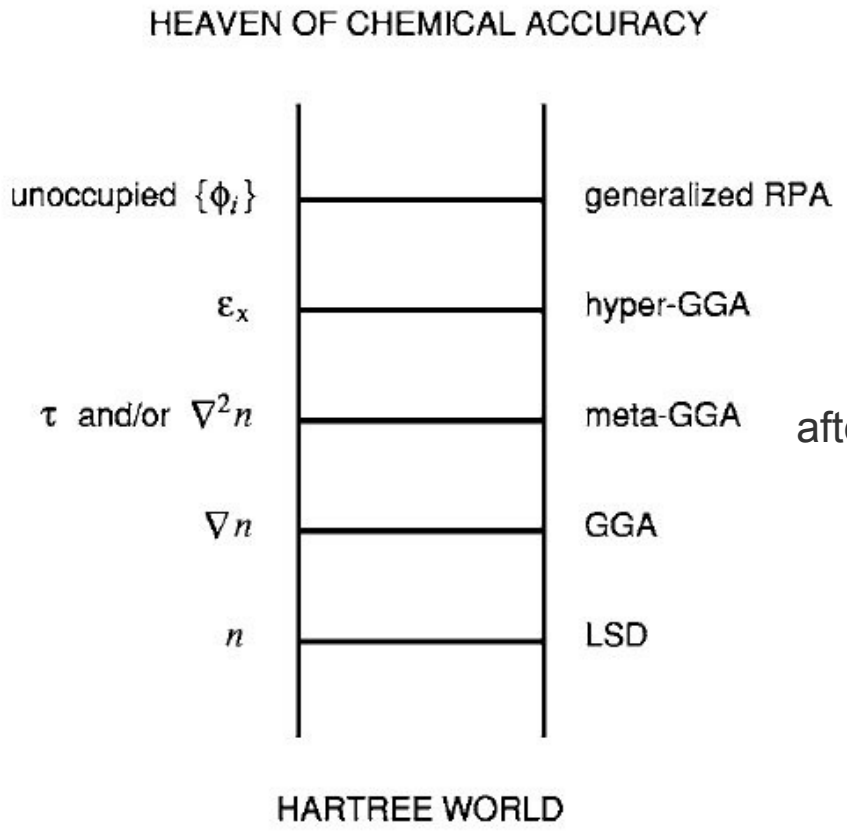


Exp.

FIG. 1. Single-particle Hartree-Fock and local density approximation eigenvalue spectra (eV) for the SiH_4 molecule.

How do go beyond within the DFT framework?

Not easy to find improvement within DFT framework
- There is no such thing as a perturbative expansion
- Perdew's Jacob's ladder does not help for the band gap



after J. Perdew JCP (2005).

FIG. 1. Jacob's ladder of density functional approximations to the exchange-correlation energy.

Need to change the overall framework!

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Many-body perturbation theory

Historically older than the DFT (1940-50's)!
Big names: Feynman, Schwinger, Hubbard, Hedin, Lundqvist

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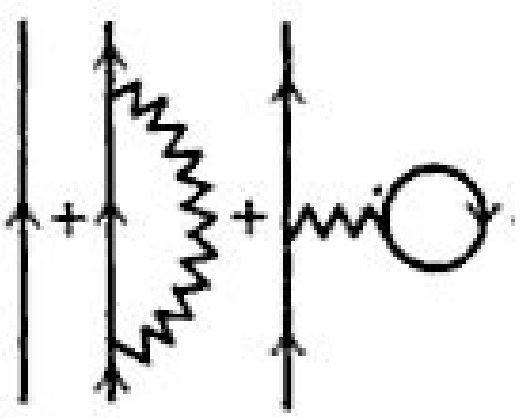
Green's functions
= propagator

$$G(\boldsymbol{r}\,t,\boldsymbol{r}'\,t')=$$



The Green's function

Exact ground state wavefunction: $|N,0\rangle$

Creation, annihilation operator: $\Psi^\dagger(\boldsymbol{r}\,t),\quad \Psi(\boldsymbol{r}\,t)$

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1 $\Psi^\dagger(\boldsymbol{r}\,t)|N,0\rangle$ is a (N+1) electron wavefunction not necessarily in the ground state

2 $\Psi^\dagger(\boldsymbol{r}'\,t')|N,0\rangle$ is another (N+1) electron wavefunction

Let's compare the two of them!

Green's function definition

$$\underbrace{\langle N,0|\Psi(\boldsymbol{r}\,t)}_{1}\underbrace{\Psi^{\dagger}(\boldsymbol{r}'t')|N,0\rangle}_{2}$$

$$=iG^{e}(\boldsymbol{r}\,t,\boldsymbol{r}'t') \quad \text{for} \quad t>t'$$

Mesures how an extra electron propagates from (*r't'*) to (*rt*).

Green's function definition

$$\underbrace{\langle N,0|\Psi^{\dagger}(r't')}_{1}\underbrace{\Psi(rt)|N,0\rangle}_{2}$$

$$= i\,G^{h}(r't',rt) \qquad \text{for} \quad t' > t$$

Mesures how a missing electron (= a hole) propagates from (*rt*) to (*r't'*).

Final expression for the Green's function

$$iG(\boldsymbol{r}t,\boldsymbol{r}'t') = \langle N,0|T\left[\Psi(\boldsymbol{r}t)\Psi^{\dagger}(\boldsymbol{r}'t')\right]|N,0\rangle$$

time-ordering operator

$$G(\boldsymbol{r}t,\boldsymbol{r}'t') = G^{e}(\boldsymbol{r}t,\boldsymbol{r}'t') - G^{h}(\boldsymbol{r}'t',\boldsymbol{r}t)$$

Compact expression that describes both the propagation of an extra electron and an extra hole

Lehman representation

$$i\,G(\boldsymbol{r},\boldsymbol{r}',t-t')=\langle N,0|\,T\left[\Psi(\boldsymbol{r}\,t)\Psi^{\dagger}(\boldsymbol{r}'\,t')\right]|N,0\rangle$$

Closure relation

$$\sum_{N,i}|N,i\rangle\langle N,i|$$

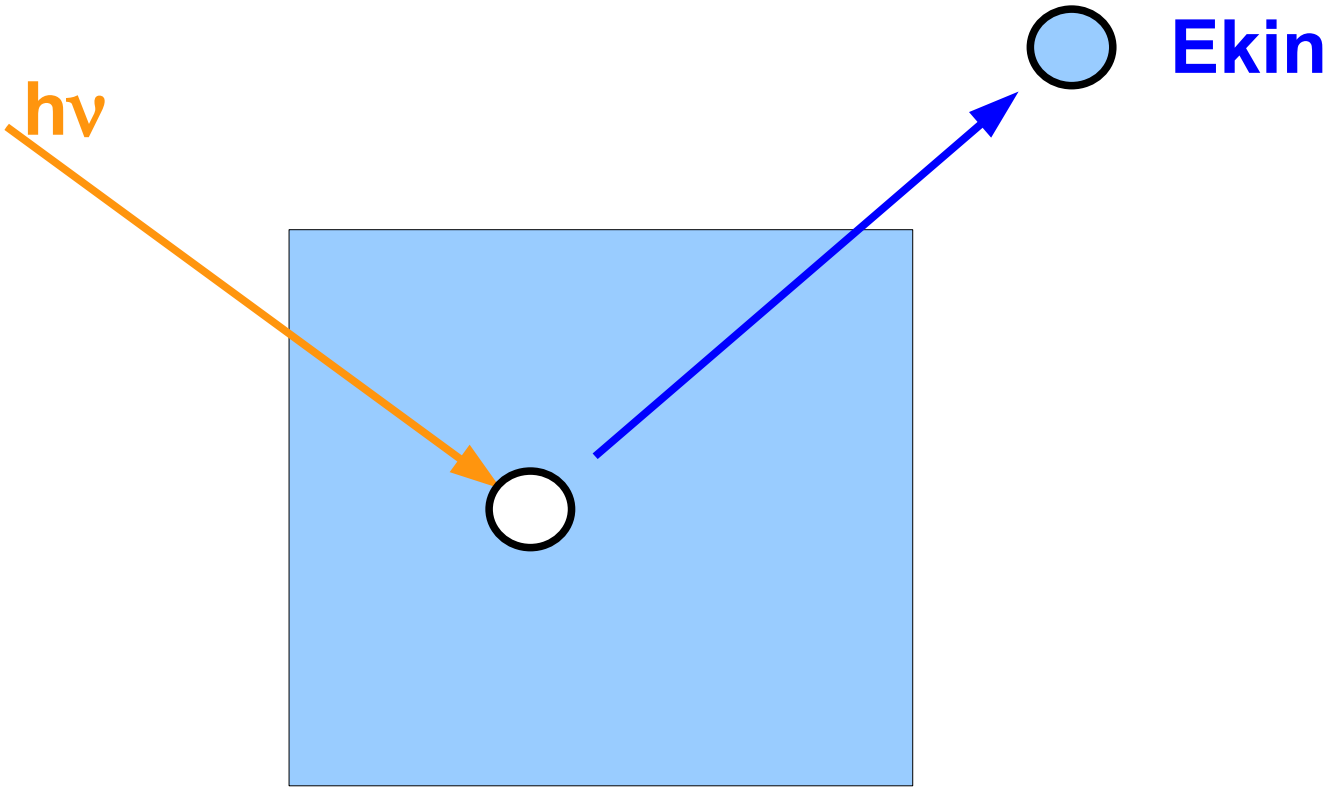
Lehman representation:

$$G(\boldsymbol{r},\boldsymbol{r}',\omega)=\sum_{i}\frac{f_i(\boldsymbol{r})\,f_i^{*}(\boldsymbol{r}')}{\omega-\epsilon_i\pm i\eta}$$

where $\epsilon_i=\begin{cases}E(N+1,i)-E(N,0)\\E(N,0)-E(N-1,i)\end{cases}$

Exact excitation energies!

Related to photoemission spectroscopy



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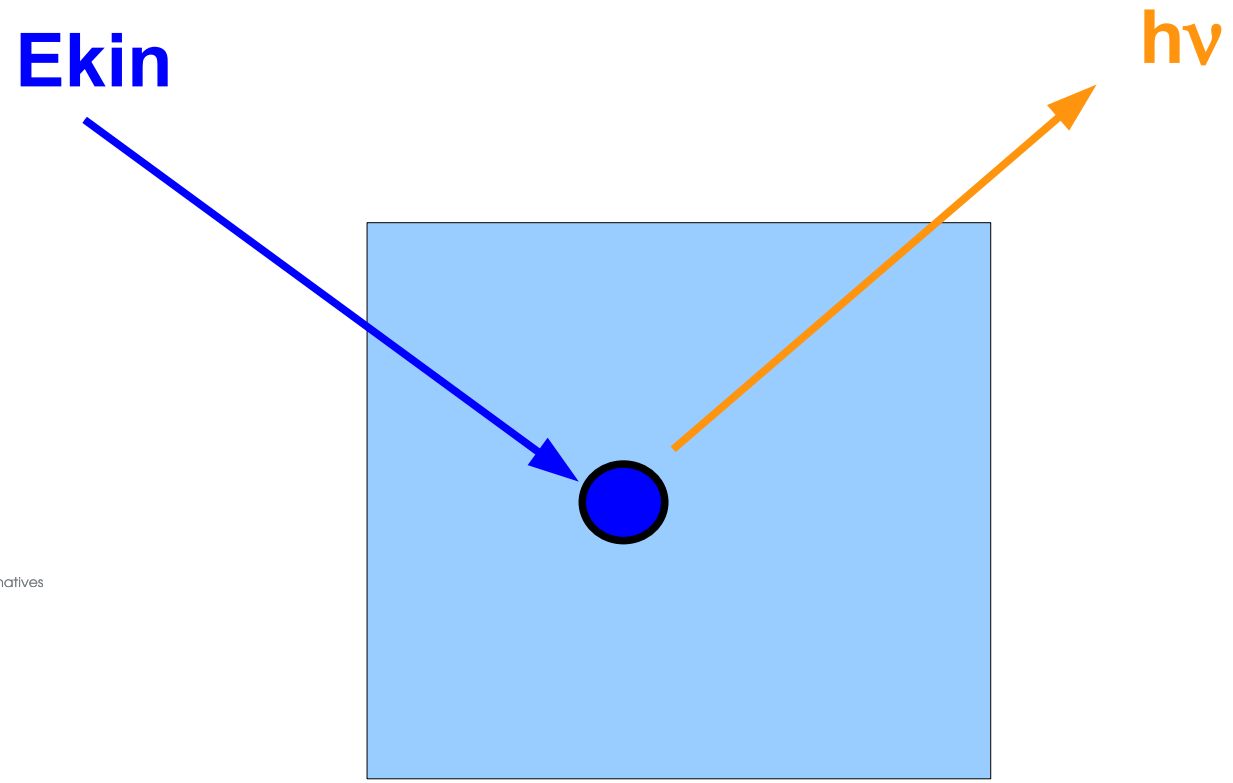
Energy conservation: before after

$$h\nu + E(N,0) = E_{kin} + E(N-1,i)$$

Quasiparticle energy: $$\epsilon_i = E(N,0) - E(N-1,i) = E_{kin} - h\nu$$

And inverse photoemission spectroscopy



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Quasiparticle energy: $$\epsilon_i = E(N+1,i) - E(N,0) = E_{kin} - h\nu$$

Other properties of the Green's function

Galitskii-Migdal formula for the total energy:

$$E_{total} = \frac{1}{\pi} \int_{-\infty}^{\mu} d\omega \, \mathrm{Tr}\left[\left(\omega - h_0 \right) \mathrm{Im}\, G(\omega) \right]$$

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Expectation value of any 1 particle operator (local or non-local)

$$\langle O \rangle = \lim_{t \to t'} Tr\left[O G \right]$$

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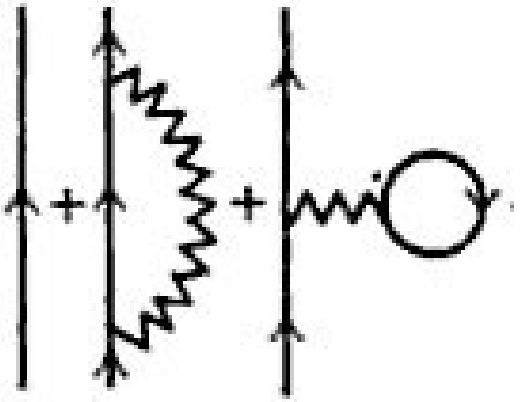
How to calculate the Green's function?

Feynman diagrams



Hedin's functional approach PRA (1965).

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Hedin's coupled equations

6 coupled equations: $1=(\boldsymbol{r}_1 t_1 \sigma_1)$ $2=(\boldsymbol{r}_2 t_2 \sigma_2)$

$$G(1,2)=G_0(1,2)+\int d34\, G_0(1,3)\Sigma(3,4)G(4,2)$$ **Dyson equation**

$$\Sigma(1,2)=i\int d34\, G(1,3)W(1,4)\Gamma(4,2,3)$$ **self-energy**

$$\Gamma(1,2,3)=\delta(1,2)\delta(1,3)+\int d4567\frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)G(5,7)\Gamma(6,7,3)$$ **vertex**

$$\chi_0(1,2)=-i\int d34\, G(1,3)G(4,1)\Gamma(3,4,2)$$ **polarizability**

$$\varepsilon(1,2)=\delta(1,2)-\int d3\, v(1,3)\chi_0(3,2)$$ **dielectric matrix**

$$W(1,2)=\int d3\,\varepsilon^{-1}(1,3)v(3,2)$$ **screened Coulomb interaction**

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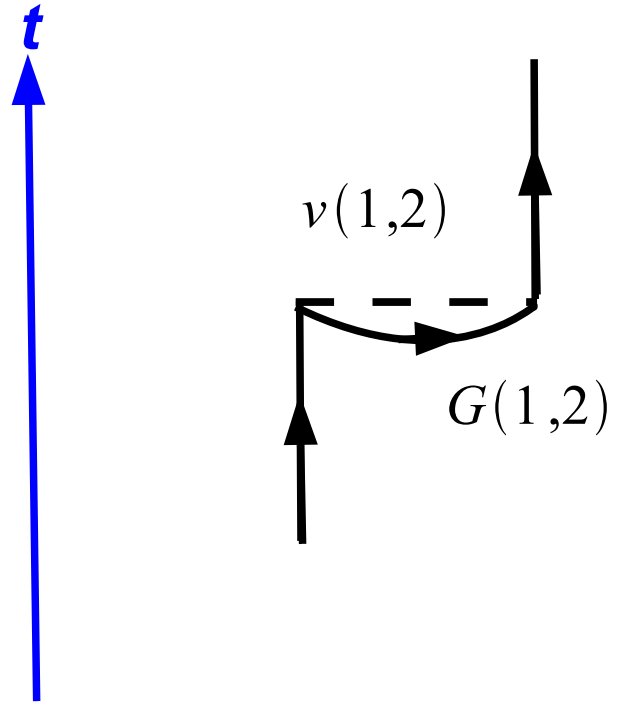
Simplest approximation

$$\Sigma(1,2) = i\,G(1^+,2)\,v(1,2) \quad \Rightarrow \quad \text{Fock exchange}$$



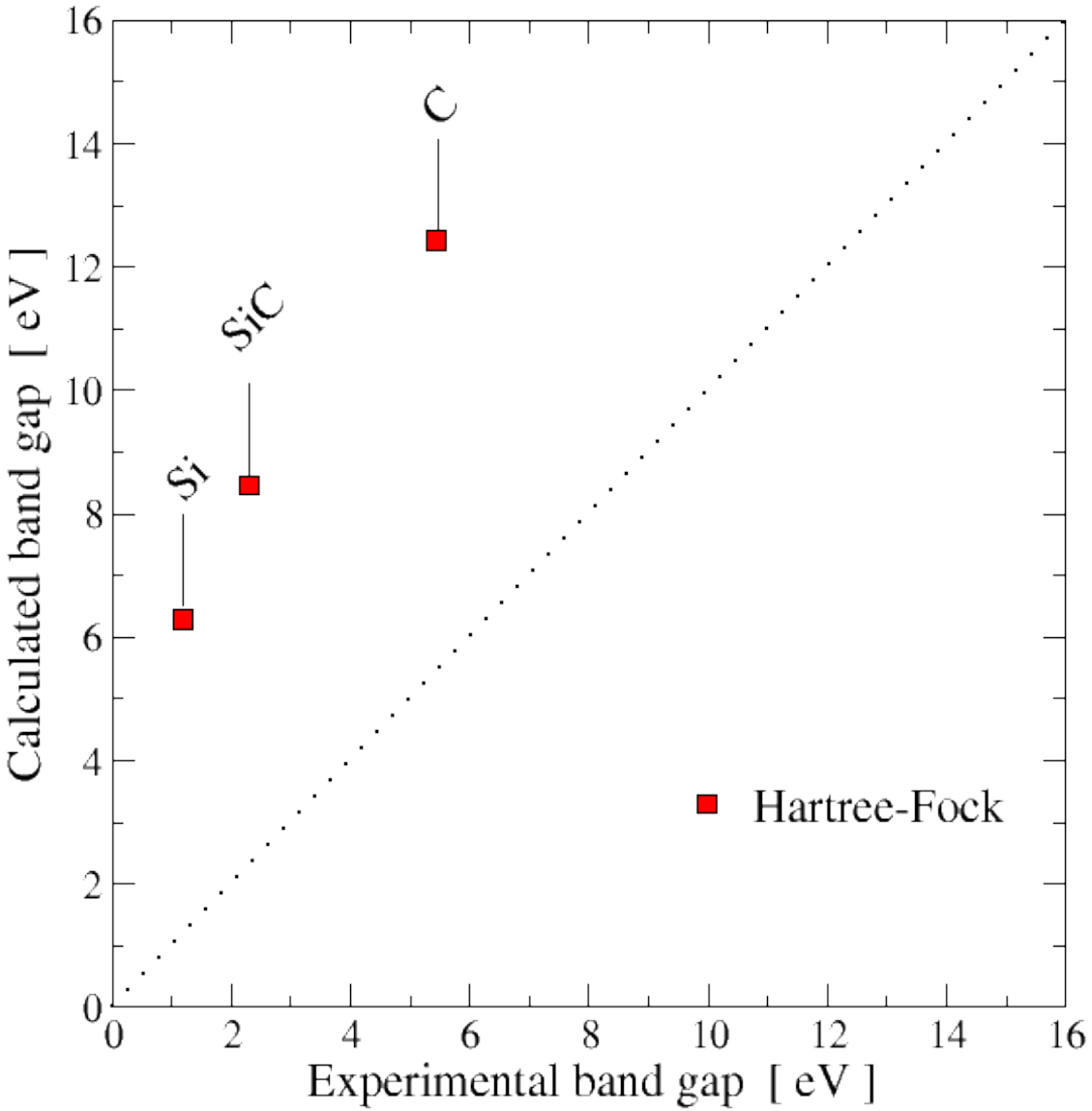
Dyson equation:

$$G = G_0 + G_0 \Sigma G$$

$$G = G_0 + G_0 \Sigma G_0 + \ldots$$

Not enough: Hartree-Fock is know to be quite bad for solids

Hartree-Fock approximation for band gaps



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Hedin's coupled equations

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$$\chi_0(1,2)=-i\int d34\, G(1,3)G(4,1)\Gamma(3,4,2)$$

$$\varepsilon(1,2)=\delta(1,2)-\int d3\, v(1,3)\chi_0(3,2)$$

$$W(1,2)=\int d3\, \varepsilon^{-1}(1,3)v(3,2)$$ **screened Coulomb interaction**

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Hedin's coupled equations

6 coupled equations:

$$G(1,2) = G_0(1,2) + \int d34\, G_0(1,3)\,\Sigma(3,4)\,G(4,2)$$ **Dyson equation**

$$\Sigma(1,2) = i \int d34\, G(1,2)\,W(1,2)\,\Gamma(4,2,3)$$ **self-energy**

$$\Gamma(1,2,3) = \delta(1,2)\,\delta(1,3) + \int d4567\, \frac{\delta\,\Sigma(1,2)}{\delta\, G(4,5)}\, G(4,6)\,G(5,7)\,\Gamma(6,7,3)$$

$$\chi_0(1,2) = -i \int d34\, G(1,2)\,G(2,1)\,\Gamma(3,4,2)$$

$$\varepsilon(1,2) = \delta(1,2) - \int d3\, v(1,3)\,\chi_0(3,2)$$

$$W(1,2) = \int d3\, \varepsilon^{-1}(1,3)\, v(3,2)$$ **screened Coulomb interaction**

Here comes the *GW* approximation

$$\Sigma(1,2) = i\,G(1,2)\,W(1,2)$$

GW approximation

$$\chi_0(1,2) = -i\,G(1,2)\,G(2,1)$$

RPA approximation

$$\varepsilon(1,2) = \delta(1,2) - \int d3\, v(1,3)\,\chi_0(3,2)$$

$$W(1,2) = \int d3\, \varepsilon^{-1}(1,3)\,v(3,2)$$

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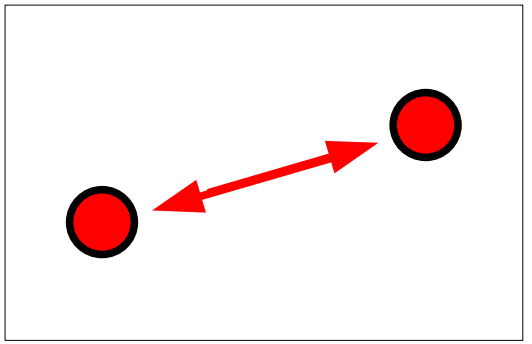
What is W?

Interaction between electrons in vacuum:

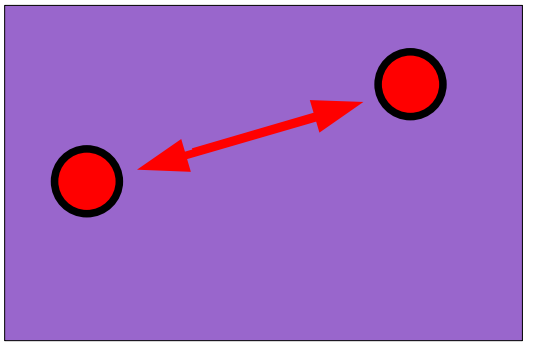
$$V(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{4\pi\epsilon_0}\frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}$$



Interaction between electrons in a homogeneous polarizable medium:

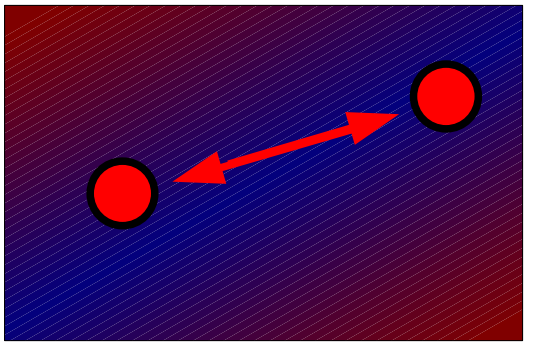
$$W(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{4\pi\varepsilon_0\varepsilon_r}\frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

Dielectric constant of the medium



Dynamically screened interaction between electrons in a general medium:

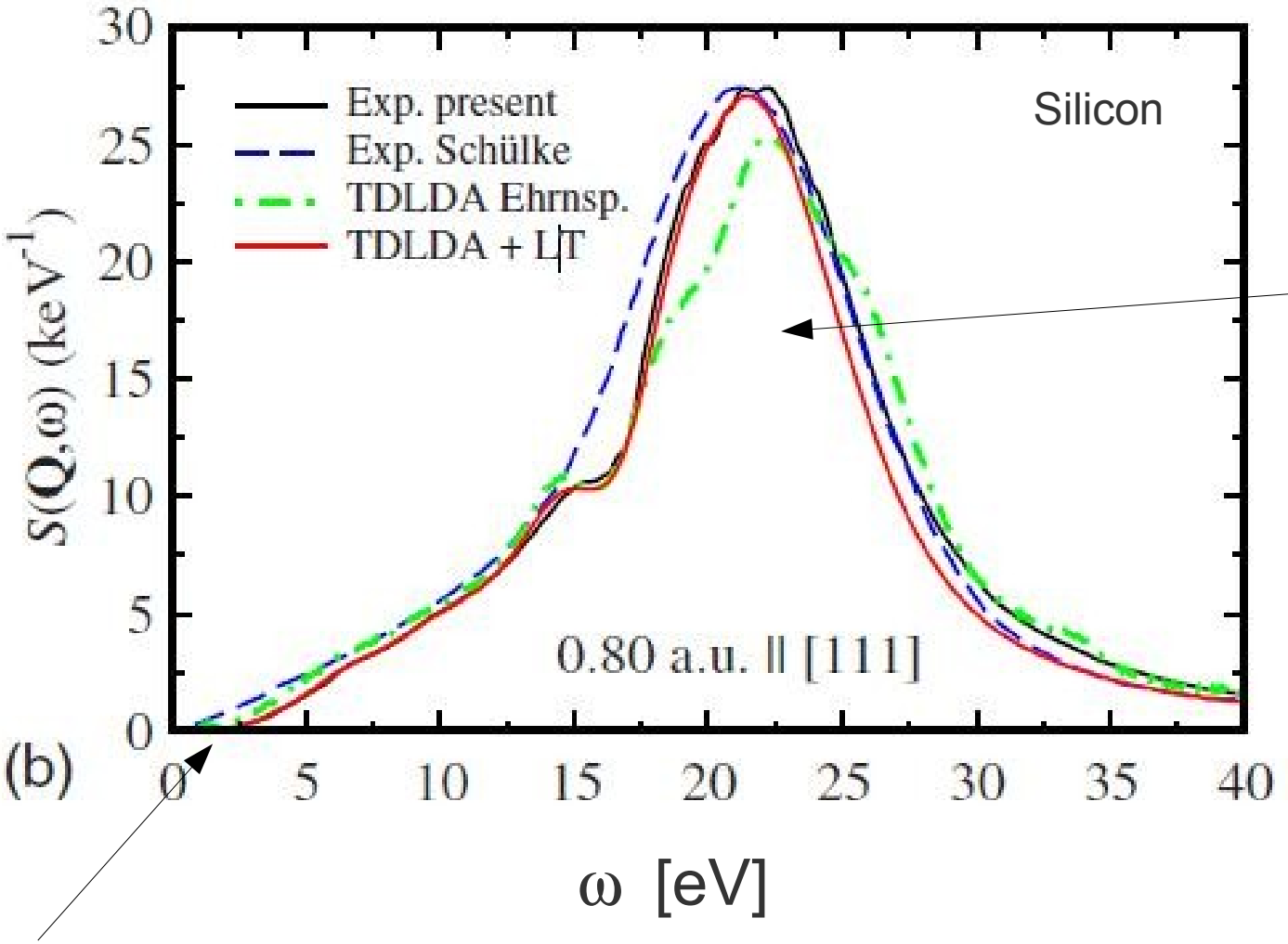
$$W(\boldsymbol{r},\boldsymbol{r}',\omega)=\frac{e^2}{4\pi\epsilon_0}\int d\boldsymbol{r}''\frac{\varepsilon^{-1}(\boldsymbol{r},\boldsymbol{r}'',\omega)}{|\boldsymbol{r}''-\boldsymbol{r}'|}$$



W is frequency dependent

W can measured directly by Inelastic X-ray Scattering

$$W(\boldsymbol{q}=0.80\,\text{a.u},\omega)$$



Plasmon frequency

Zero below the band gap

H-C Weissker et al. PRB (2010)

GW has a "super" Hartree-Fock

Hartree-Fock Approximation

$$\Sigma_x(\boldsymbol{r}_1,\boldsymbol{r}_2)=$$

$$\frac{i}{2\pi}\int_{-\infty}^{\mu} d\,\omega' G(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega')v(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

= bare exchange

GW Approximation

$$\Sigma_{xc}(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega)=$$

$$\frac{i}{2\pi}\int d\,\omega' G(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega+\omega')W(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega')$$

$\Sigma_x(\boldsymbol{r}_1,\boldsymbol{r}_2)$

Bare exchange

$\Sigma_c(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega)$

+ correlation

Non Hermitian dynamic

***GW* is nothing else but a "screened" version of Hartree-Fock.**

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Summary: DFT vs *GW*

Electronic density $\rho(\boldsymbol{r})$

Local and static

Green's function $G(\boldsymbol{r}t, \boldsymbol{r}'t')$

Non-local, dynamic
Depends onto empty states

exchange-correlation potential $v_{xc}(\boldsymbol{r})$

exchange-correlation operator = self-energy $\Sigma_{xc}(\boldsymbol{r}, \boldsymbol{r}', \epsilon)$

Approximations:

LDA, GGA, hybrids

GW approximation

$$\Sigma_{GW}(\boldsymbol{r}t, \boldsymbol{r}'t') = iG(\boldsymbol{r}t, \boldsymbol{r}', t')W(\boldsymbol{r}t, \boldsymbol{r}'t')$$

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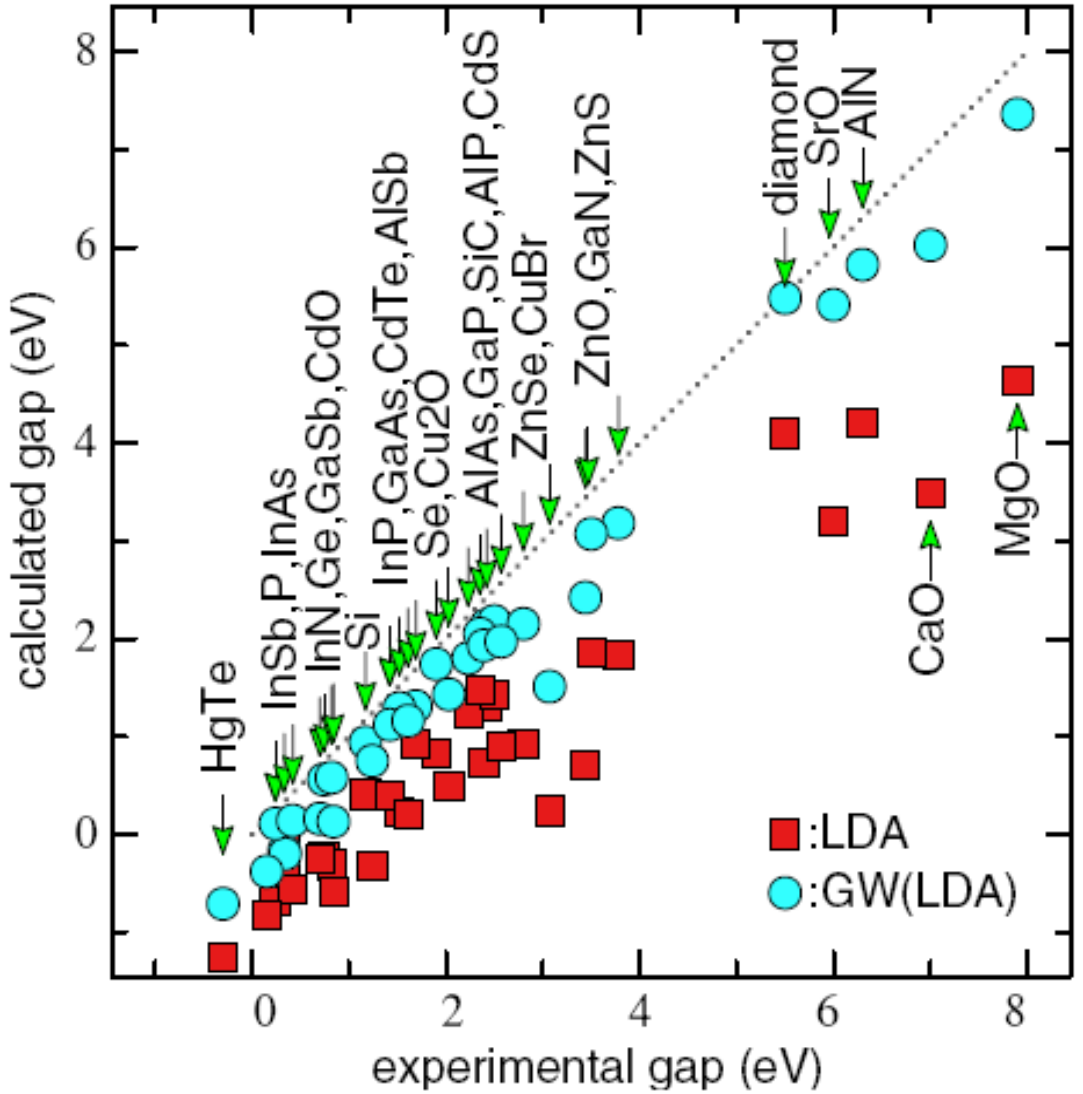
GW approximation gets good band gap



after van Schilfgaarde *et al* PRL **96** 226402 (2008)

No more a band gap problem !

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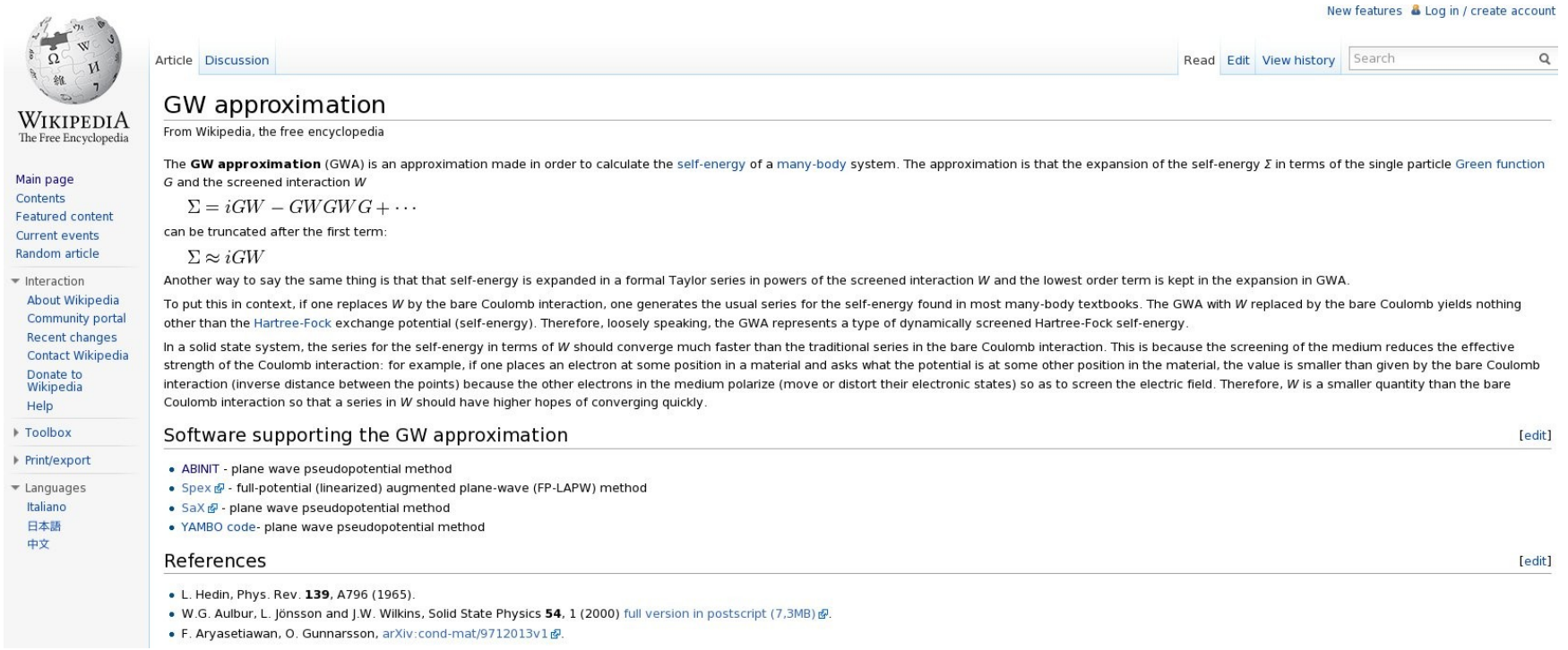
Available *GW* codes



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GW approximation

From Wikipedia, the free encyclopedia

The **GW approximation** (GWA) is an approximation made in order to calculate the self-energy of a many-body system. The approximation is that the expansion of the self-energy Σ in terms of the single particle Green function G and the screened interaction W

$$\Sigma = iGW - GWGWG + \cdots$$

can be truncated after the first term:

$$\Sigma \approx iGW$$

Another way to say the same thing is that that self-energy is expanded in a formal Taylor series in powers of the screened interaction W and the lowest order term is kept in the expansion in GWA.

To put this in context, if one replaces W by the bare Coulomb interaction, one generates the usual series for the self-energy found in most many-body textbooks. The GWA with W replaced by the bare Coulomb yields nothing other than the Hartree-Fock exchange potential (self-energy). Therefore, loosely speaking, the GWA represents a type of dynamically screened Hartree-Fock self-energy.

In a solid state system, the series for the self-energy in terms of W should converge much faster than the traditional series in the bare Coulomb interaction. This is because the screening of the medium reduces the effective strength of the Coulomb interaction: for example, if one places an electron at some position in a material and asks what the potential is at some other position in the material, the value is smaller than given by the bare Coulomb interaction (inverse distance between the points) because the other electrons in the medium polarize (move or distort their electronic states) so as to screen the electric field. Therefore, W is a smaller quantity than the bare Coulomb interaction so that a series in W should have higher hopes of converging quickly.

Software supporting the GW approximation [edit]

- ABINIT - plane wave pseudopotential method
- Spex - full-potential (linearized) augmented plane-wave (FP-LAPW) method
- SaX - plane wave pseudopotential method
- YAMBO code- plane wave pseudopotential method

References [edit]

- L. Hedin, Phys. Rev. **139**, A796 (1965).
- W.G. Aulbur, L. Jönsson and J.W. Wilkins, Solid State Physics **54**, 1 (2000) full version in postscript (7,3MB).
- F. Aryasetiawan, O. Gunnarsson, arXiv:cond-mat/9712013v1.

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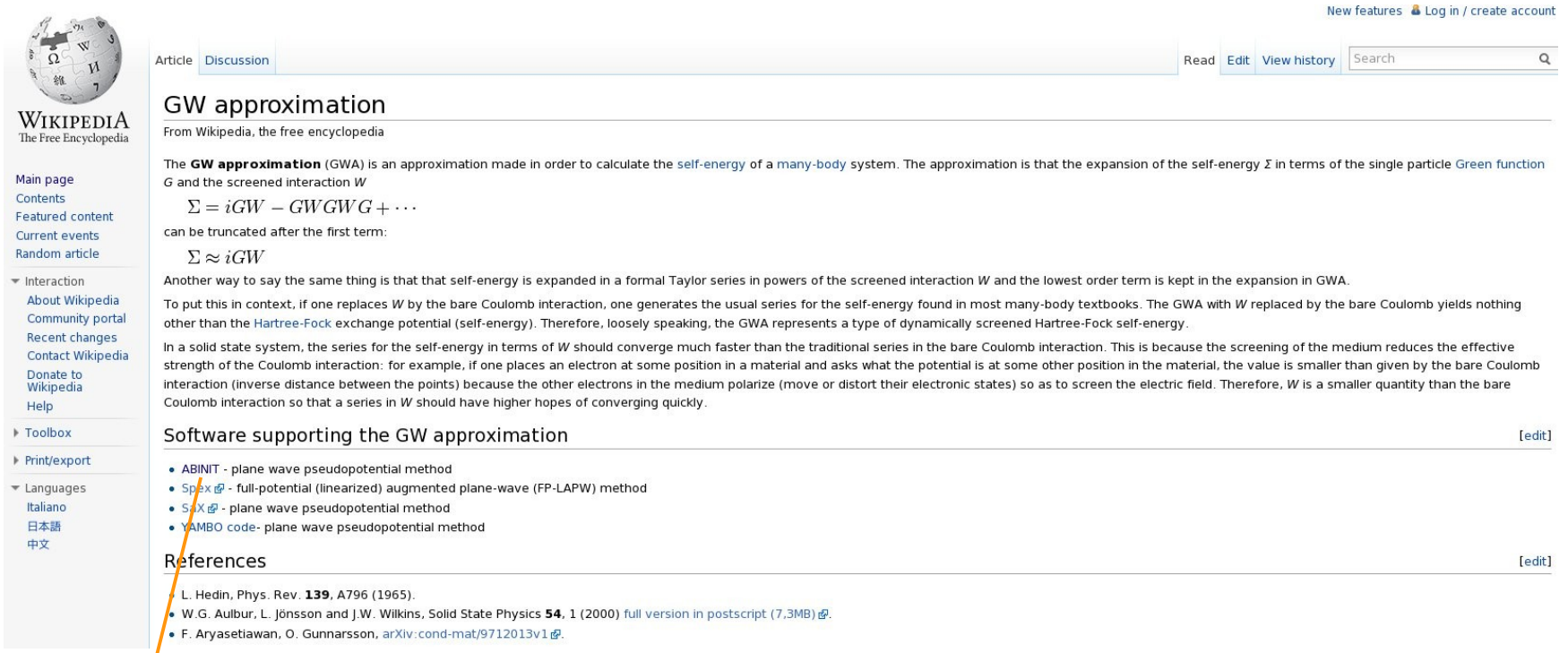

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GW approximation

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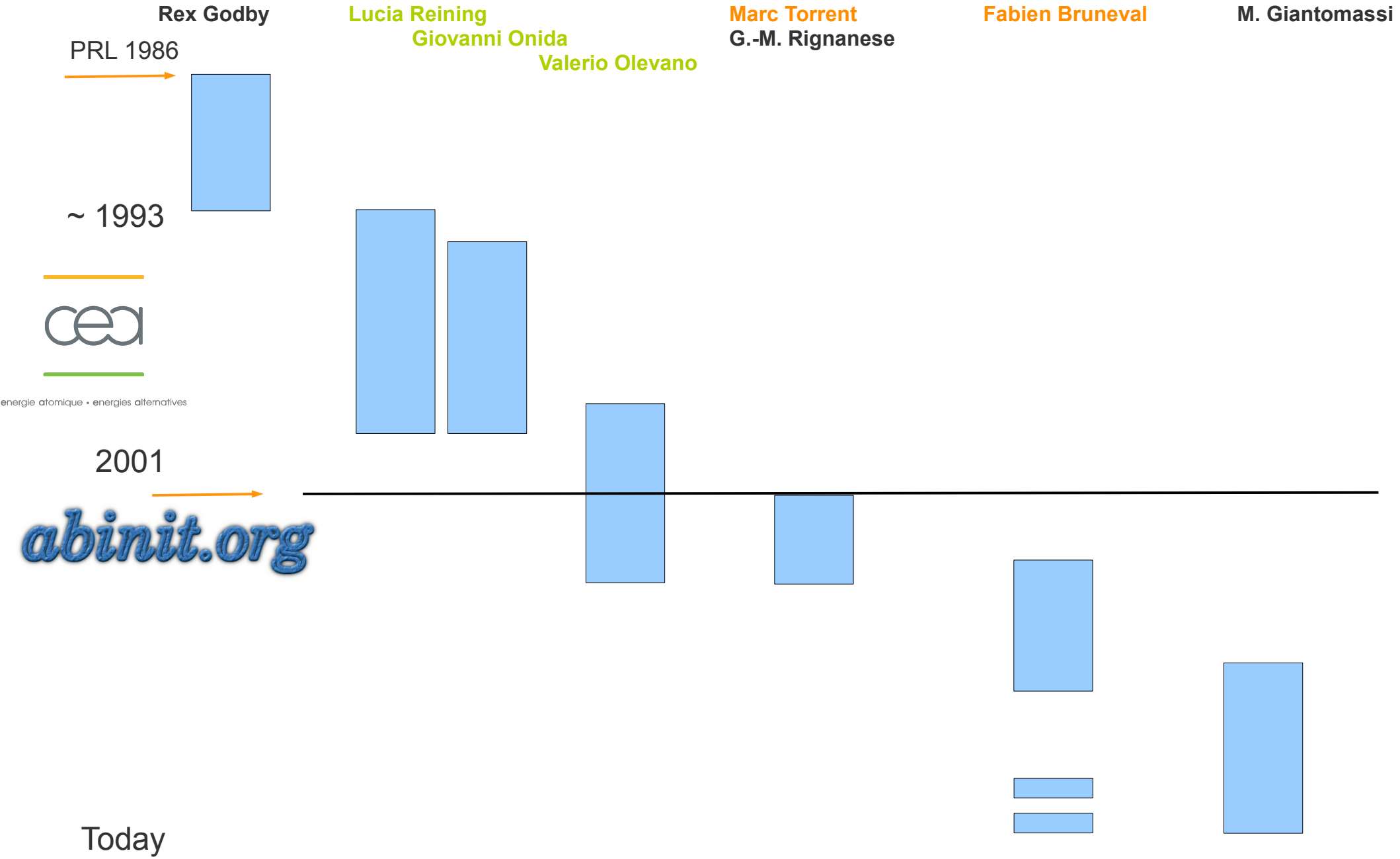
- F. Aryasetiawan, O. Gunnarsson, arXiv:cond-mat/9712013v1.

abinit.org

has a GW code inside

Code history



How to get *G*?

Remember the **Lehman representation**:

$$G(\boldsymbol{r},\boldsymbol{r}',\omega)=\sum_i \frac{f_i(\boldsymbol{r})f_i^*(\boldsymbol{r}')}{\omega-\epsilon_i\pm i\eta}$$

where the $f_i(\boldsymbol{r})$ and the ϵ_i are complicated quantities

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But for **independent electrons** like Kohn-Sham electrons:

$$G^{KS}(\boldsymbol{r},\boldsymbol{r}',\omega)=\sum_i \frac{\varphi_i^{\mathrm{KS}}(\boldsymbol{r})\varphi_i^{KS*}(\boldsymbol{r}')}{\omega-\epsilon_i^{\mathrm{KS}}\pm i\eta}$$

This can be considered as the best guess for *G*

One can get W and Σ^{GW}

GW as a perturbation with respect to LDA

GW quasiparticle equation:

$$\left[h_0+\Sigma_{xc}\left(\epsilon_i^{GW}\right)\right]\left|\varphi_i^{GW}\right\rangle=\epsilon_i^{GW}\left|\varphi_i^{GW}\right\rangle$$

KS equation:

$$\left[h_0+v_{xc}^{\mathrm{LDA}}\right]\left|\varphi_i^{\mathrm{LDA}}\right\rangle=\epsilon_i^{\mathrm{LDA}}\left|\varphi_i^{\mathrm{LDA}}\right\rangle$$

Approximation : $\varphi_i^{GW}\approx\varphi_i^{\mathrm{LDA}}$

GW as a perturbation with respect to LDA

GW quasiparticle equation:

$$\left\langle \varphi_i^{\mathrm{LDA}} \middle| \left[h_0 + \Sigma_{xc}(\epsilon_i^{GW}) \right] \middle| \varphi_i^{\mathrm{LDA}} \right\rangle = \epsilon_i^{GW}$$

KS equation:

$$\left\langle \varphi_i^{\mathrm{LDA}} \middle| \left[h_0 + v_{xc}^{\mathrm{LDA}} \right] \middle| \varphi_i^{\mathrm{LDA}} \right\rangle = \epsilon_i^{\mathrm{LDA}}$$

$$\epsilon_i^{GW} - \epsilon_i^{\mathrm{LDA}} = \left\langle \varphi_i^{\mathrm{LDA}} \middle| \left[\Sigma_{xc}(\epsilon_i^{GW}) - v_{xc}^{\mathrm{LDA}} \right] \middle| \varphi_i^{\mathrm{LDA}} \right\rangle$$

Linearization of the energy dependance

$$\epsilon_i^{GW} - \epsilon_i^{\mathrm{LDA}} = \left\langle \varphi_i^{\mathrm{LDA}} \middle| \left[\Sigma_{xc}\left(\epsilon_i^{GW}\right) - v_{xc}^{\mathrm{LDA}} \right] \middle| \varphi_i^{\mathrm{LDA}} \right\rangle$$

Not yet known

Taylor expansion:

$$\Sigma_{xc}\left(\epsilon_i^{GW}\right) = \Sigma_{xc}\left(\epsilon_i^{\mathrm{LDA}}\right) + \left(\epsilon_i^{GW} - \epsilon_i^{\mathrm{LDA}}\right) \frac{\partial \Sigma_{xc}}{\partial \epsilon} + \ldots$$

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Final result:

$$\epsilon_i^{GW} = \epsilon_i^{\mathrm{LDA}} + Z_i \left\langle \varphi_i^{\mathrm{LDA}} \middle| \left[\Sigma_{xc}\left(\epsilon_i^{\mathrm{LDA}}\right) - v_{xc}^{\mathrm{LDA}} \right] \middle| \varphi_i^{\mathrm{LDA}} \right\rangle$$

where $$Z_i = 1 \Big/ \left(1 - \frac{\partial \Sigma_{xc}}{\partial \epsilon} \right)$$

Quasiparticle equation

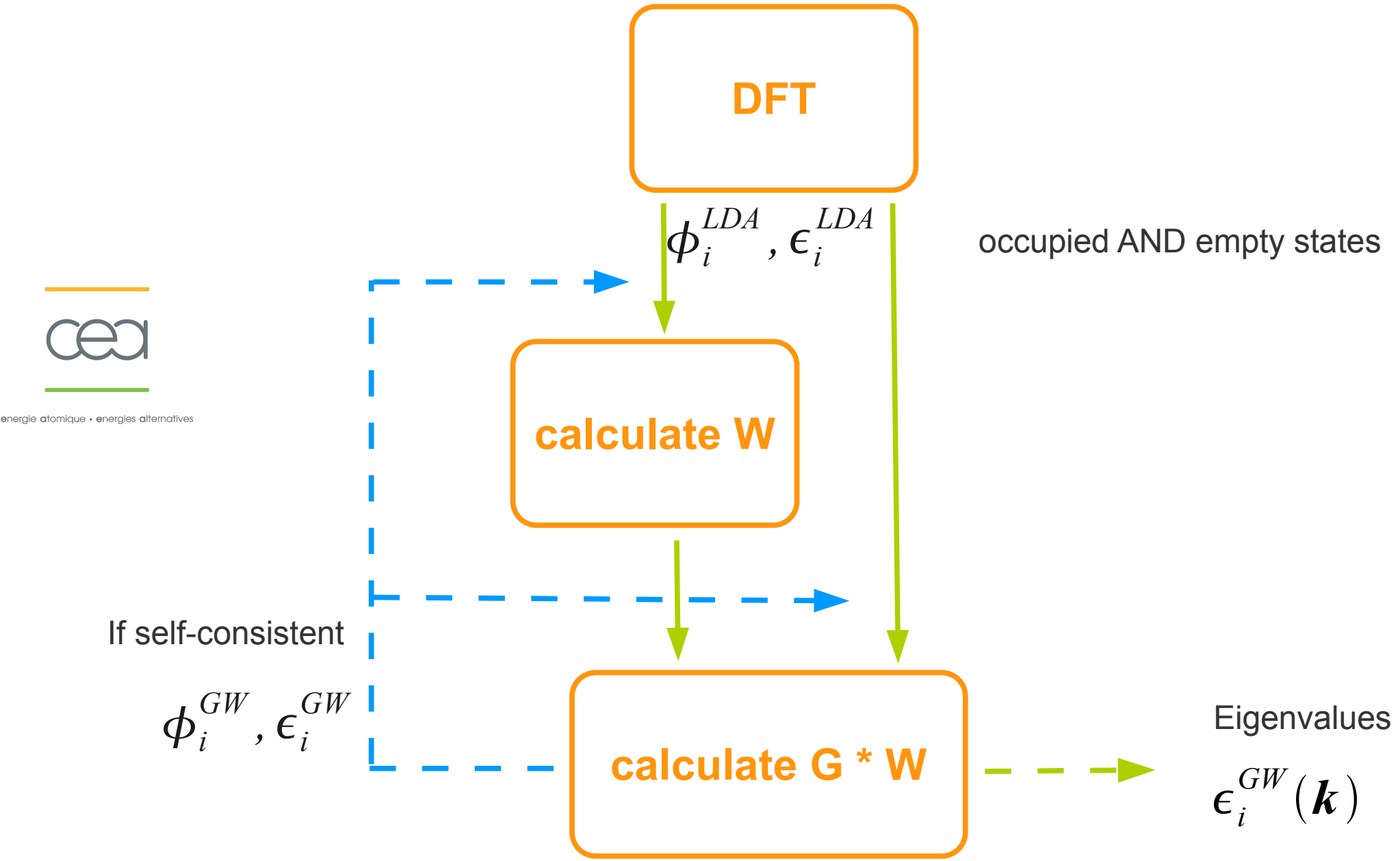
A typical ABINIT ouptput for Silicon at Gamma point

```
k =     0.000   0.000   0.000
Band      E0 <VxcLDA>   SigX SigC(E0)       Z dSigC/dE  Sig(E)    E-E0        E
   4   0.506 -11.291 -12.492   0.744   0.775  -0.291 -11.645  -0.354   0.152
   5   3.080 -10.095  -5.870  -3.859   0.775  -0.290  -9.812   0.283   3.363

E^0_gap         2.574
E^GW_gap        3.212
```

$$\epsilon_i^{GW} = \epsilon_i^{\mathrm{LDA}} + Z_i \left\langle \varphi_i^{\mathrm{LDA}} \middle| \left[\Sigma_{xc}(\epsilon_i^{\mathrm{LDA}}) - v_{xc}^{\mathrm{LDA}} \right] \middle| \varphi_i^{\mathrm{LDA}} \right\rangle$$

Flow chart of a typical *GW* calculation



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Outline

I. Standard DFT suffers from the band gap problem

II. Introduction of the Green's function

III. The *GW* approximation

IV. The *GW* code in ABINIT and the G_0W_0 method

V. Some applications

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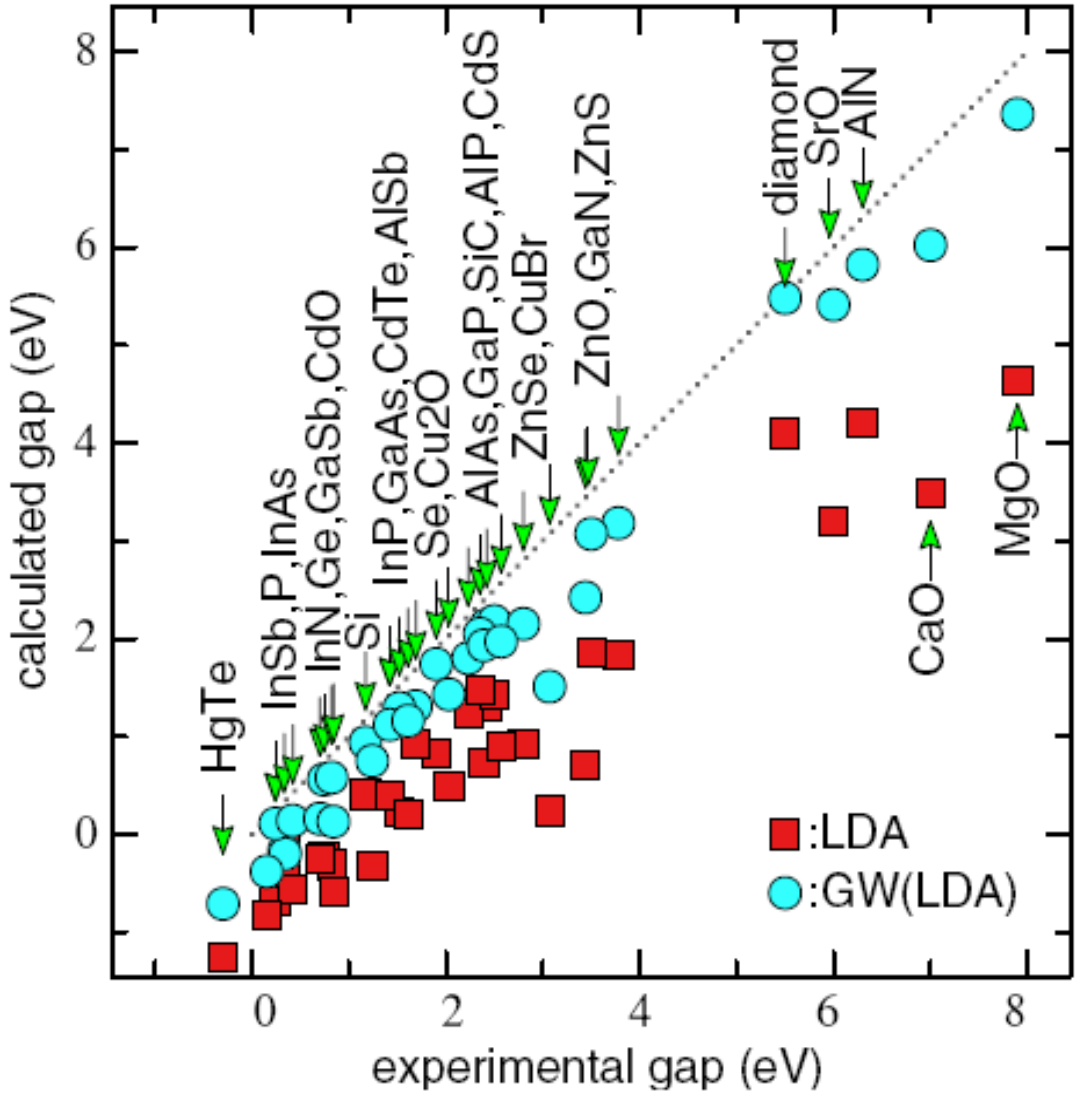
GW approximation gets good band gap



after van Schilfgaarde *et al* PRL **96** 226402 (2008)

No more a band gap problem !

Clusters de sodium

$$Na_4^+ + e^- \Leftrightarrow Na_4$$

$$E_0(Na_4) - E_0(Na_4^+) = \begin{cases} \epsilon(\mathbf{HOMO}, \mathbf{Na_4}) \\ \epsilon(\mathbf{LUMO}, \mathbf{Na_4^+}) \end{cases}$$

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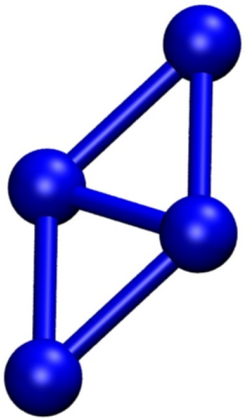
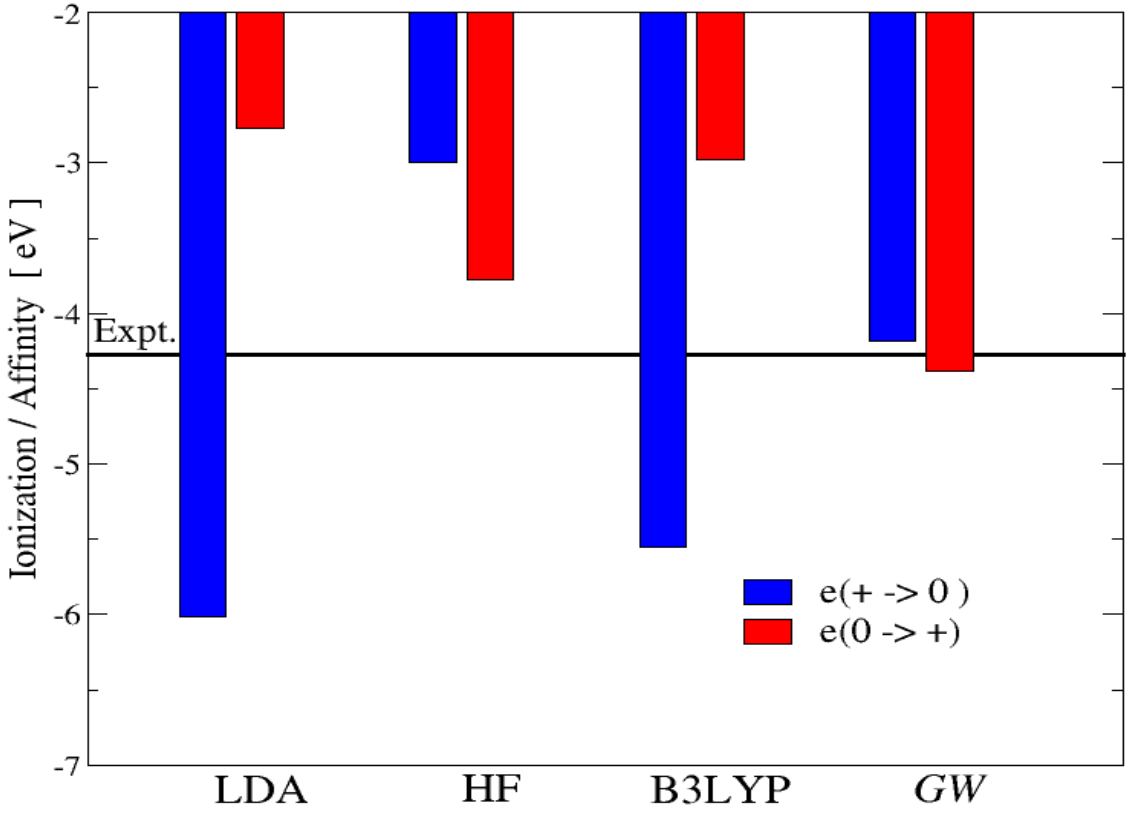


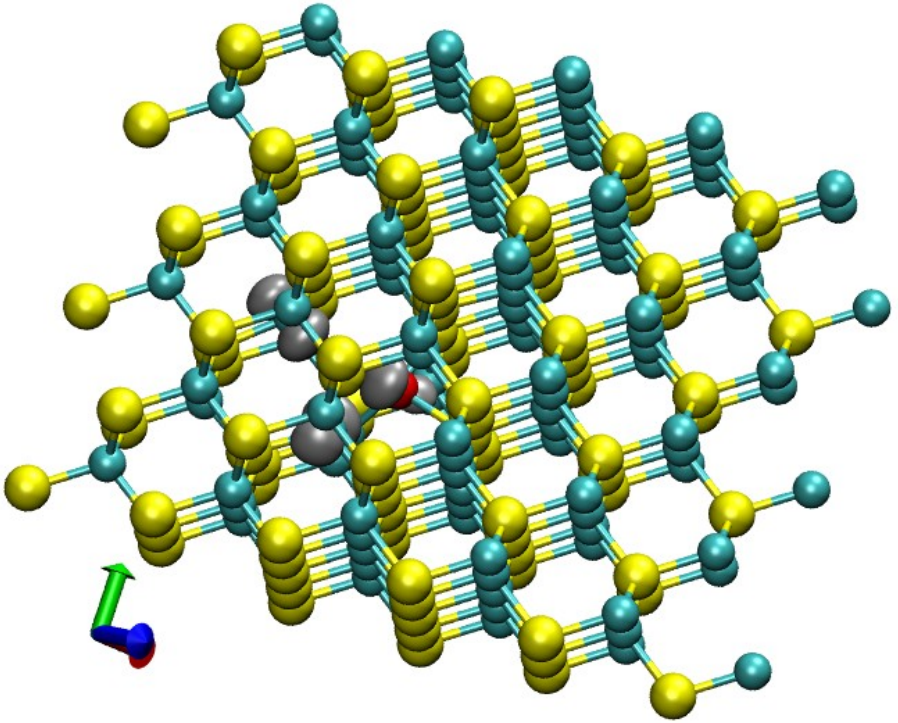
Na_4^+/Na_4



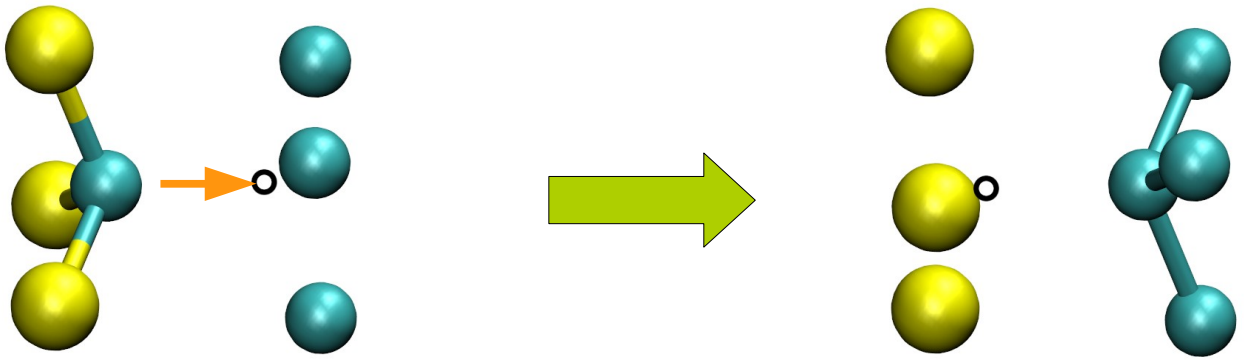
Bruneval PRL (2009)

Calculs de défauts avec l'approximation *GW*

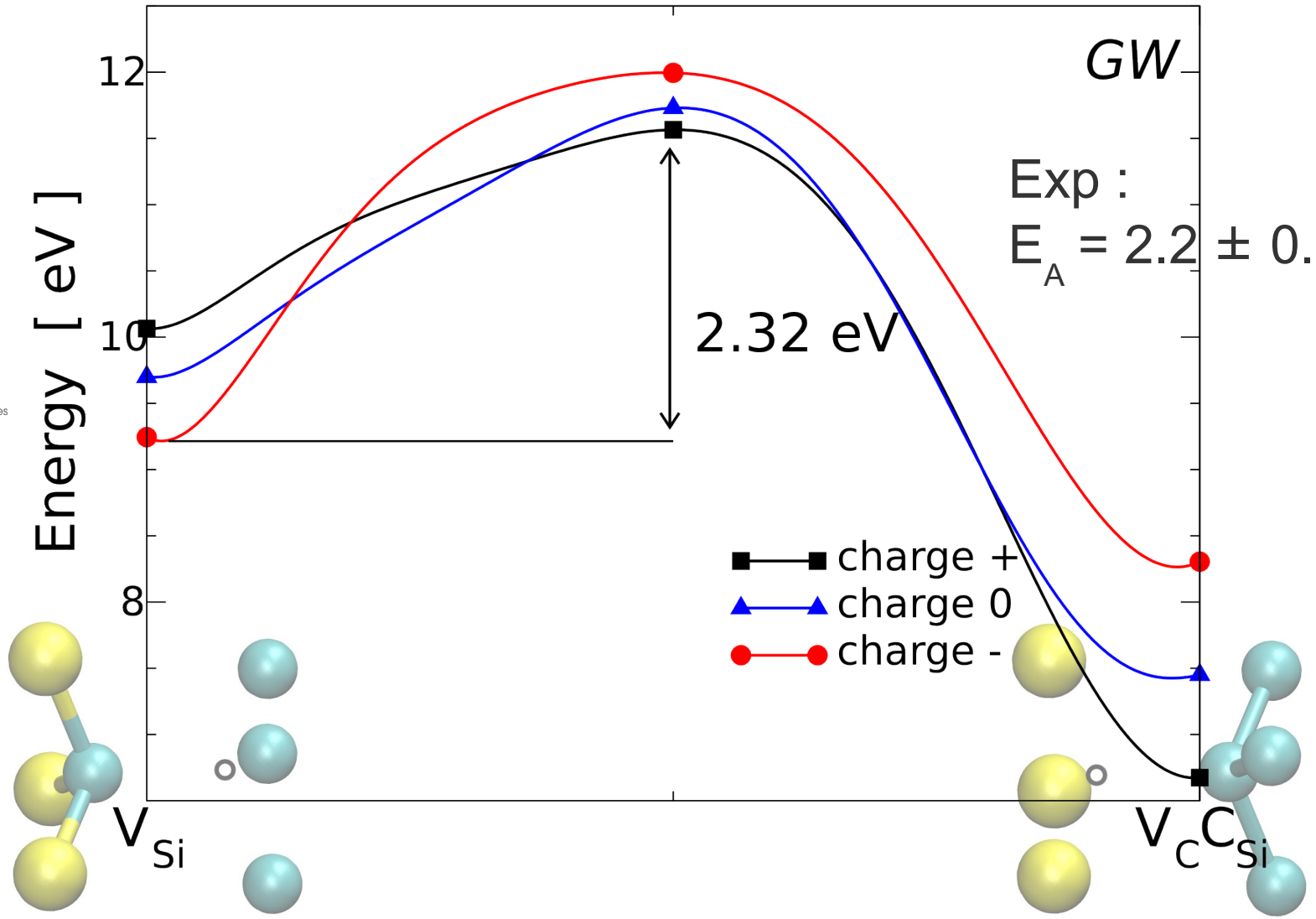
Calcul d'un système à 215 atomes



Carbure de Silicium cubique
3C-SiC



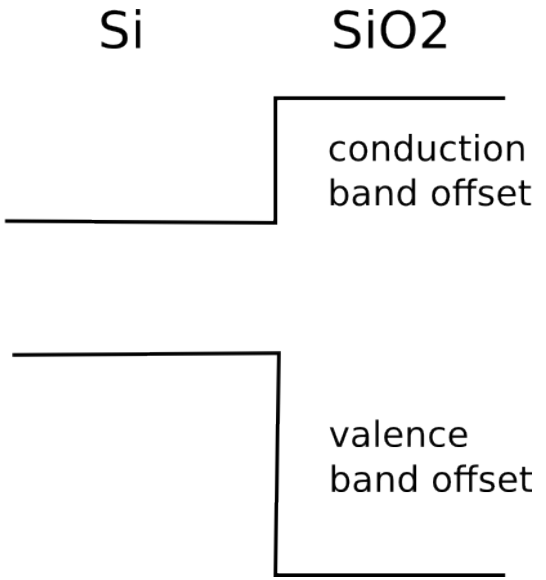
Barrière de transformation



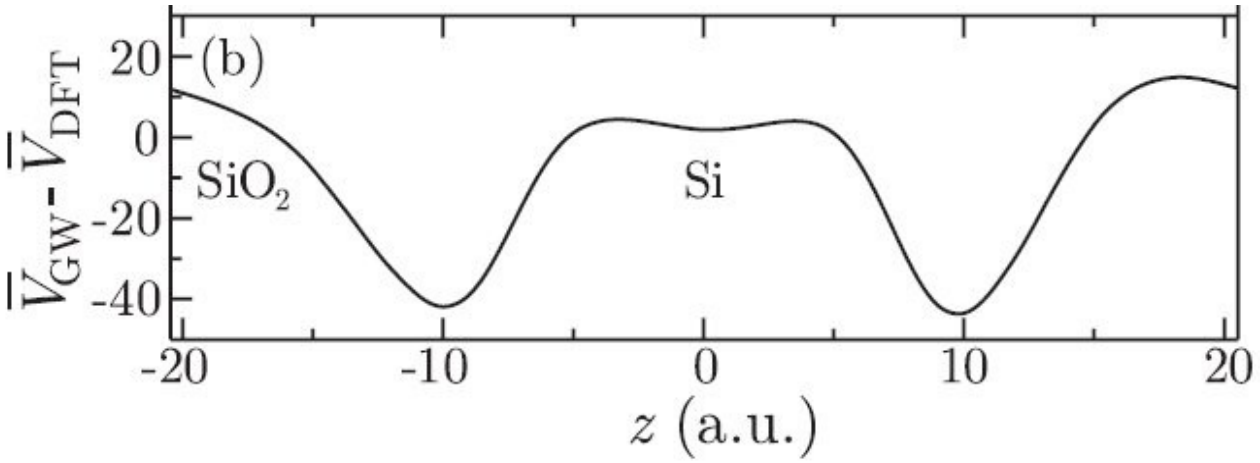
Bruneval et Roma soumis (2010)

Band Offset at the interface between two semiconductors

Very important for electronics!



Example: Si/SiO_2 interface for transistors



GW correction with respect to LDA

R. Shaltaf PRL (2008).

Summary

- The *GW* approximation **solves the band gap problem!**
- The calculations are extremely heavy, so that we resort to many additional technical approximations: **method named G_0W_0**
- The complexity comes from
  - Dependance upon empty states
  - Non-local operators
  - Dynamic operators that requires freq. convolutions
- There are still some other approximations like the Plasmon-Pole model... that I'll discuss during the practical session...

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