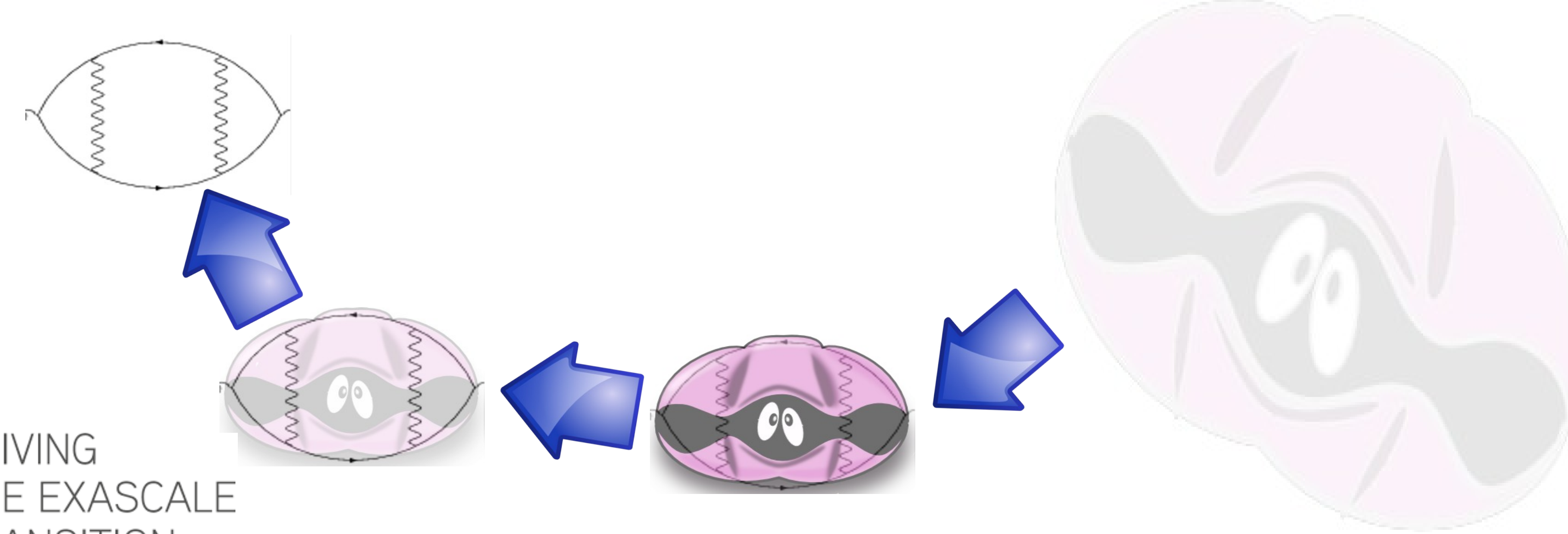

MaX DRIVING THE EXASCALE TRANSITION

Overview of the Yambo code: main features and performance

D. Sangalli
Istituto di Struttura della Materia (CNR),
Area della Ricerca di Roma 1, Monterotondo Scalo, Italy.

the Yambo team

CNR Istituto di Struttura della Materia

ENCSS MaX School
14-17 November 2022

Outline

I. The yambo code

II. abintio MBPT & the QP concept

III. Excitons: the BSE

Part I
The yambo code

Theory

Many-Body perturbation Theory

Time-dependent density functional theory

Interfaces

Planewave Pseudopotential codes:

Abinit

QUANTUM ESPRESSO

www.yambo-code.eu

MaX flagship code

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Libraries

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netCDF

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Different projects

Developers

the Yambo team

Properties

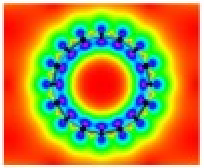
GPL

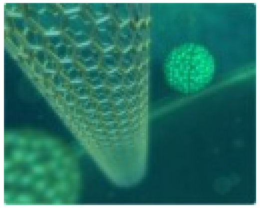
Quasi-particles
Optics and excitons
Magneto-optics & dichroism
Electron-phonon coupling
Real-time propagation
Non-linear optics

Development (pre-GPL) version

Exciton-phonon coupling
Pump and probe experiments
Defects withing MBPT
Ehrenfest dynamics
Magnons

Applications





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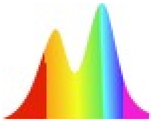
MaX flagship code

Properties



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Schools

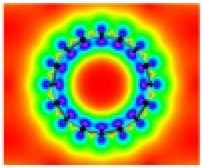
Community & Publications

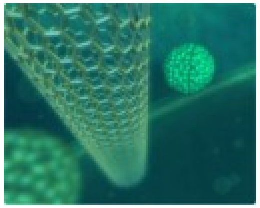
Growing community of users using Yambo for fore-front research. More than 200 publications.

www.yambo-code.eu

MaX flagship code

Applications





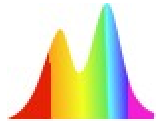
Support & reach out

Git repository

Dedicated User Forum

Online documentation and tutorials

Properties



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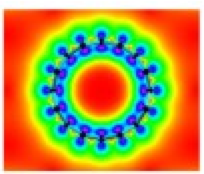
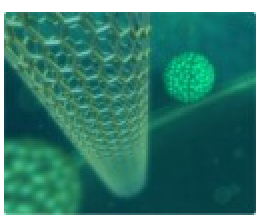
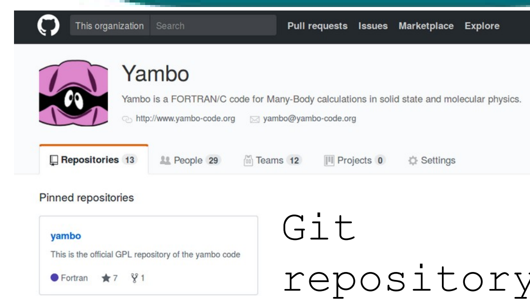




Support & reach out



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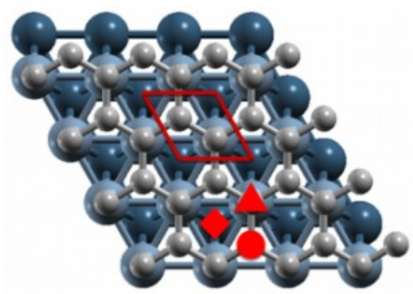
Perfomances

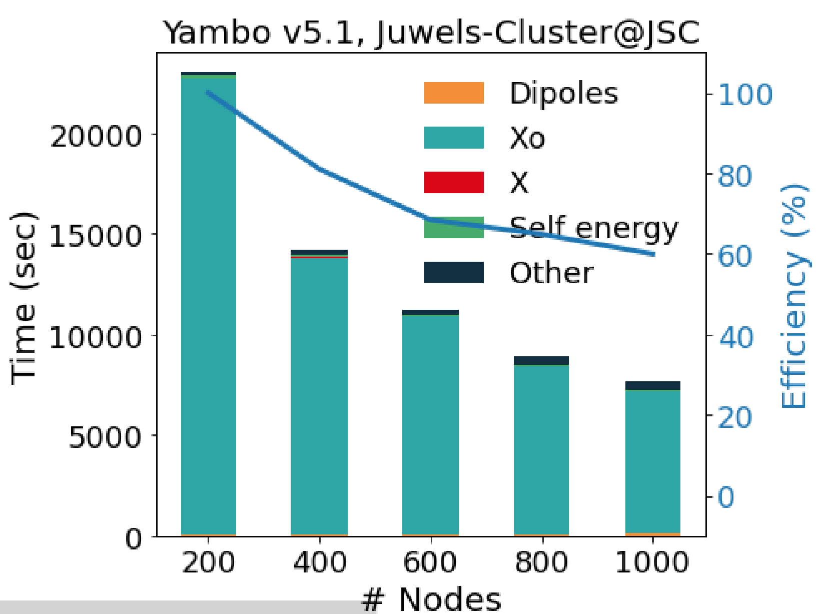
GW study of
Graphene @ Co(0001) interface



Yambo compiled with ifort (**intel**).
MPI + OpenMP

mpirun -np #MPI
#MPI=4
#THREADS=24 (2*#cores / #MPI)

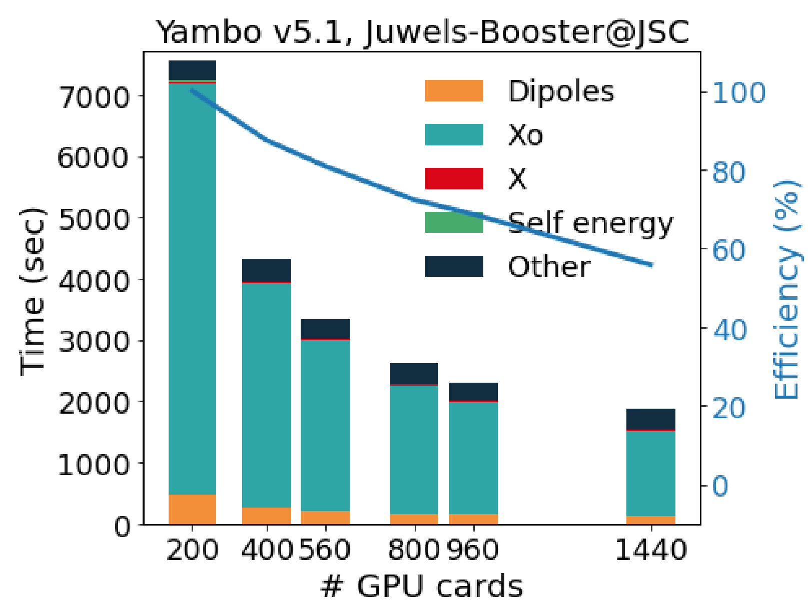
Juwels-Cluster.
48 **Intel** cores per node



Yambo compiled with nvfortran (**nvidia**).
MPI + OpenMP **+ Cudafortran**
(working on OpenACC)

mpirun -np #MPI
#MPI=4 (= #cards per node)
#THREADS=8 (no effect here)

Juwels-Booster.
48 AMD cores per node
4 **Nvidia** A100 cards per node



Data available at: http://www.gitlab.com/max-centre/Benchmarks

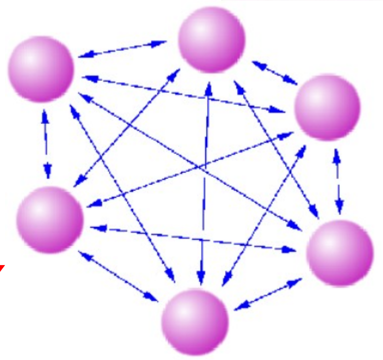
Part II
Abinitio Many-body Perturbation-Theory

Many-Body Perturbation-Theory

$$H = \sum_{i=1}^{N} h(\mathbf{r}_i) + \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V(\mathbf{r}_i, \mathbf{r}_j)$$

1 - Define the Green function (GF)

$$G(\mathbf{r}', t'; \mathbf{r}, t) = -i \left\langle \phi_0^N \left| \hat{T} \left[\hat{\psi}(\mathbf{r}', t') \hat{\psi}^\dagger(\mathbf{r}, t) \right] \right| \phi_0^N \right\rangle$$



Interacting particles
Ground state

Many-Body Perturbation-Theory

$$H = \sum_{i=1}^{N} h(\mathbf{r}_i) + \sum_{\substack{i,j=1 \\ i\neq j}}^{N} V(\mathbf{r}_i, \mathbf{r}_j)$$

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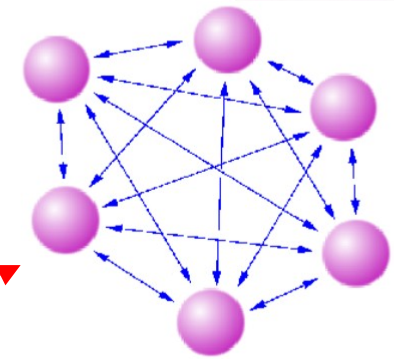
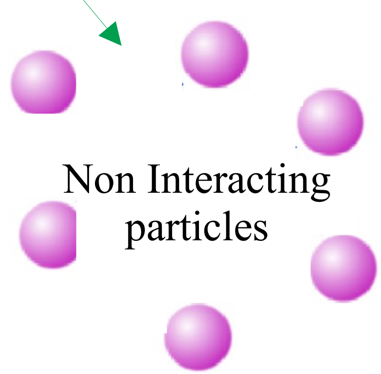


Interacting particles
Ground state

2 – Use Gell-Mann & Low theorem

$$G(\mathbf{r}, t, \mathbf{r}', t') = -\frac{\mathrm{i}}{\left\langle \psi_0 \middle| \hat{U} \middle| \psi_0 \right\rangle} \sum_{n=0}^{+\infty} \frac{(-\mathrm{i})^n}{n!} \int_{-\infty}^{+\infty} \mathrm{d}t_1 \cdots \mathrm{d}t_n e^{-\eta(|t_1|+\cdots+|t_n|)} \times$$

$$\left\langle \psi_0 \middle| \mathrm{T} \left[\hat{V}(t_1) \cdots \hat{V}(t_n) \hat{\psi}(t) \hat{\psi}^\dagger(t') \right] \middle| \psi_0 \right\rangle$$



$$+\Sigma^{xc}[G](r, r', \omega)$$

Why the GF?

Leehman's representation

$$G(\mathbf{r},\mathbf{r}',\omega) = \lim_{\eta\to 0^+} \sum_n \left\{ \frac{\chi_0^{N+1}(\mathbf{r})\left[\chi_0^{N+1}(\mathbf{r}')\right]^*}{\omega - \epsilon_n(N+1) - \mu + i\eta} + \frac{\left[\chi_0^{N-1}(\mathbf{r})\right]^* \chi_0^{N-1}(\mathbf{r}')}{\omega - \epsilon_n(N-1) - \mu - i\eta} \right\}$$

Phys. Rev. B 92, 125440 (2015)

Why the GF?

Leehman's representation

$$G(\mathbf{r},\mathbf{r}',\omega) = \lim_{\eta\to 0^+} \sum_n \left\{ \frac{\chi_0^{N+1}(\mathbf{r})\left[\chi_0^{N+1}(\mathbf{r}')\right]^*}{\omega - \epsilon_n(N+1) - \mu + i\eta} + \frac{\left[\chi_0^{N-1}(\mathbf{r})\right]^* \chi_0^{N-1}(\mathbf{r}')}{\omega - \epsilon_n(N-1) - \mu - i\eta} \right\}$$

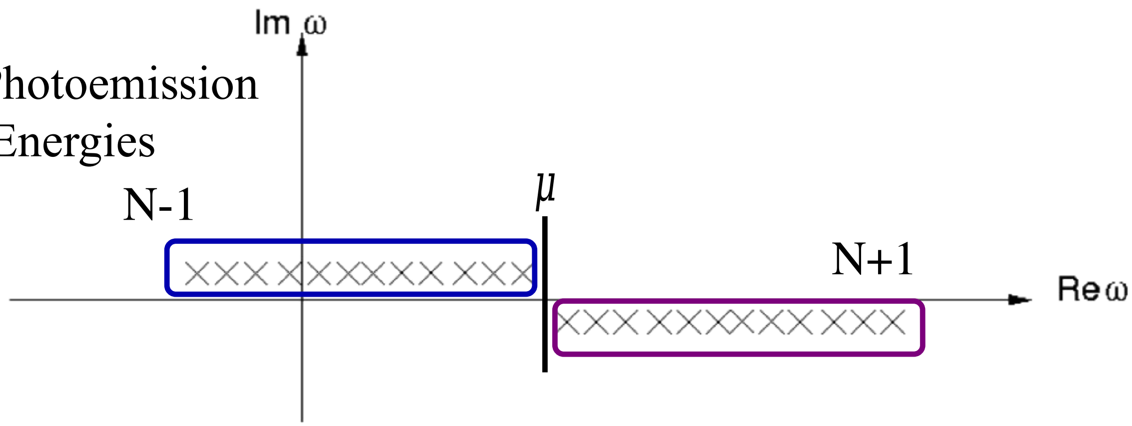
Excitation energies

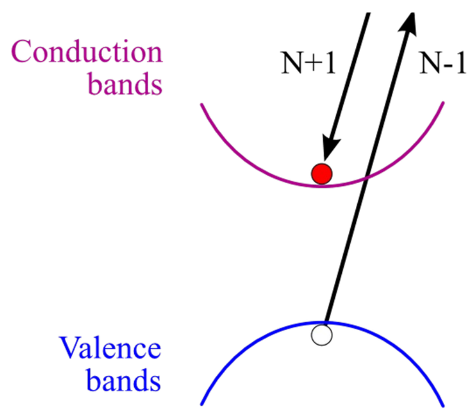
$$\epsilon_n(N \pm 1) = E_n(N \pm 1) - E_0(N \pm 1)$$

Chemical potential

$$\mu = \begin{cases} E_0(N+1) - E_0(N) \\ E_0(N) - E_0(N-1) \end{cases}$$

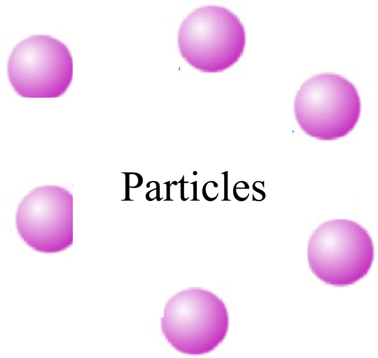
Photoemission Energies





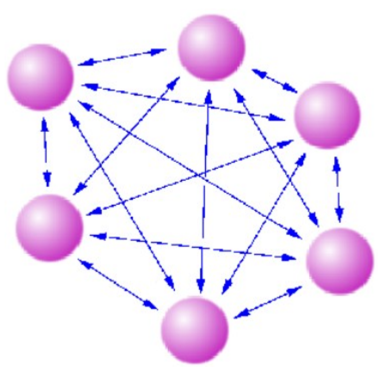
Phys. Rev. B 92, 125440 (2015)

The QP concept



$$+\Sigma^{xc}[G](\omega)$$

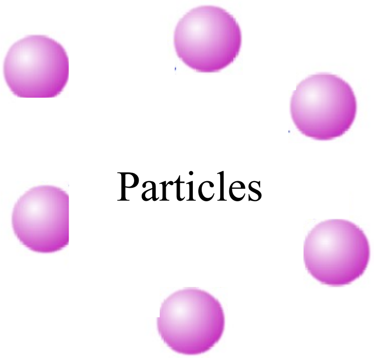
Interacting particles



$$G(\omega)=G^{0}(\omega)+G^{0}(\omega)\Sigma^{xc}[G](\omega)G(\omega)$$

#poles of G >> #poles of G^0

The QP concept

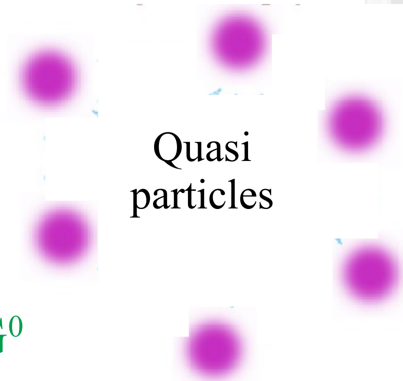


Particles

$$+\Sigma^{xc}[G](\epsilon^{qp})$$

$$G^{qp} = G^0 + G^0 \Sigma^{xc}(\epsilon_{qp}) G^{qp}$$

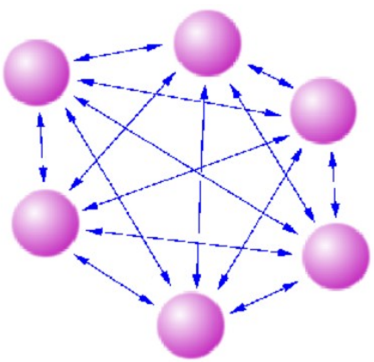
#poles of G^{qp} = #poles of G^0



Quasi particles

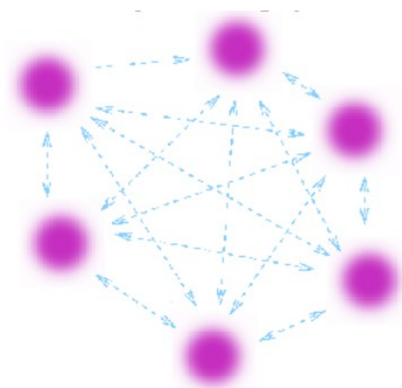
$$+\Sigma^{xc}[G](\omega)$$

Interacting particles



$$+\Sigma^{xc}(\omega) - \Sigma^{xc}(\epsilon^{qp})$$

Weakly interacting quasi-particles



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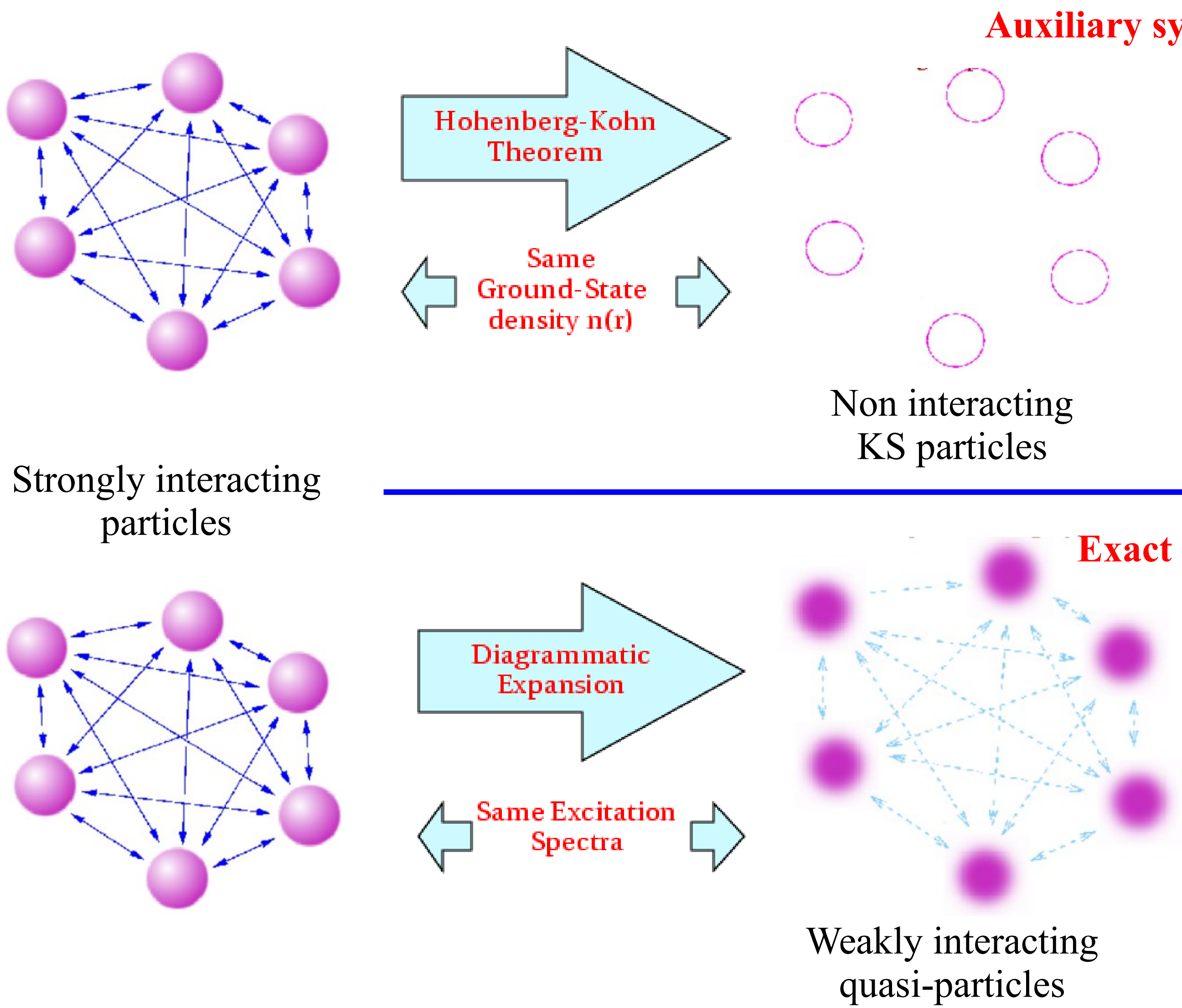
Adapted from F. Sottile PhD thesis

the Yambo team

DFT vs MBPT



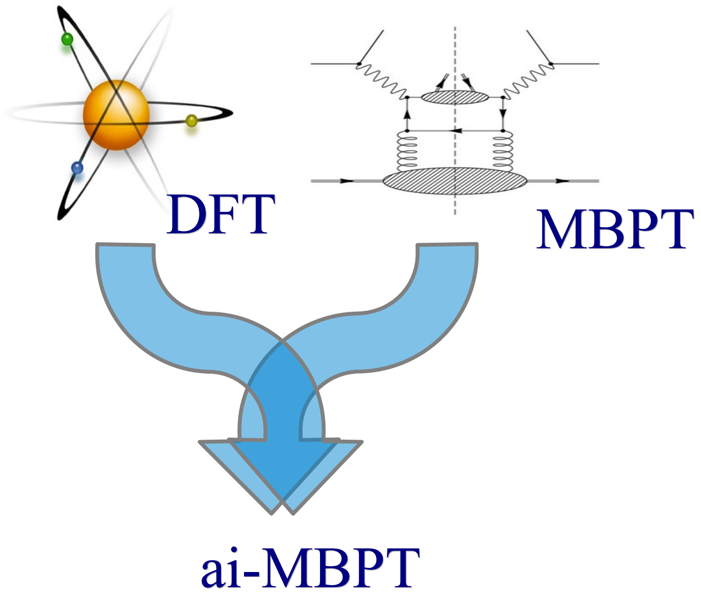
DFT

$$v^{xc}[\rho](r)$$

MBPT

$$\Sigma^{xc}[G](r,r',\omega)$$

DFT + MBPT



G. Onida, L. Reining, and A. Rubio,
Rev. Mod. Phys. 74, 601 (2002)

DFT

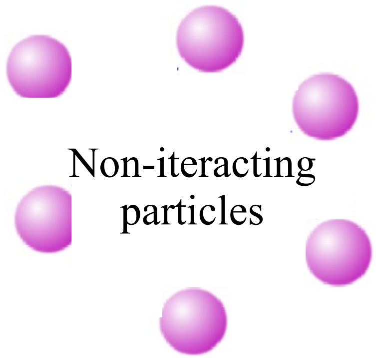
$$\left[\frac{-\nabla^2}{2}+v^{ext}+v^{Hxc}\right]\psi_{nk}(r)=\epsilon_{nk}\psi_{nk}(r)$$

MBPT

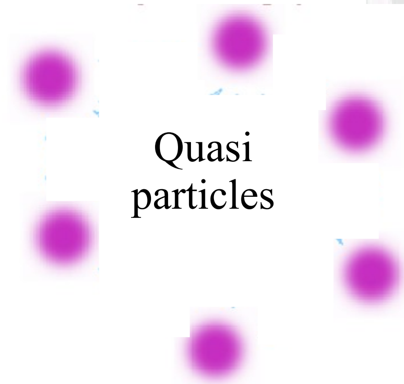
$$G^{KS}(r,r',\omega)=\sum_{nk}\frac{\psi^*_{nk}(r)\psi_{nk}(r')}{\omega-\epsilon^{KS}_{nk}+i\eta}$$

$$G=G^{KS}+G^{KS}(\Sigma^{xc}-v^{xc})G$$

MBPT



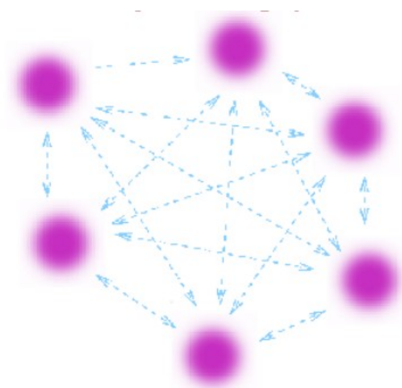
$$+\Sigma^{xc}[G](\epsilon^{qp})$$



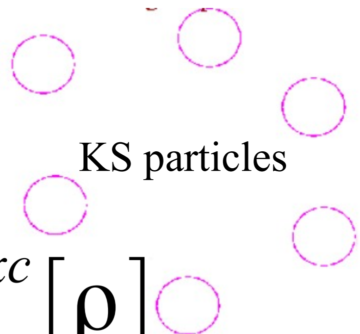
$$+\Sigma^{xc}(\omega) - \Sigma^{xc}(\epsilon^{qp})$$

$$G = G^0 + G^0 \Sigma^{Hxc} G$$

Weakly interacting
quasi-particles

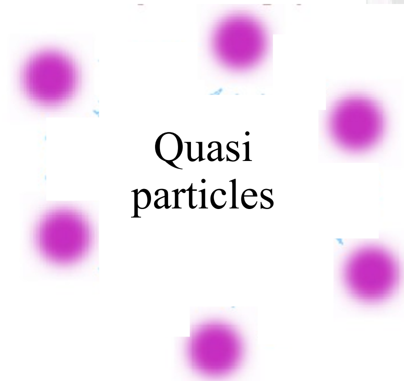


abinitio MBPT



$$v^{xc}[\rho]$$

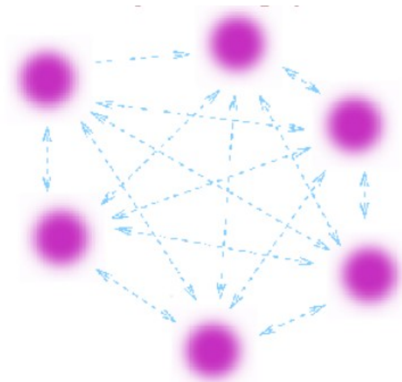
$$+\Sigma^{xc}[G](\epsilon^{qp}) - v^{xc}[\rho]$$



$$+\Sigma^{xc}(\omega) - \Sigma^{xc}(\epsilon^{qp})$$

$$G = G^{KS} + G^{KS}(\Sigma^{xc} - v^{xc})G$$

Weakly interacting
quasi-particles



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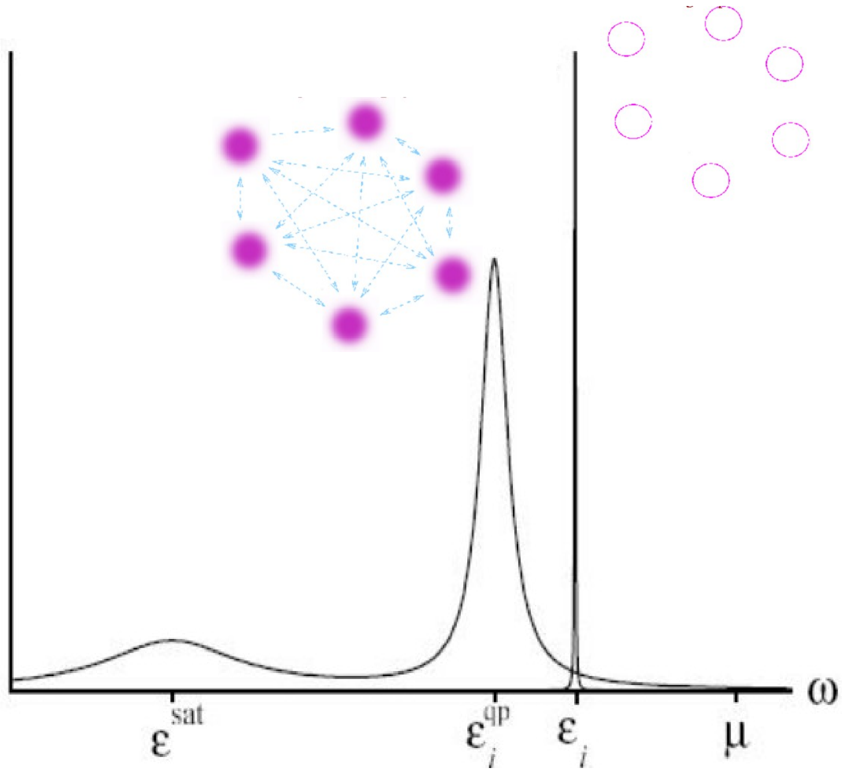
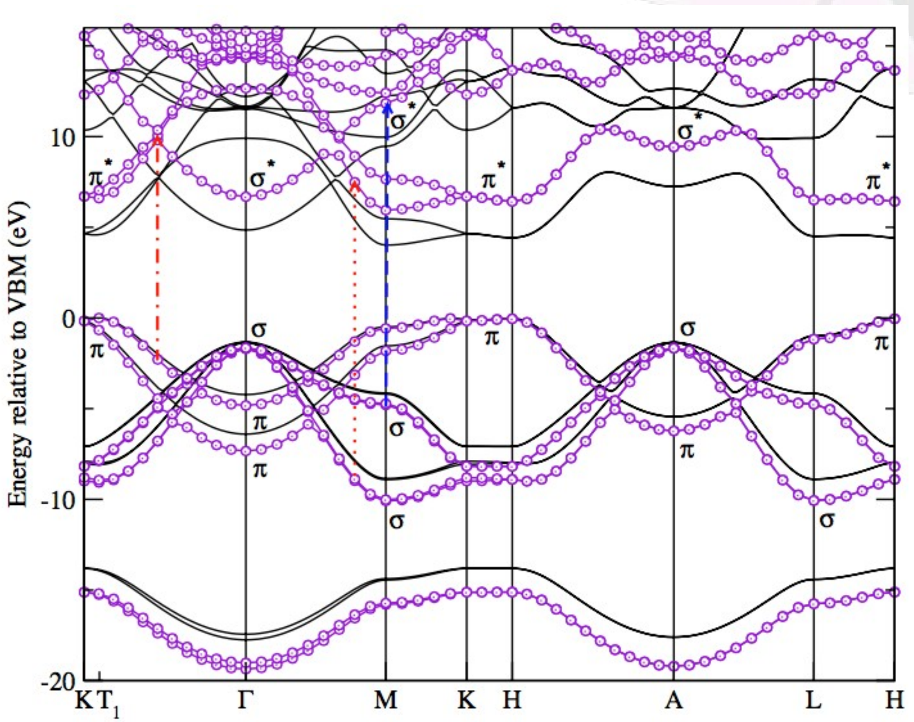
DFT and GW bands

Photoemission spectral function



DFT vs GW band structure in hBN

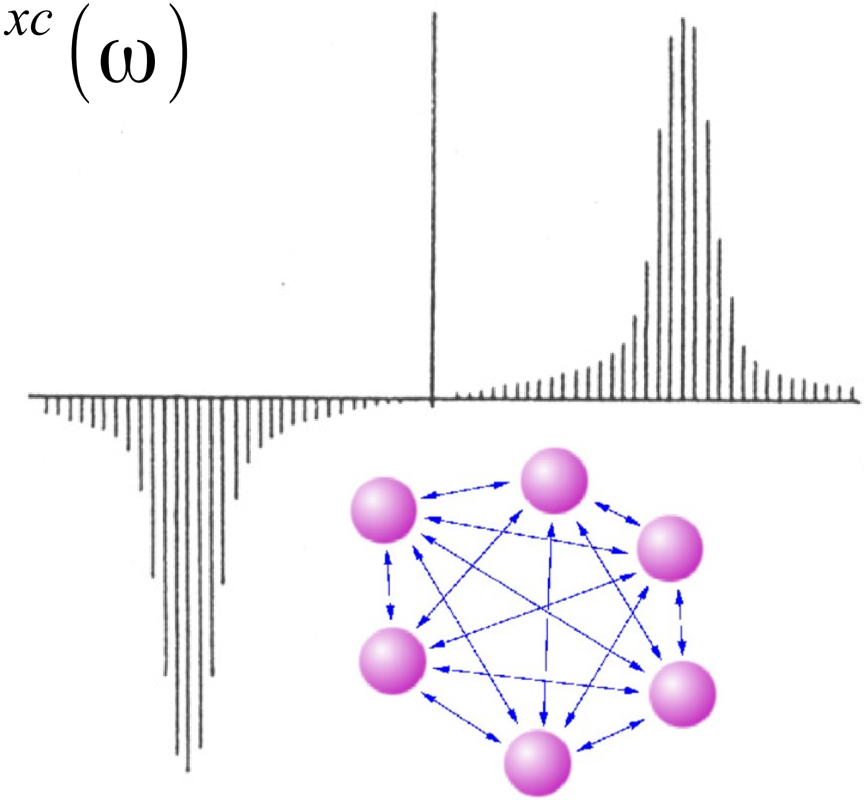


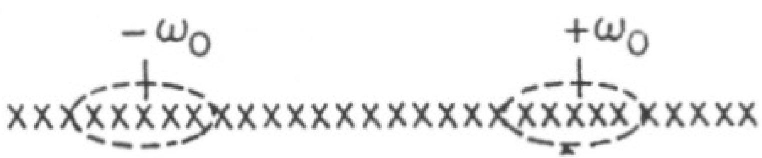
Phys, Rev. Lett. 96, 026402 (2006)

See more in the next talk

QP complex energies

$$\Sigma^{xc}(\omega)$$





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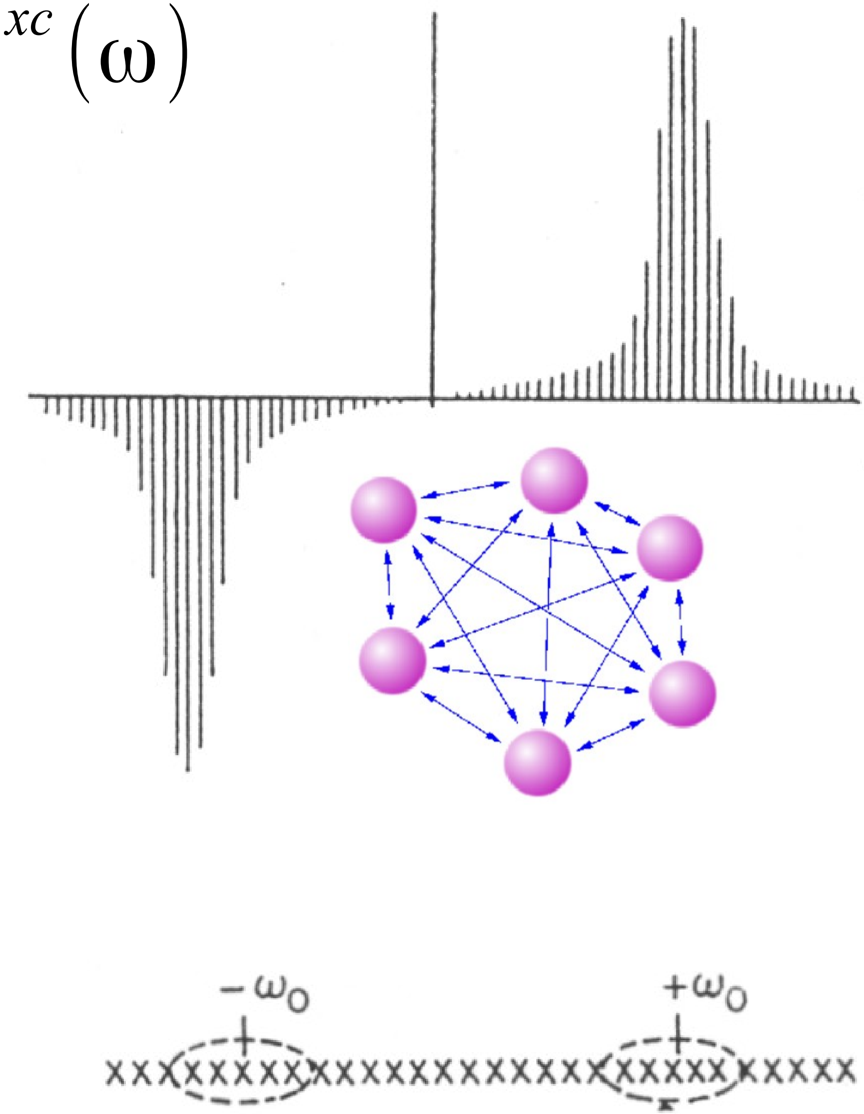
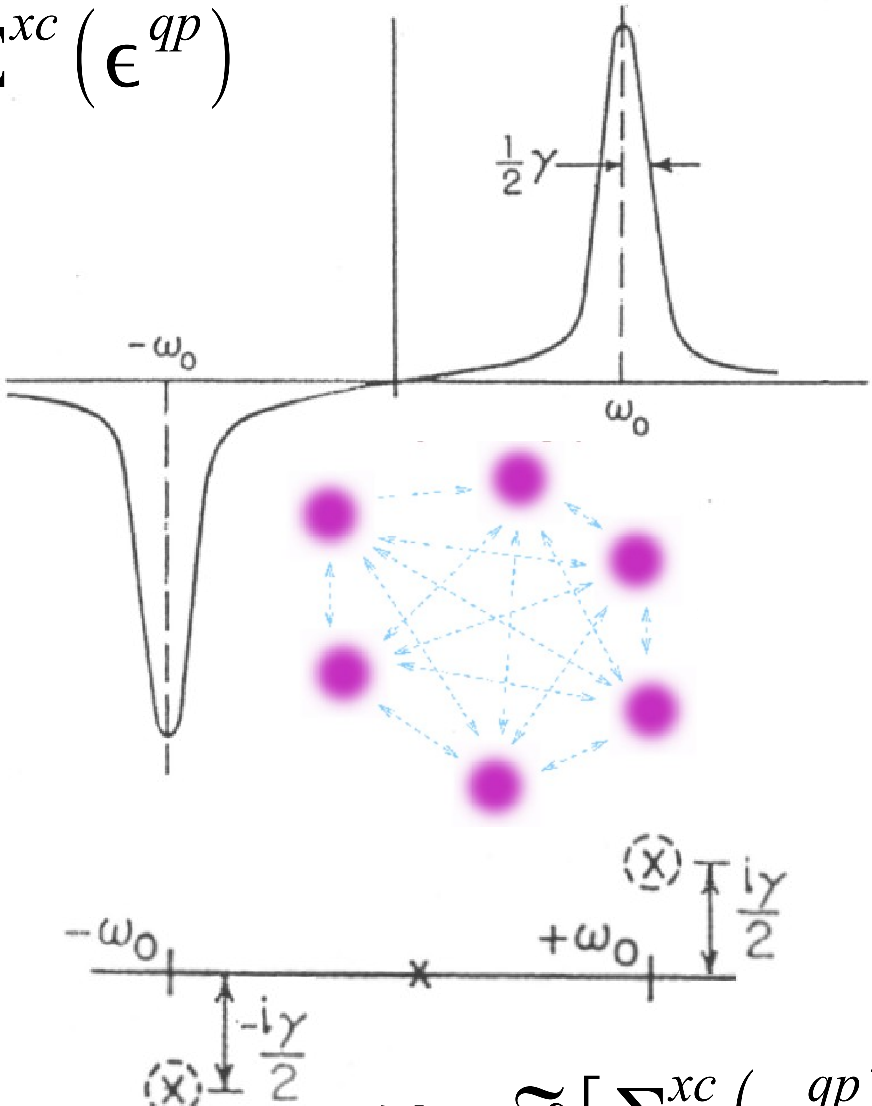
Adapted from M. Gatti PhD thesis

QP complex energies

$\Sigma^{xc}(\omega)$



$\Sigma^{xc}(\epsilon^{qp})$



$$\gamma = \Im\left[\Sigma^{xc}\left(\epsilon^{qp}\right)\right]$$

Adapted from M. Gatti PhD thesis

The role of screening

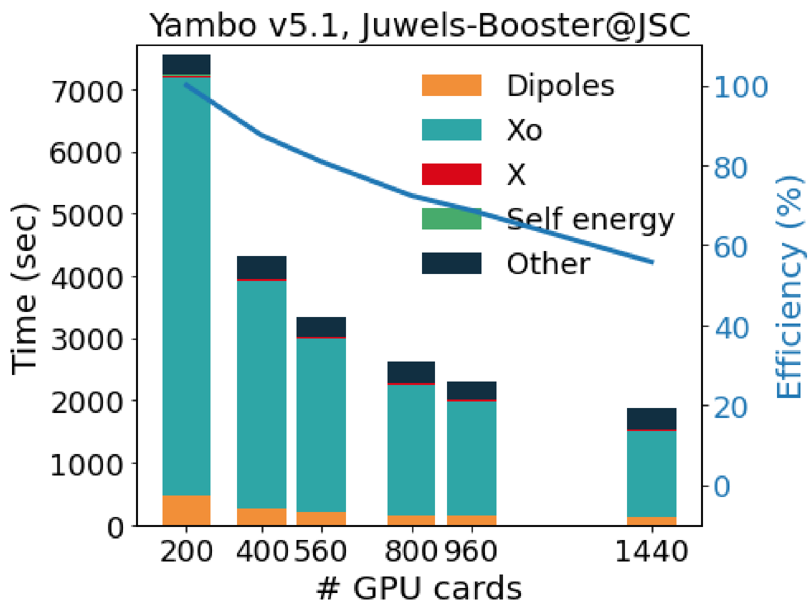
$$\Sigma^{xc}[G] = G W \Gamma$$

Screened electron-hole interaction

$$W^{RPA} = v + v \chi^{RPA} v$$

$$\chi^{RPA}_{GG'}(q, \omega)$$

$$\chi^{RPA} = \chi_0 + \chi_0 v \chi^{RPA}$$



the Yambo team

Part III

Excitons:

The Bethe-Salpeter equation

Neutral excitations

1 - Define a two body response function

$$G(1,2,3,4) = (-i)^2 \left\langle N \left| T \left[\psi(1)\psi(3)\psi^\dagger(4)\psi^\dagger(2) \right] \right| N \right\rangle$$

$$1 = (x_1, t_1, \sigma_1)$$

$$L(1,2,3,4) = L^0(1,2,3,4) - G(1,2,3,4)$$

Strongly interacting
(quasi)electron – (quasi)hole

Neutral excitations

1 - Define a two body response function

$$G(1,2,3,4) = (-i)^2 \langle N \left| T \left[\psi(1)\psi(3)\psi^\dagger(4)\psi^\dagger(2) \right] \right| N \rangle$$

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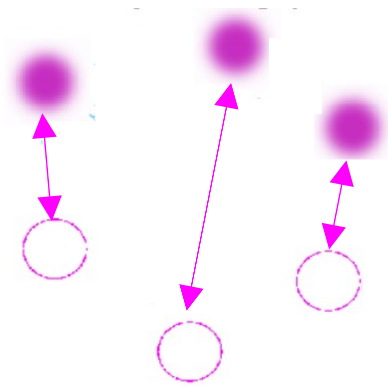

2- Define a Kernel

$$K^{Hxc}[G](1,2;3,4) = \frac{\delta \Sigma(1,2)}{\delta G(3,4)}$$

Neutral excitations

1 - Define a two body response function

$$G(1,2,3,4) = (-i)^2 \langle N | T \left[\psi(1)\psi(3)\psi^\dagger(4)\psi^\dagger(2) \right] | N \rangle$$

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$$L(1,2,3,4) = L^0(1,2,3,4) - G(1,2,3,4)$$

Strongly interacting
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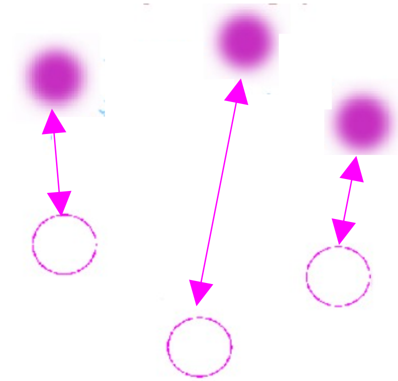

2- Define a Kernel

$$K^{Hxc}[G](1,2;3,4) = \frac{\delta \Sigma(1,2)}{\delta G(3,4)}$$

3- Spectral representation $(t_1 = t_2)$ $(t_3 = t_4)$

$L(\omega)$ ⟶ poles $\omega_I = E_I(N) - E_0(N)$

Bethe-Salpeter Equation

The Dyson equation for L, or Bethe Salpeter Equation (BSE)

$$L = L^{qp} + L^{qp} K^{Hxc} L \qquad K^{Hxc}(\omega=0) = (v - W)$$

can be rewritten as an eigenvalue problem

$$\left[\left(\epsilon_{ck} - \epsilon_{vk-q} \right) + v_{cvk,\,c'v'k'} - W_{cvk,\,c'v'k'} \right] A^{\lambda q}_{c'v'k'} = \omega_{\lambda q} A^{\lambda q}_{cvk}$$

Bethe-Salpeter Equation

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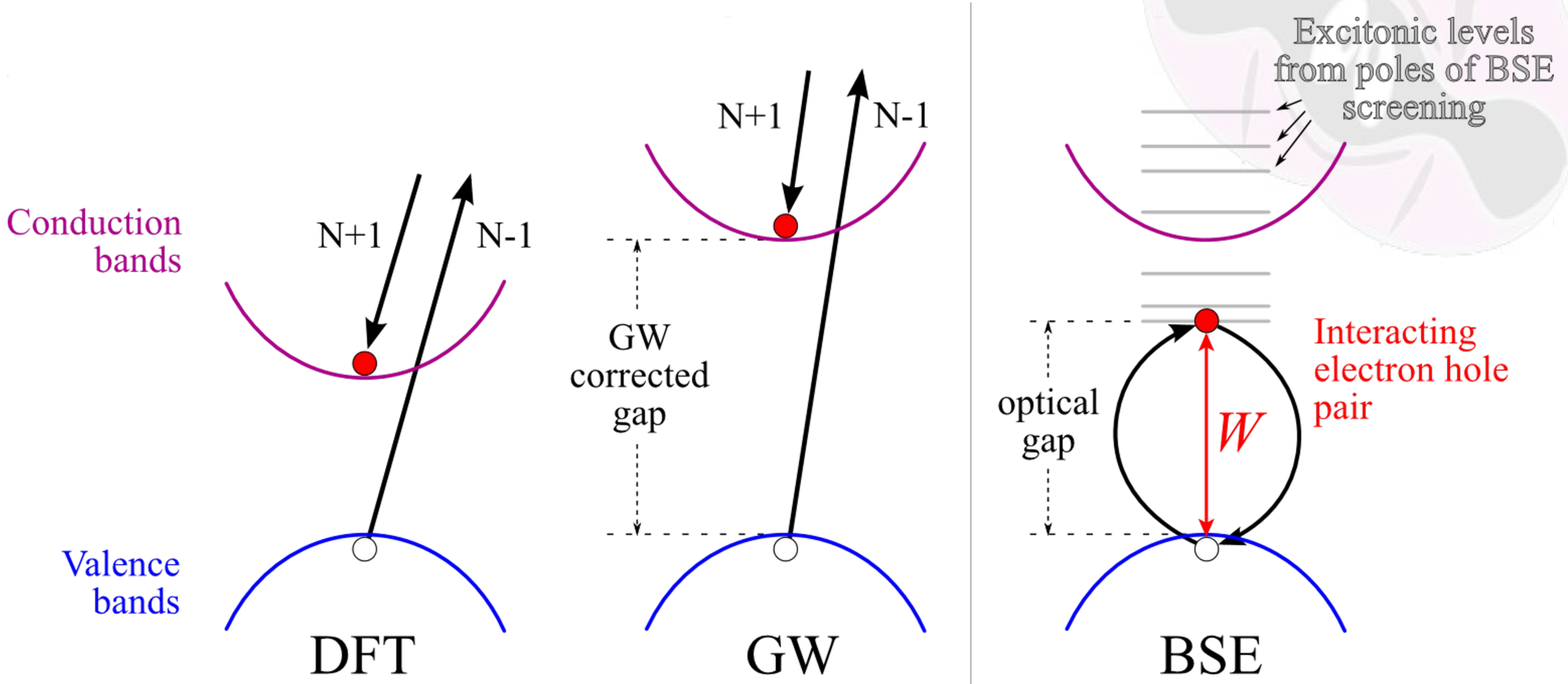
$$\left[(\epsilon_{ck} - \epsilon_{vk-q}) + v_{cvk,c'v'k'} - W_{cvk,c'v'k'} \right] A^{\lambda q}_{c'v'k'} = \omega_{\lambda q} A^{\lambda q}_{cvk}$$

$$|\Psi^{\lambda q}(k)|^2 = \sum_{cv} |A^{\lambda q}_{cvk}|^2$$

Excitation wave-function

$$\Psi^{\lambda q}(x_h, x_e) = \sum_{cvk} A^{\lambda q}_{cvk} \psi^*_{ck-q}(x_e) \psi_{vk}(x_h)$$

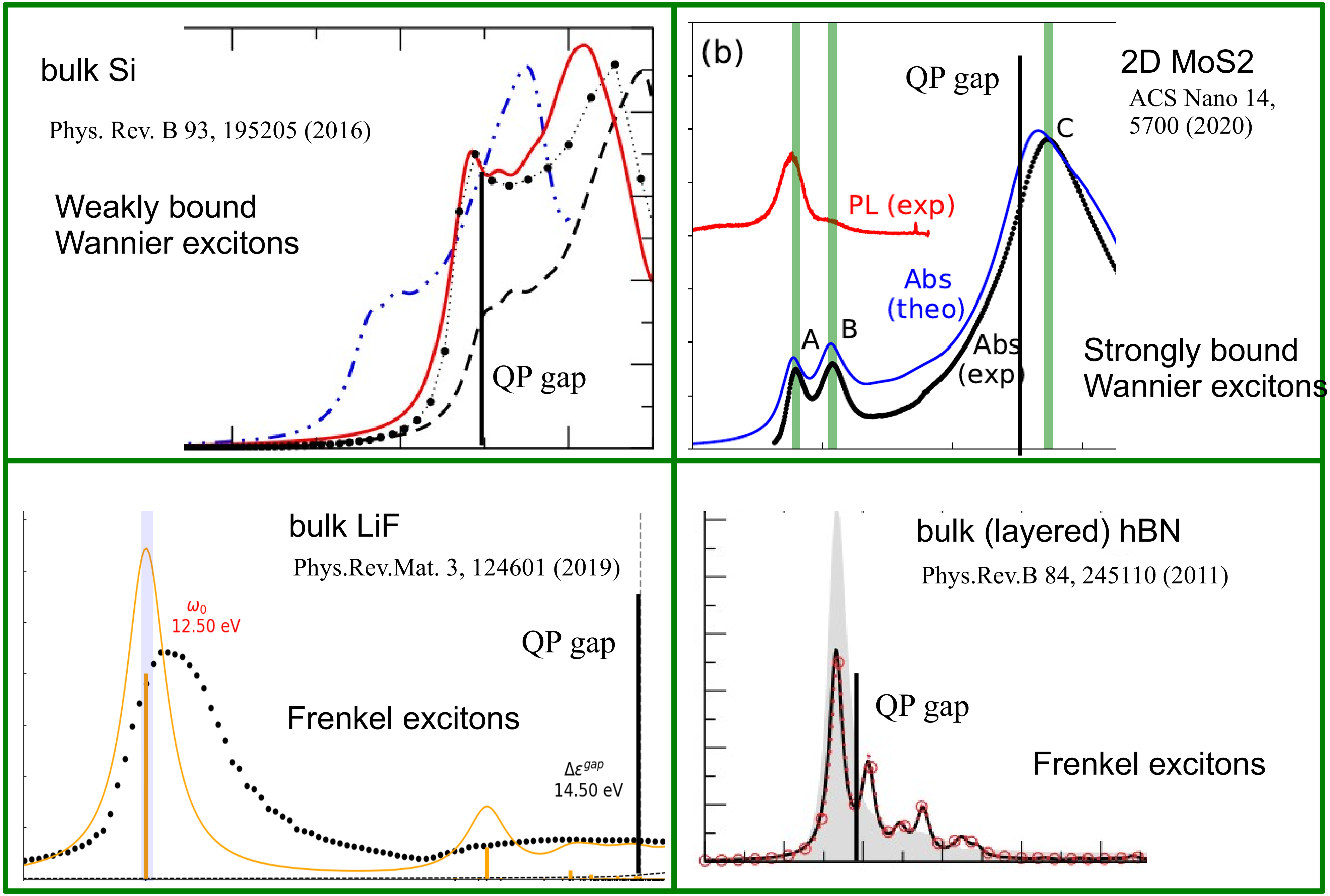
abinitio GW+BSE



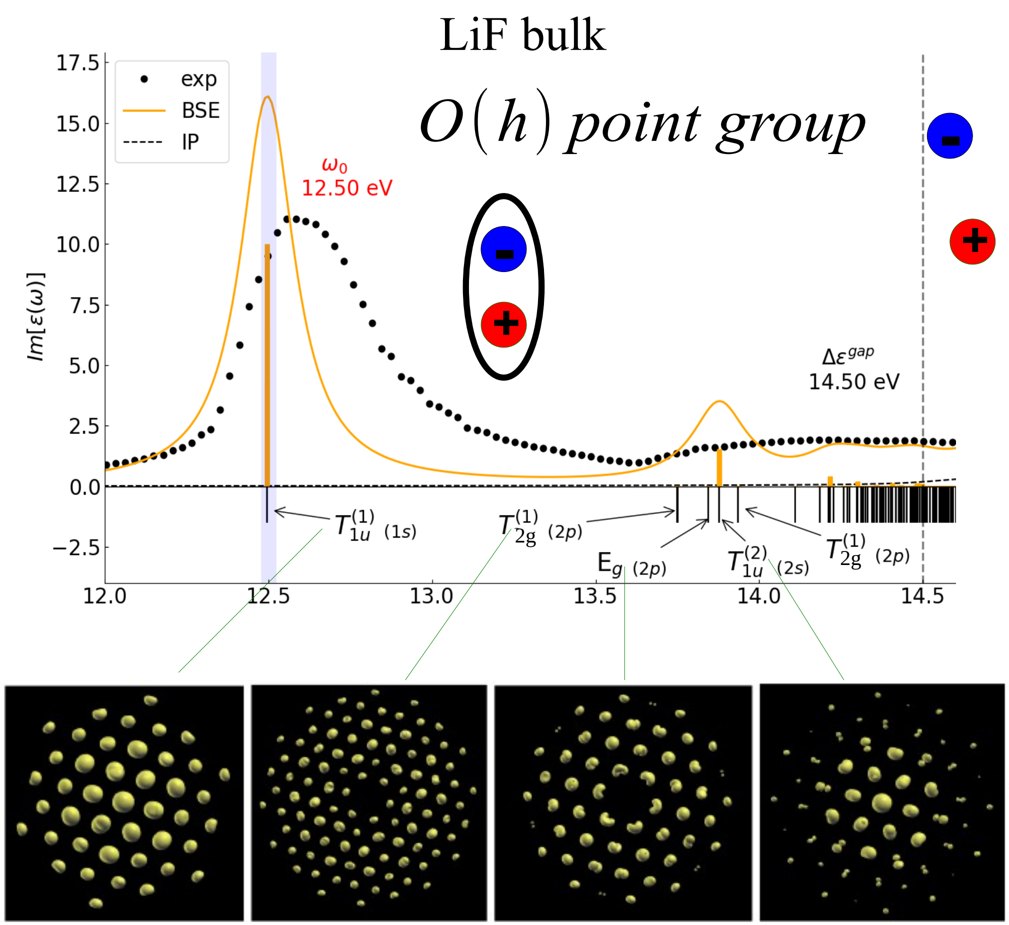
$$\epsilon_I = E_I(N \pm 1) - E_0(N)$$

$$\omega_I = E_I(N) - E_0(N)$$

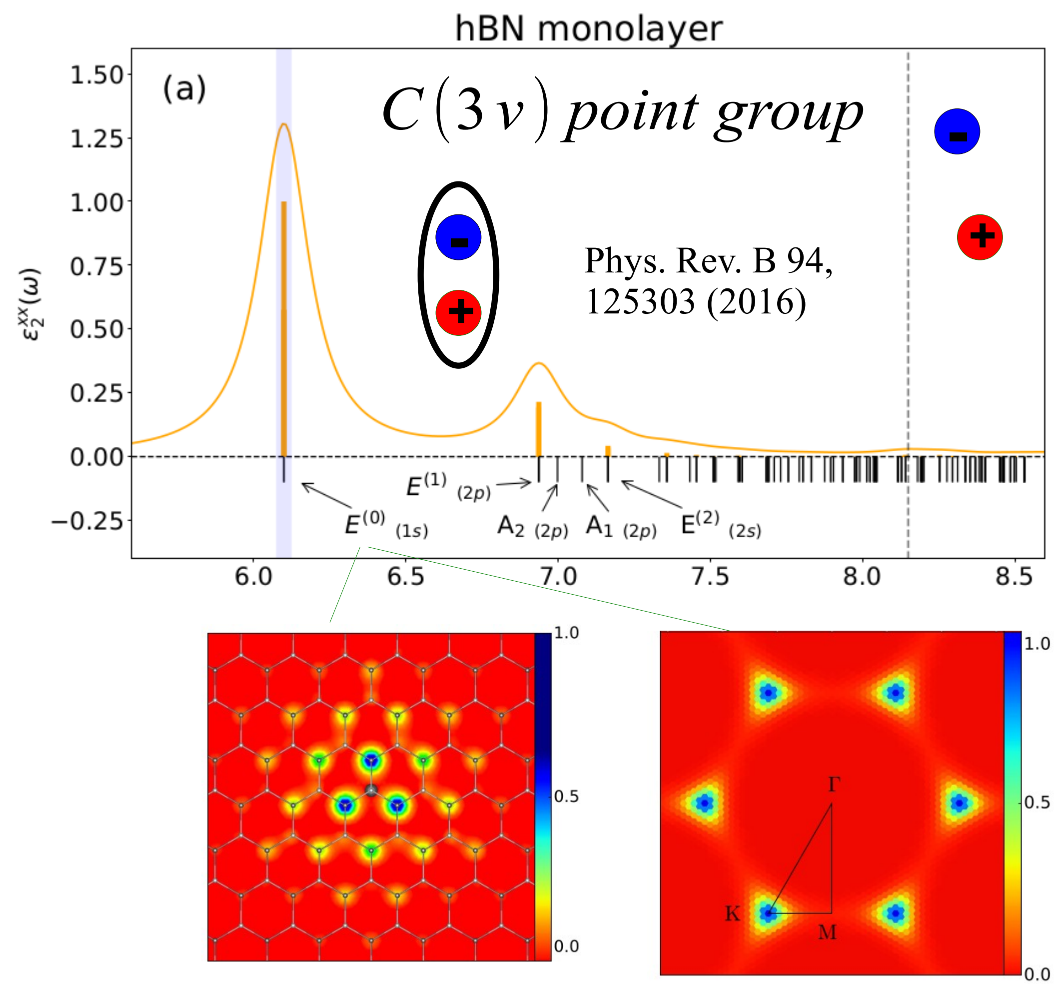
BSE overview



Exciton wave-function



$$\left|\Psi^{\lambda\, q=0}(x_h^0, x)\right|^2$$



$$\left|\Psi^{\lambda\, q=0}(x_h^0, x)\right|^2 \qquad \left|\Psi^{\lambda\, q=0}(k)\right|^2$$

the Yambo team

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* Claudio Attaccalite
* Miki Bonacci
* Elena Cannuccia
* Andrea Ferretti
* Myrta Gruening
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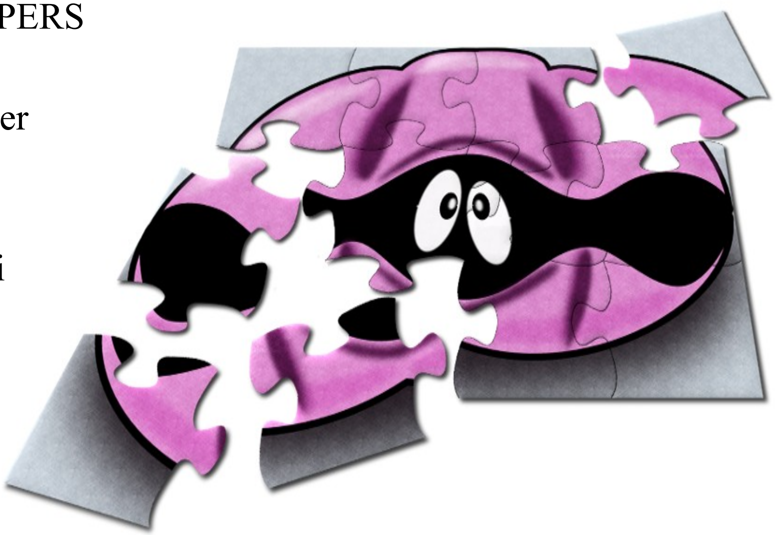

Thank you for your attention

the Yambo team

1. Many-body perturbation theory calculations using the yambo code
   Journal of Physics: Condensed Matter 31, 325902 (2019)
2. Yambo: an ab initio tool for excited state calculations
   Comp. Phys. Comm. 144, 180 (2009)

More slides

the Yambo team

1. Many-body perturbation theory calculations using the yambo code
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2. Yambo: an ab initio tool for excited state calculations
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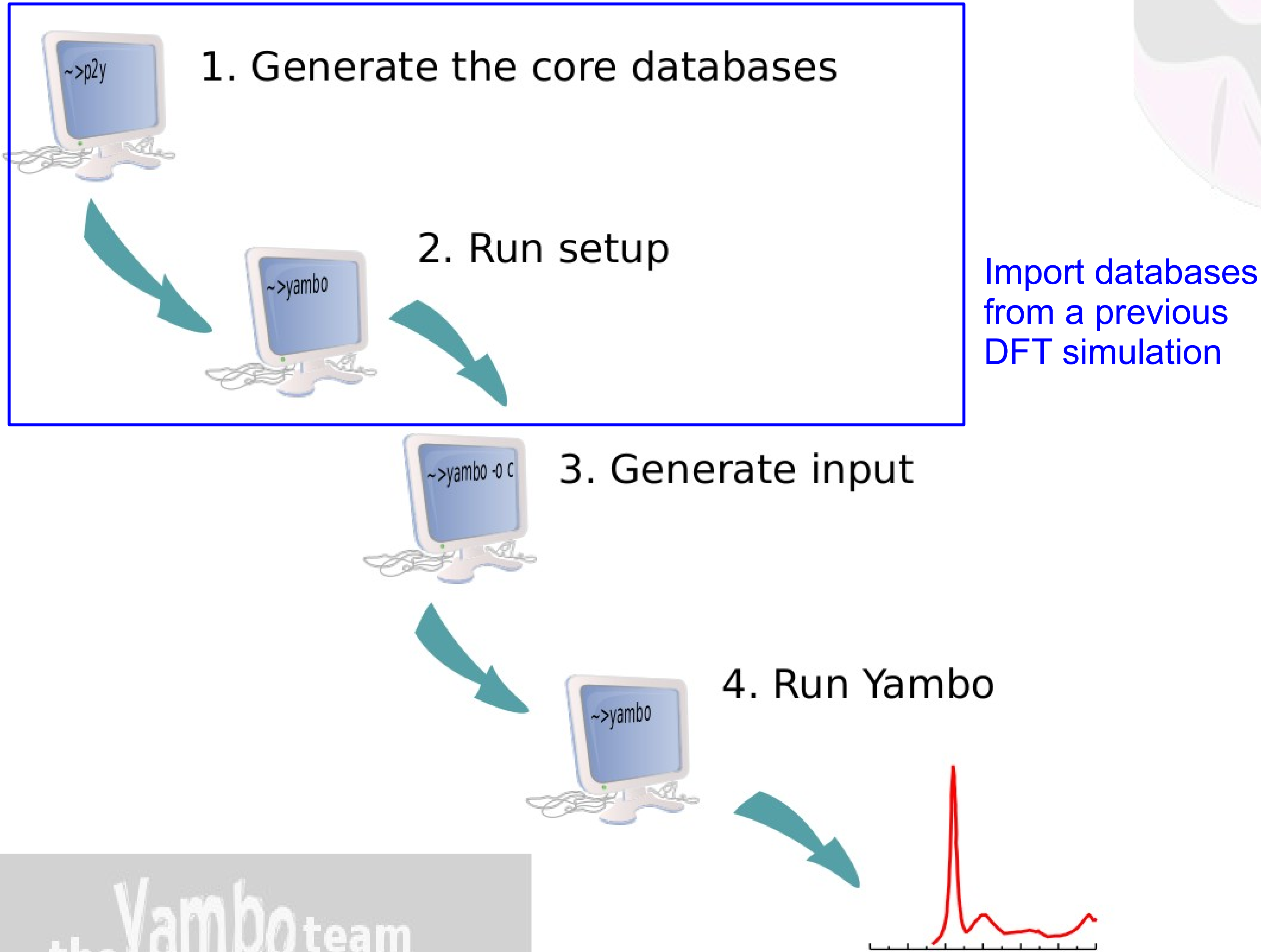
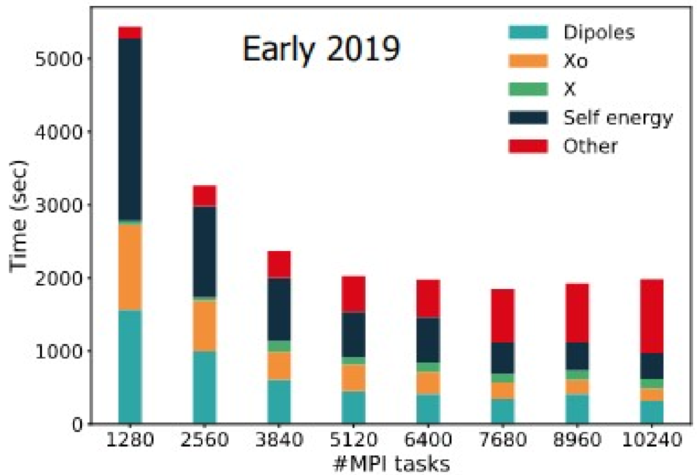
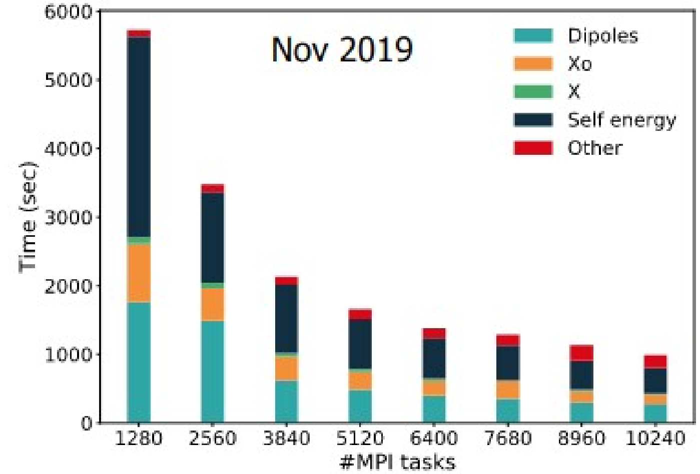
How the code works



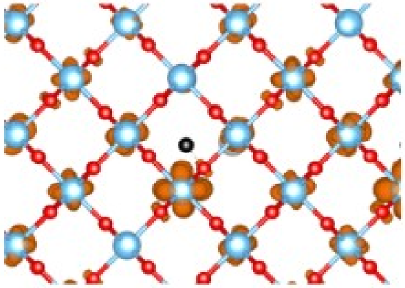
Yambo parallel performance

heterogeneous architectures: **MPI** + OpenMP + CUDA





- **optimisation of MPI+OpenMP** parallelism
- working at scale (bottleneck identification and solution)



system size: 72+1 atoms, 2000 bands, 6 Ry for Xo repr (N=1317); ~290 occ states, 8 kpts.

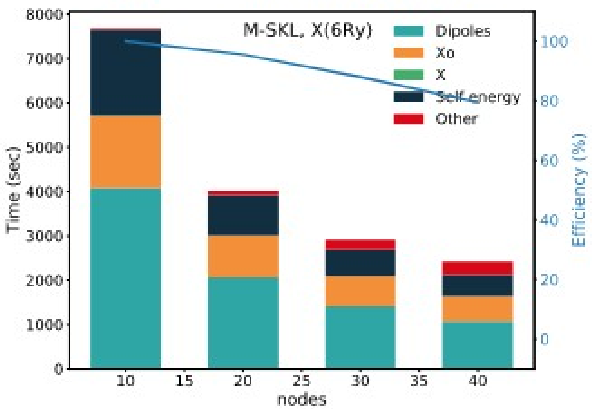
data available at: http://www.gitlab.com/max-centre/Benchmarks

Yambo: performance (GPU)

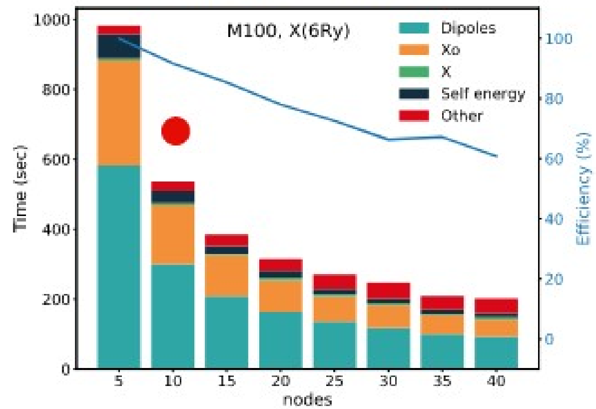
heterogeneous architectures: **MPI + OpenMP + CUDA**

x14 wrt SKL (10 nodes) **x1.4 wrt V100 (2 nodes)**

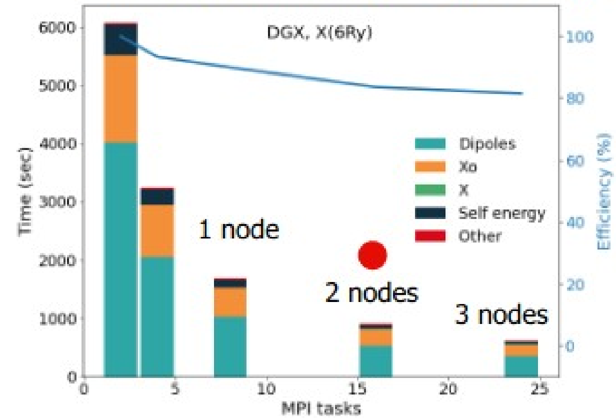
CPU: **Skylake**



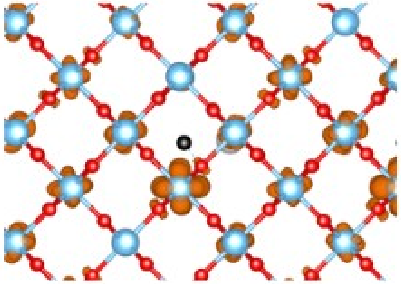
GPU: P9+**V100**



GPU: AMD-Rome + **A100** (DGX)



- complete **GW workflow** for defected TiO_2 (rutile)
- small system, **stress test**
- 1 MPI task/GPU
- data obtained on Marconi100, 4 V100 GPUs/node
- and DGX arch, 8 A100 GPUs/node



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Part IV
More applications