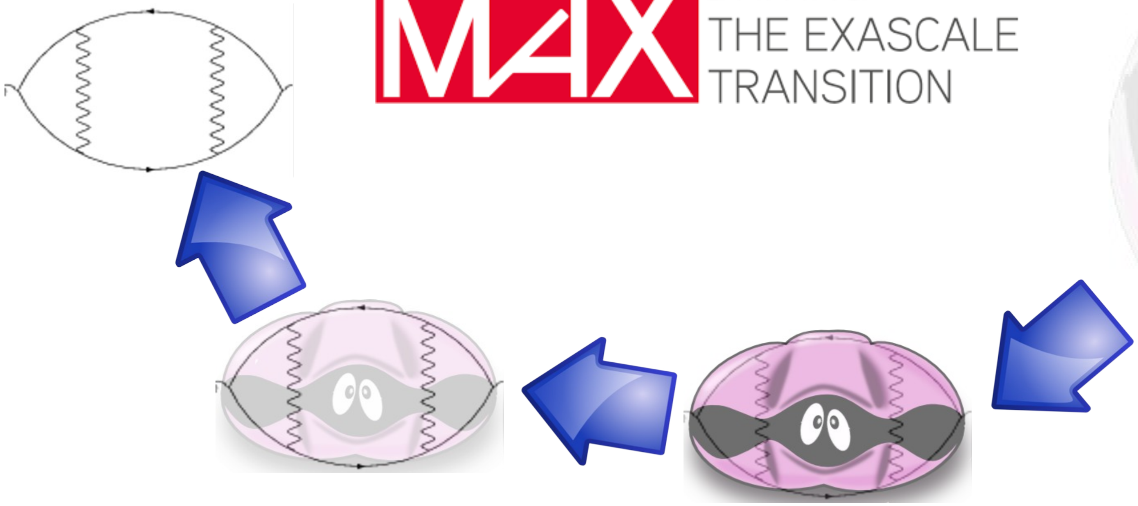
Efficient materials modelling on HPC with Quantum ESPRESSO, Siesta and Yambo

ENCCS
EuroCC National Competence Centre Sweden

MAX DRIVING THE EXASCALE TRANSITION



Overview of the Yambo code: main features and performance

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

the Yambo team

CNR
Istituto di Struttura
della Materia

11 – 15 March 2024

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:

www.yambo-code.eu

MaX flagship code

Theory

Many-Body perturbation Theory

Time-dependent density functional theory

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Abinit

QUANTUMESPRESSO

Libraries

ScaLAPACK

netCDF

ioth

libxc

FFTW

HDF

ETSF-IO

MPI2

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MaX flagship code

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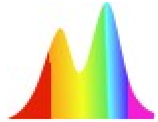
MaX flagship code

Different projects

Developers

the Yambo team

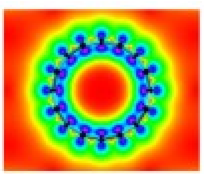
Properties

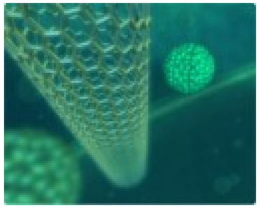


GPL
Quasi-particles
Optics and excitons
Magneto-optics & dichroism
Electron-phonon coupling
Real-time propagation
Non-linear optics
Pump and probe experiments

Development (pre-GPL) version
Exciton-phonon coupling
Carrier dynamics
Ehrenfest dynamics
Magnons

Applications





www.yambo-code.eu

MaX flagship code

the Yambo team

Properties

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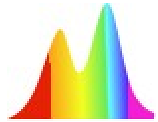

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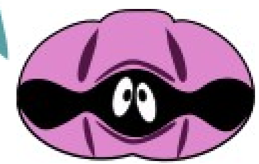
Schools

Community & Publications

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



www.yambo-code.eu

MaX flagship code

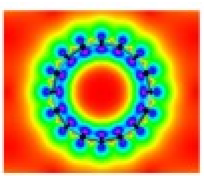
Support & reach out

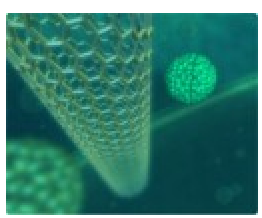
Git repository

Dedicated User Forum

Online documentation and tutorials

Applications





the Yambo team

Properties

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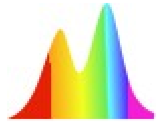

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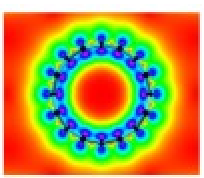
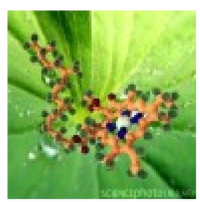
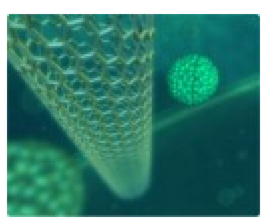
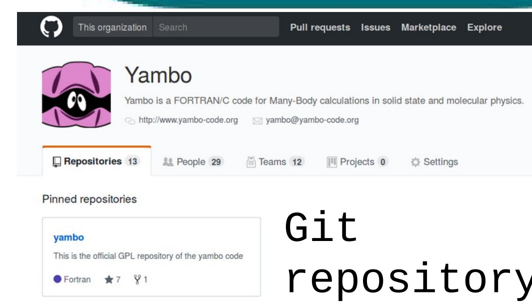






Support & reach out



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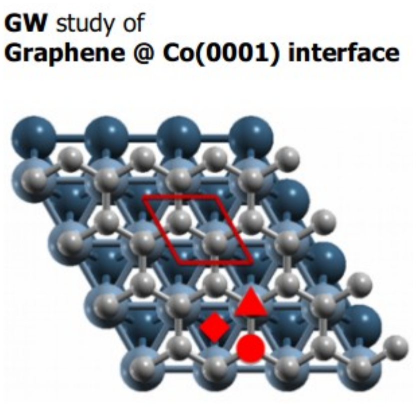
Perfomances



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

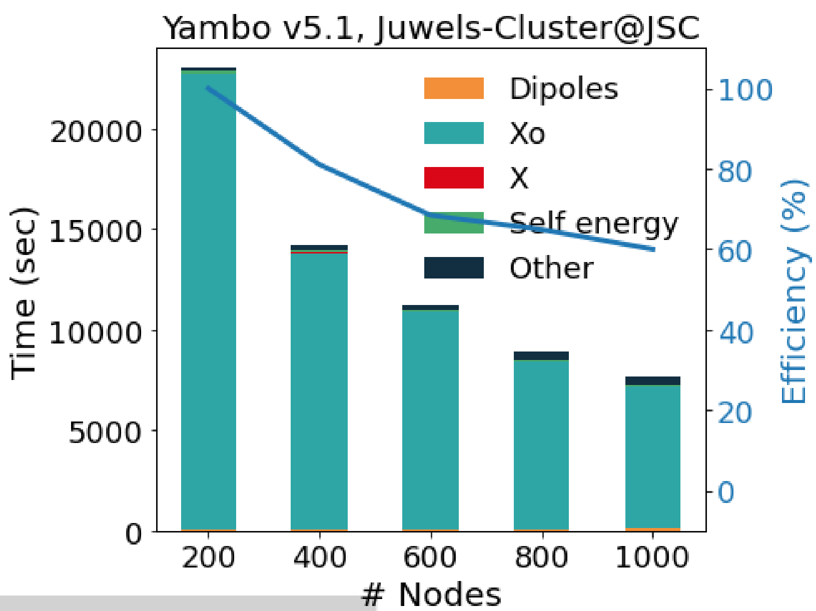
mpirun -np #MPI
#MPI=4
#THREADS=24 (2*#cores / #MPI)

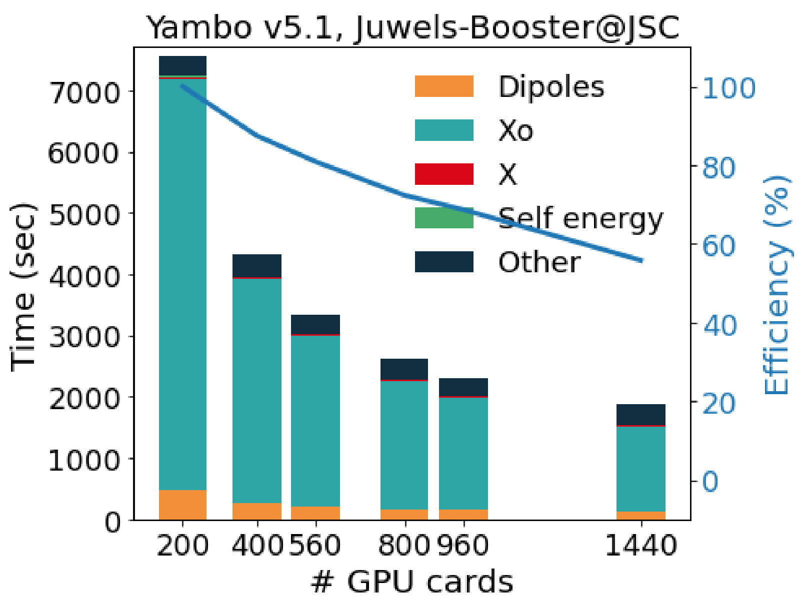
Juwels-Cluster.
48 **Intel** cores per node

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

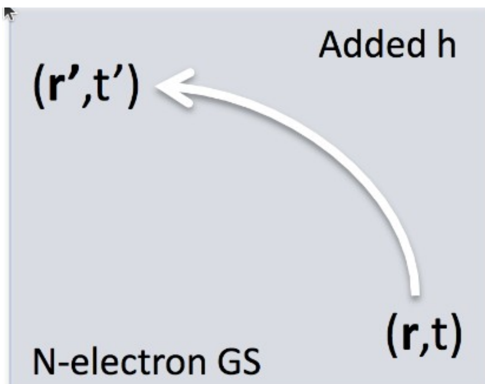
the Yambo team

The Many Body Green Function

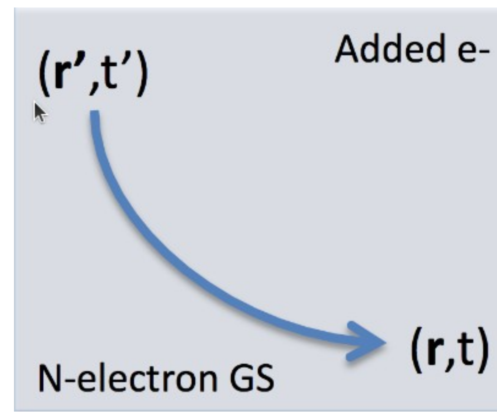
Time ordered Green function

$$iG(r,t;r',t') = \langle \phi_0^N | T[\hat{\psi}(r,t)\hat{\psi}^+(r',t')] | \phi_0^N \rangle$$

$$-\theta(t'-t)\langle \phi_0^N | \hat{\psi}^+(r',t')\hat{\psi}(r,t) | \phi_0^N \rangle + \theta(t-t')\langle \phi_0^N | \hat{\psi}(r,t)\hat{\psi}^+(r',t') | \phi_0^N \rangle$$

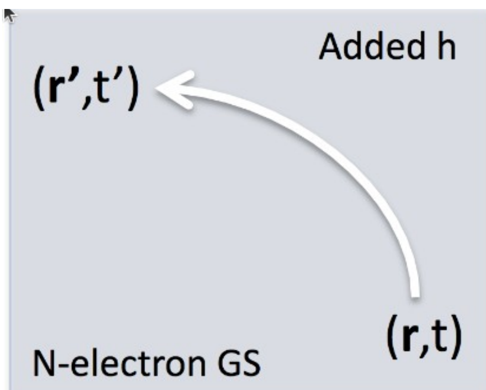


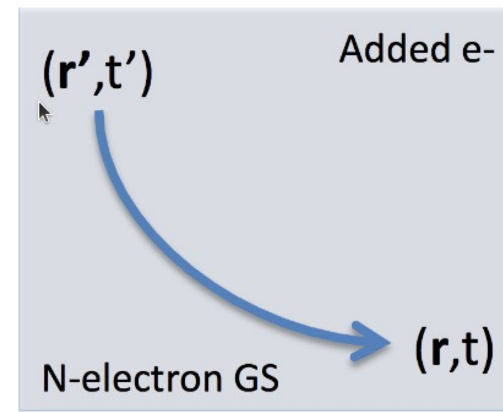
$iG^<(r,t;r',t')$



$iG^>(r,t;r',t')$

Lehmann Representation





$$-\theta(t'-t)\langle \phi_0^N | \hat{\psi}^+(r',t')\hat{\psi}(r,t)|\phi_0^N\rangle + \theta(t-t')\langle \phi_0^N | \hat{\psi}(r,t)\hat{\psi}^+(r',t')|\phi_0^N\rangle$$

$$iG(r,t;r',t') = \theta(t'-t)\sum_{\lambda}\langle \phi_0^N | \hat{\psi}^+(r',t')|\phi_\lambda^{N-1}\rangle\langle \phi_\lambda^{N-1}|\hat{\psi}(r,t)|\phi_0^N\rangle$$

$$-\theta(t-t')\sum_{\lambda}\langle \phi_0^N | \hat{\psi}(r,t)|\phi_\lambda^{N+1}\rangle\langle \phi_\lambda^{N+1}|\hat{\psi}^+(r',t')|\phi_0^N\rangle$$

Lehmann Representation

$$iG(r,t;r',t')=\theta(t'-t)\sum_{\lambda}\langle\phi_0^N|\hat{\psi}^+(r',t')|\phi_\lambda^{N-1}\rangle\langle\phi_\lambda^{N-1}|\hat{\psi}(r,t)|\phi_0^N\rangle$$

$$-\theta(t-t')\sum_{\lambda}\langle\phi_0^N|\hat{\psi}(r,t)|\phi_\lambda^{N+1}\rangle\langle\phi_\lambda^{N+1}|\hat{\psi}^+(r',t')|\phi_0^N\rangle$$

$$\hat{\psi}(r,t)=e^{i\hat{H}t}\hat{\psi}(r)e^{-i\hat{H}t}$$

$$f_\lambda^{N-1}(r)=\langle\phi_\lambda^{N-1}|\hat{\psi}(r)|\phi_0^N\rangle$$

$$\boxed{G(r,r',\omega)=\lim_{\eta\to 0}\sum_{\lambda}\frac{[f_\lambda^{N-1}(r)]^* f_\lambda^{N-1}(r')}{\omega+(E_\lambda^{N-1}-E_0^N)-i\eta}+\frac{f_\lambda^{N+1}(r)[f_\lambda^{N+1}(r')]^*}{\omega-(E_\lambda^{N+1}-E_0^N)+i\eta}}$$

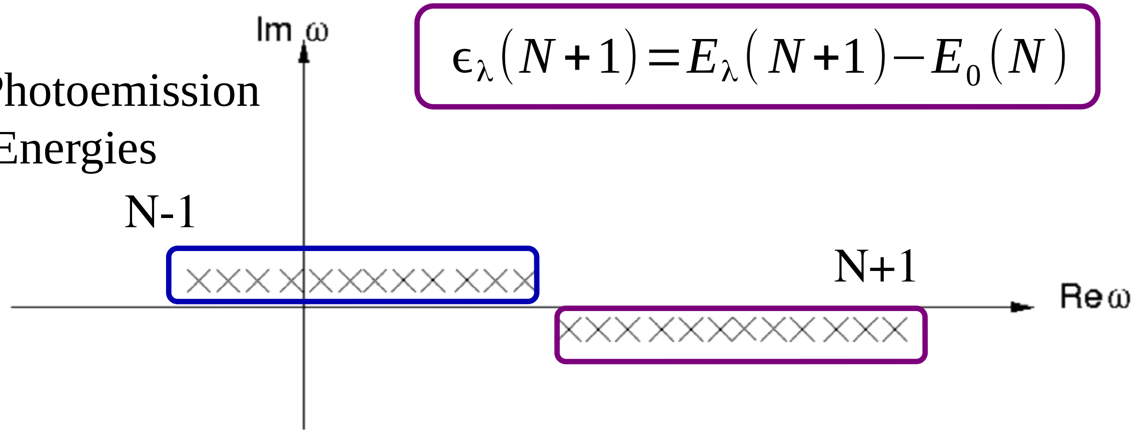
Poles of the GF

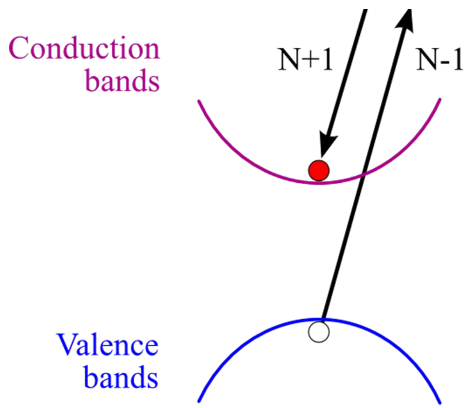
$$\boxed{G(r,r',\omega)=\lim_{\eta\to 0}\sum_{\lambda}\frac{[f_{\lambda}^{N-1}(r)]^{*}f_{\lambda}^{N-1}(r')}{\omega+(E_{\lambda}^{N-1}-E_{0}^{N})-i\eta}+\frac{f_{\lambda}^{N+1}(r)[f_{\lambda}^{N+1}(r')]^{*}}{\omega-(E_{\lambda}^{N+1}-E_{0}^{N})+i\eta}}$$

$$\boxed{\epsilon_{\lambda}(N-1)=-(E_{\lambda}(N-1)-E_{0}(N))} \quad G^{<}$$

$$\boxed{\epsilon_{\lambda}(N+1)=E_{\lambda}(N+1)-E_{0}(N)} \quad G^{>}$$

Photoemission
Energies

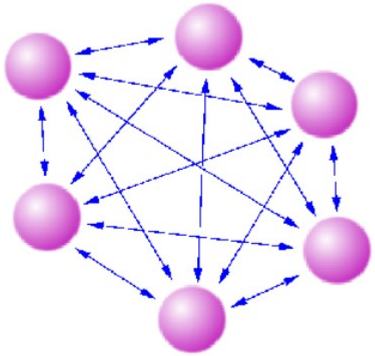




Many-Body Perturbation-Theory

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

Interacting particles
Ground state



$$iG(r,t;r',t') = \langle \phi_0^N | T[\hat{\psi}(r,t)\hat{\psi}^+(r',t')] | \phi_0^N \rangle$$

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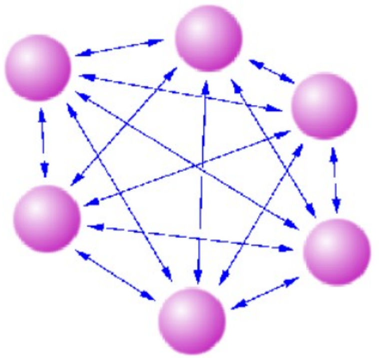
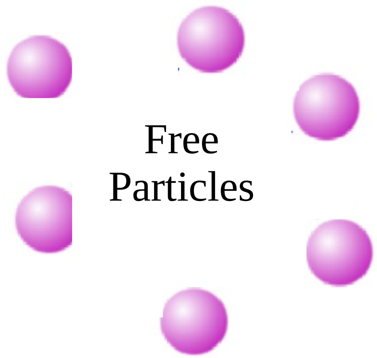


$$iG(r,t;r',t') = \langle \phi_0^N | T[\hat{\psi}(r,t)\hat{\psi}^{+}(r',t')] | \phi_0^N \rangle$$

Gell-Mann & Low theorem

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

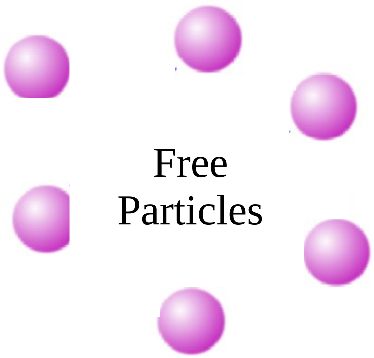
$$\left\langle \psi_0 \middle| \mathrm{T}\left[\hat{V}(t_1)\cdots\hat{V}(t_n)\hat{\psi}(t)\hat{\psi}^{\dagger}(t')\right] \middle| \psi_0 \right\rangle$$



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

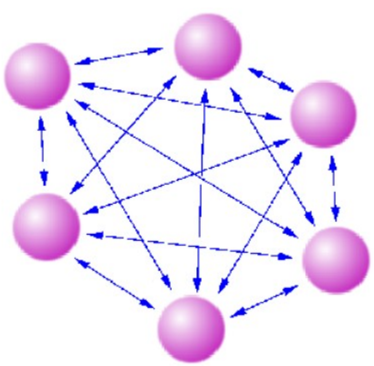
$$G^0(r,r',\omega) = \sum_{nk} \frac{\psi_{nk}^{*}(r)\psi_{nk}(r')}{\omega - \epsilon_{nk}^{0} + i\eta\theta(k-k_F)}$$

The QP concept



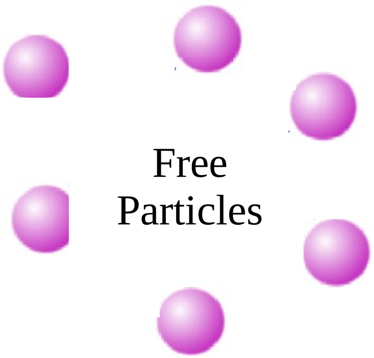
$$\Sigma^{Hxc}[G](\omega)$$

Interacting particles



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

The QP concept



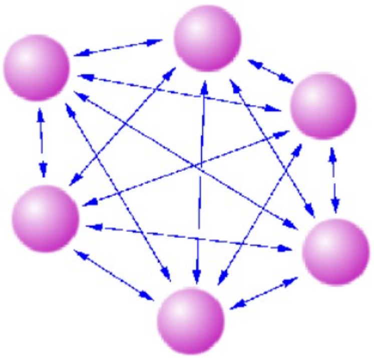
$$G^0(r,r',\omega)=\sum_{nk}\frac{\psi^*_{nk}(r)\psi_{nk}(r')}{\omega-\epsilon^0_{nk}+i\eta\theta(k-k_F)}$$

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

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

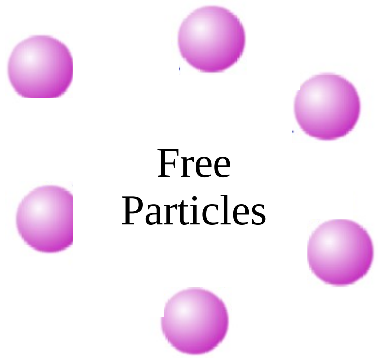
Interacting particles

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



$$G(r,r',\omega)=\sum_{\lambda}\frac{[f_\lambda^{N-1}(r)]^* f_\lambda^{N-1}(r')}{\omega-\epsilon_\lambda^{N-1}-i\eta}+\frac{f_\lambda^{N+1}(r)[f_\lambda^{N+1}(r')]^*}{\omega-\epsilon_\lambda^{N+1}+i\eta}$$

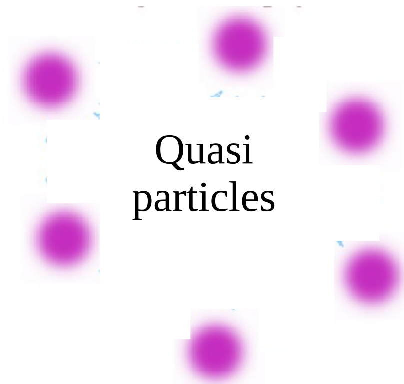
The QP concept



$$\Sigma^{Hxc}[G](\epsilon^{qp}) \longrightarrow$$

$$G^{QP} = G^{0} + G^{0}\,\Sigma^{Hxc}(\epsilon_{QP})\,G^{QP}$$

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



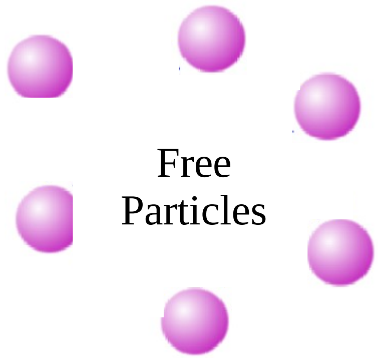
$$\Sigma^{Hxc}[G](\omega)$$

Interacting particles

NB: this is trivial only for static self-energies
For dynamical self-energies evaluated at the QP energy
we assume that well defined quasi-particle poles exist
[no strongly correlated materials]

$$G^{QP}(r, r', \omega) = \sum_{nk} \frac{[f^{QP}_{nk}(r)]^{*} f^{QP}_{nk}(r')}{\omega - \epsilon^{QP}_{nk} + i\eta\theta(k - k_F)}$$

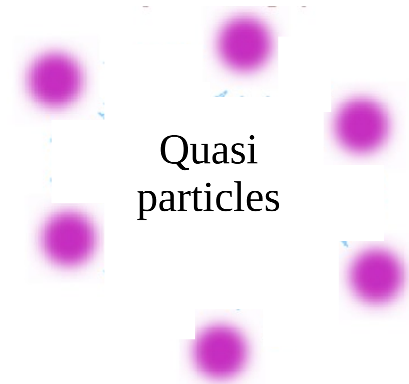
The QP concept



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

$$G^{QP} = G^{0} + G^{0}\,\Sigma^{Hxc}(\epsilon_{QP})\,G^{QP}$$

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

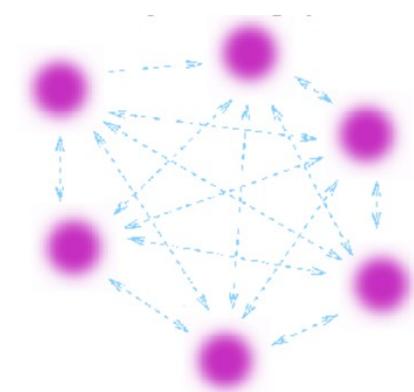


$$\Sigma^{Hxc}[G](\omega)$$

Interacting particles

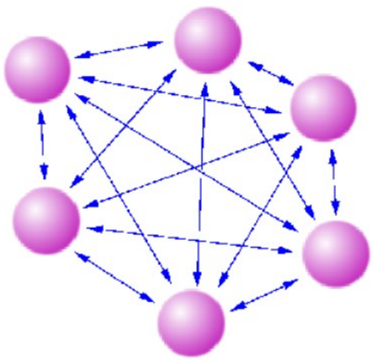
$$\Sigma^{xc}(\omega) - \Sigma^{xc}(\epsilon^{qp})$$

Weakly interacting
quasi-particles

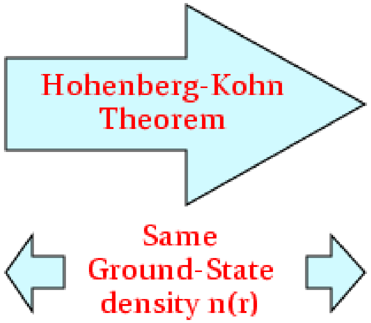


Adapted from F. Sottile PhD thesis

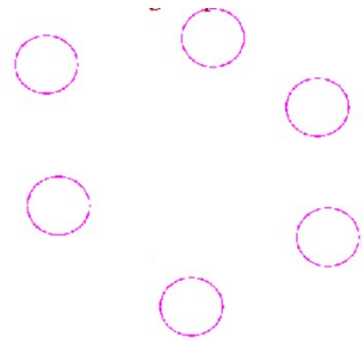
DFT vs MBPT



Strongly interacting particles



Auxiliary system

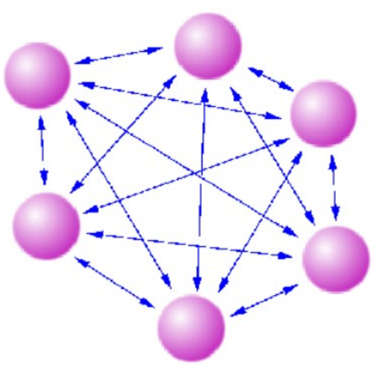


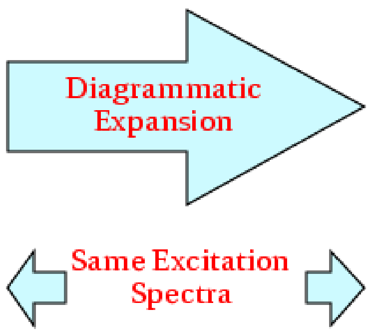
Non interacting KS particles

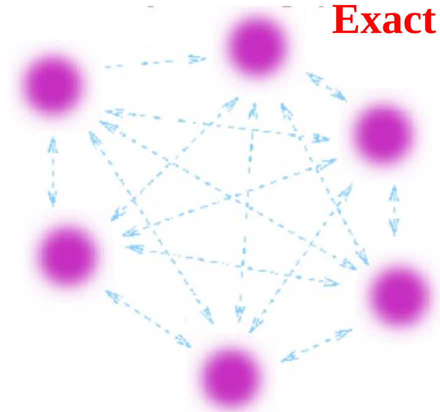
DFT

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

Exact





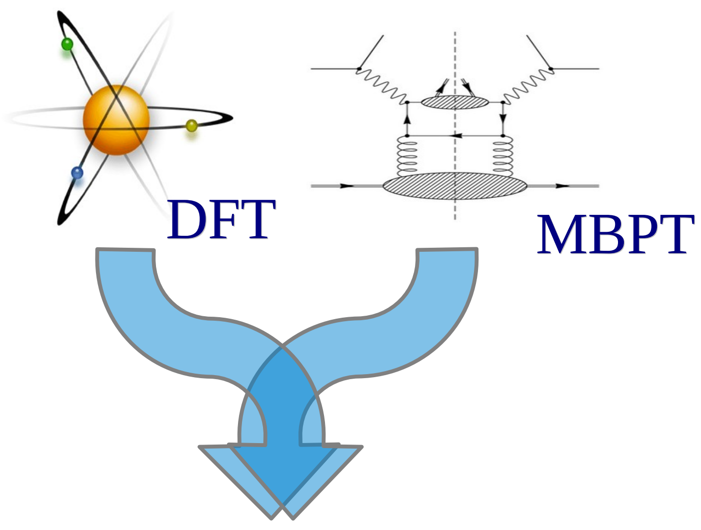


Weakly interacting quasi-particles

MBPT

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

DFT + MBPT



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

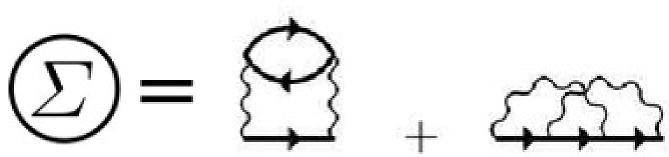
DFT

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

MBPT

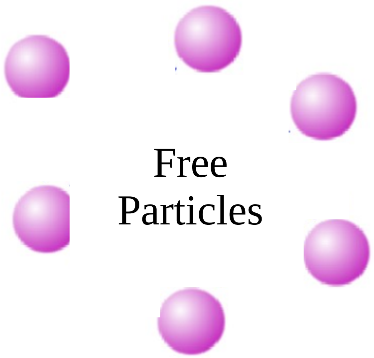
$$G^{KS}(r,r',\omega)=\sum_{nk}\frac{\psi^*_{nk}(r)\,\psi_{nk}(r')}{\omega-\epsilon^{KS}_{nk}+i\eta}$$

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

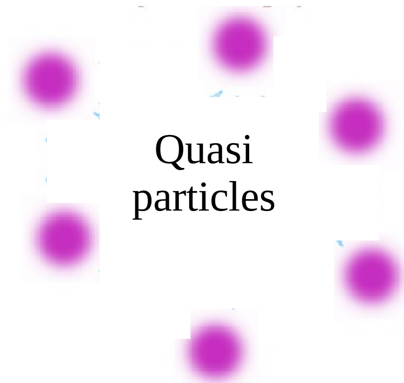


the Yambo team

MBPT

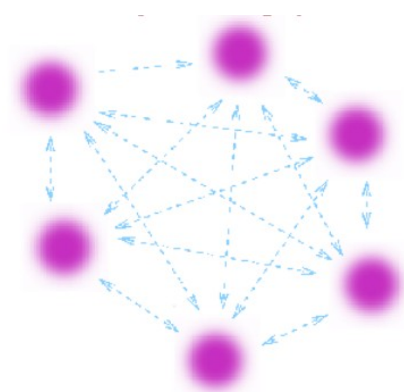


$$\Sigma^{xc}[G](\epsilon^{qp})$$



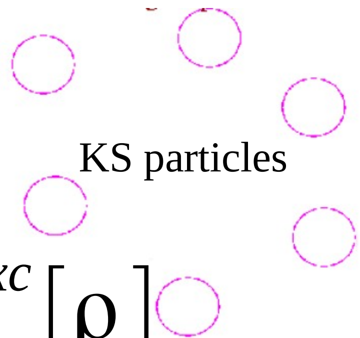
$$\Sigma^{xc}(\omega)-\Sigma^{xc}(\epsilon^{qp})$$

Weakly interacting
quasi-particles



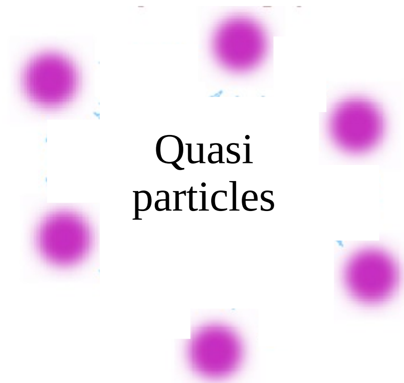
$$G=G^0+G^0\Sigma^{Hxc}G$$

abinitio MBPT



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

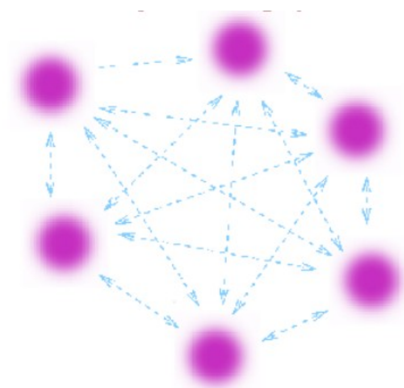
$$\Sigma^{xc}[G](\epsilon^{qp})-v^{xc}[\rho]$$



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

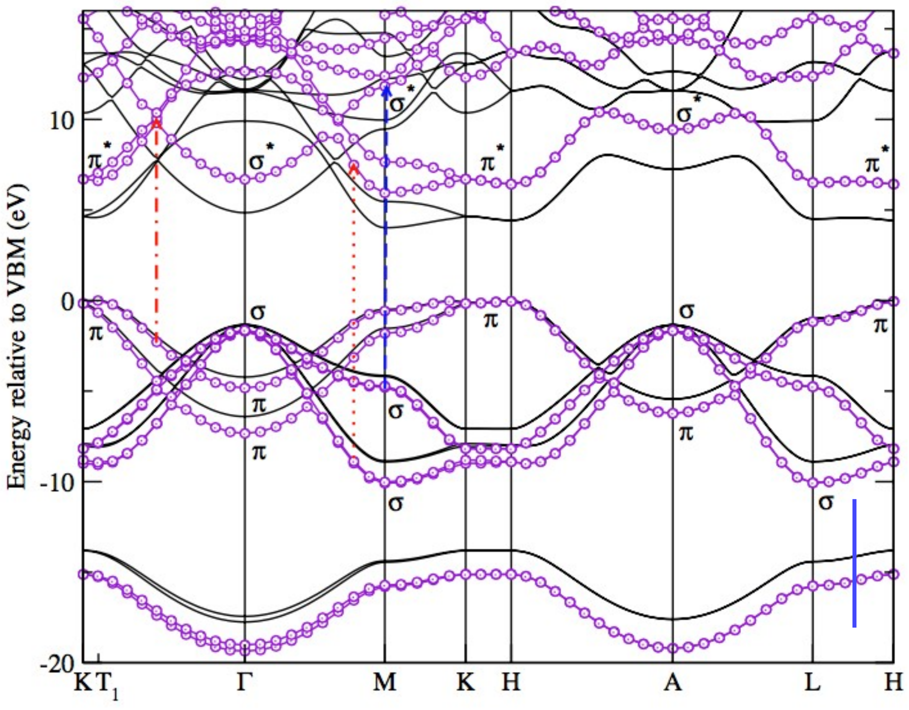
$$G=G^{KS}+G^{KS}(\Sigma^{xc}-v^{xc})G$$

Weakly interacting
quasi-particles



DFT and MBPT bands

DFT vs **MBPT** band structure in hBN



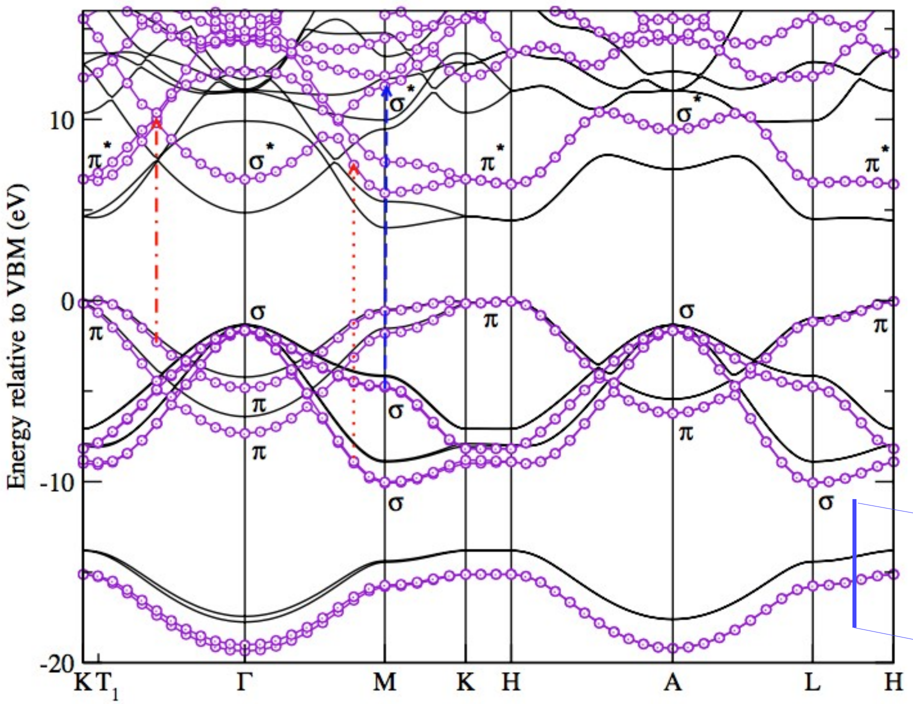
B. Arnaud, S. Lebègue, P. Rabiller, and M. Alouani, Phys, Rev. Lett. **96**, 026402 (2006)

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

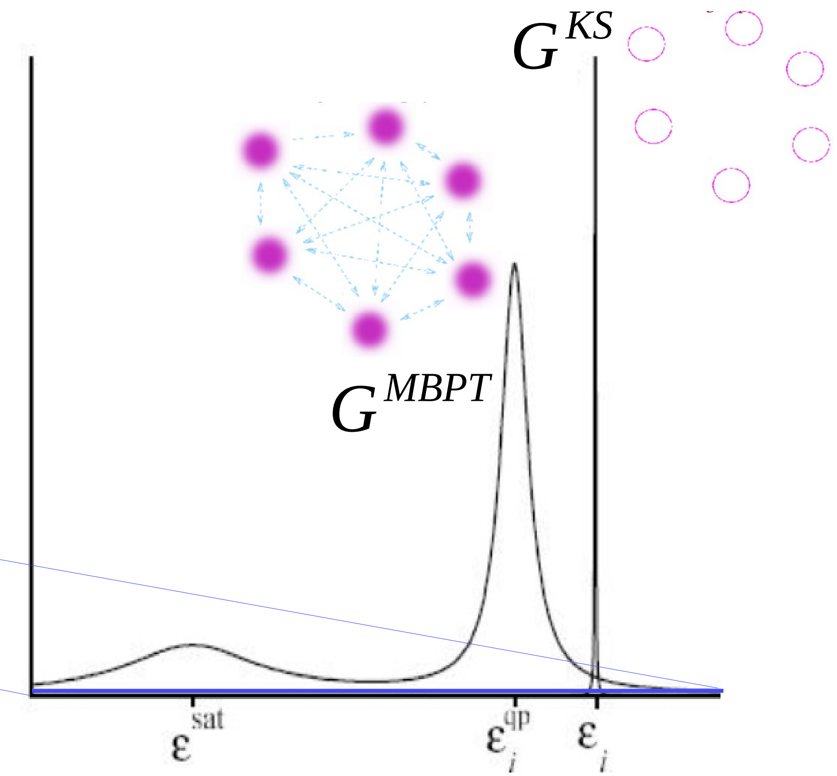
DFT and MBPT bands

$$\Im[G(k,\omega)]$$

DFT vs **MBPT** band structure in hBN



Angle resolved photoemission spectral function



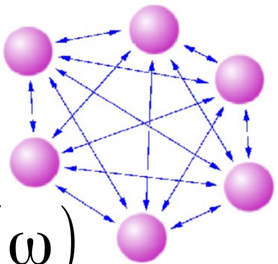
B. Arnaud, S. Lebègue, P. Rabiller, and M. Alouani,
Phys, Rev. Lett. **96**, 026402 (2006)

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

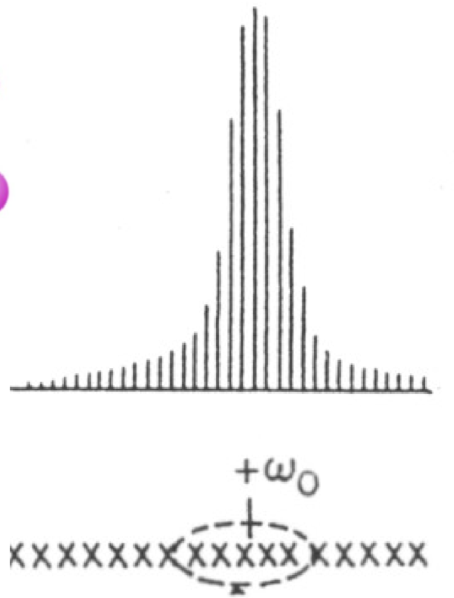
$$\Sigma^{xc}(\omega)-\Sigma^{xc}(\epsilon^{qp})$$

QP complex energies

$$\Im[G(k,\omega)]$$



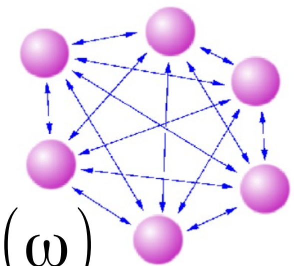
$$\Sigma(\omega)$$



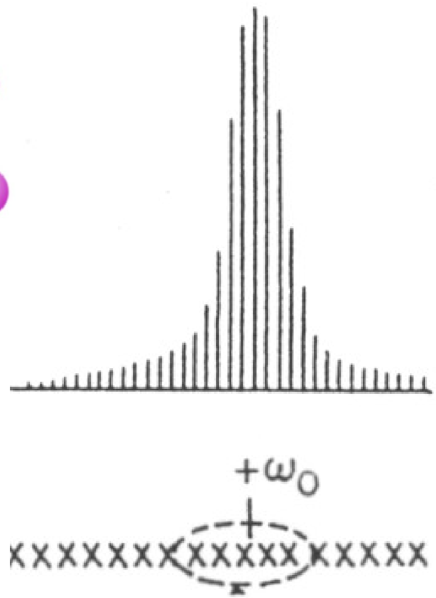
Images Adapted from
M. Gatti PhD thesis

QP complex energies

$$\Im[G(k,\omega)]$$



$\Sigma(\omega)$

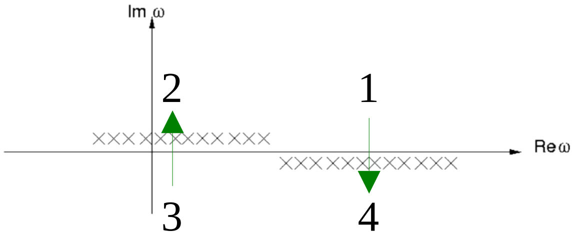


Analitic continuation $\Sigma(z)$

$$[h_0+\Sigma(z)]\psi^r_\lambda(z)=E_\lambda(z)\psi^r_\lambda(z)$$

$$\begin{cases} G^<(r,r',z)=\sum_\lambda \dfrac{\psi^l_\lambda(r,z)\psi^r_\lambda(r',z)}{z-E_\lambda(z)} \\ E_\lambda(z)=z \end{cases}$$

Multivalued functions

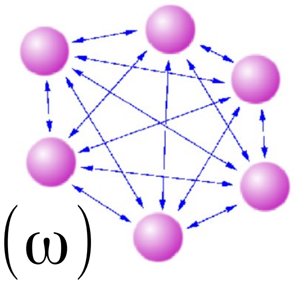


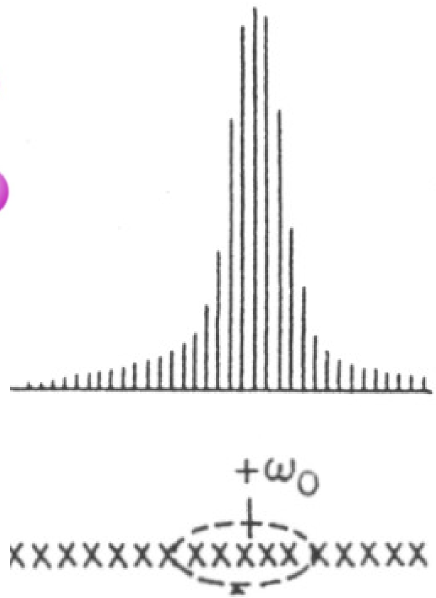
Images Adapted from
M. Gatti PhD thesis

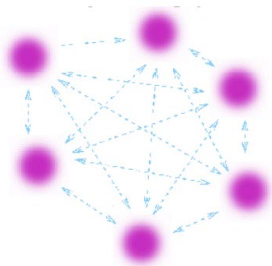
QP complex energies

$\Im[G(k,\omega)]$

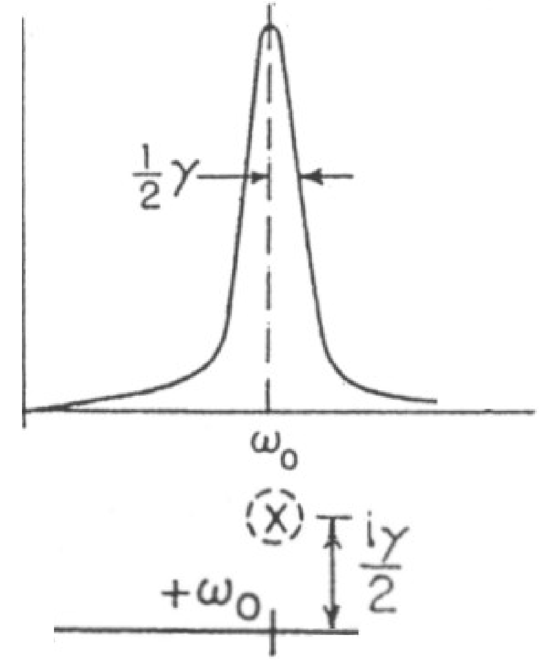
$\Sigma(\omega)$







$\Im[G^c(k,z)]$



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

$E_\lambda(z) = z$

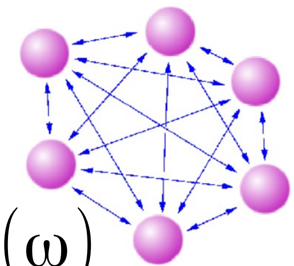
G. Onida, L. Reining, Lucia, A. Rubio, Rev. Mod. Phys. **74**, 601 (2002)
B. Farid, Phyl. Mag. B **79**, 1097 (1999) [arXiv 0004476 (2000)]
B. Farid, Phyl. Mag. B **82**, 1413 (2002) [arXiv 0110481 (2002)]

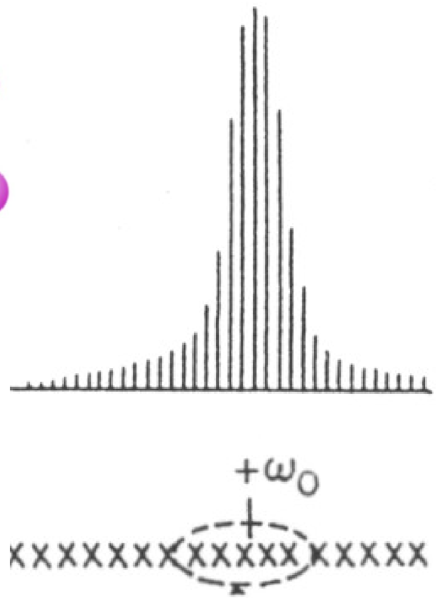
Images Adapted from
M. Gatti PhD thesis

QP complex energies

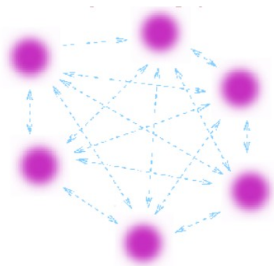
$$\Im[G(k,\omega)]$$

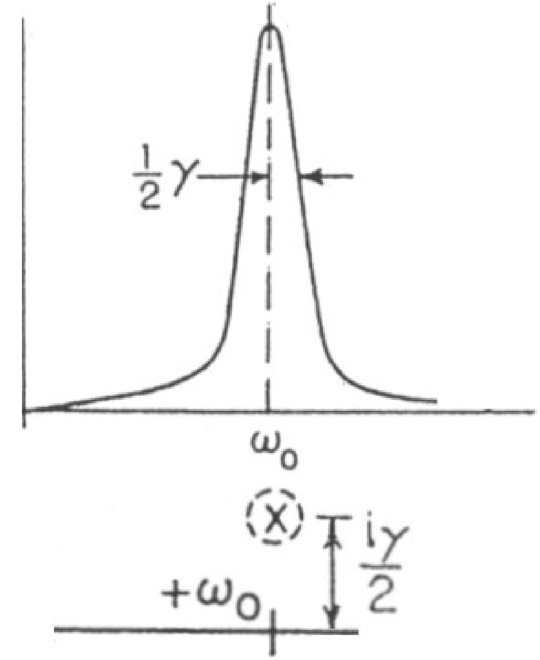
$\Sigma(\omega)$





$$\Im[G^c(k,z)]$$





Example

$$G(\omega)=\sum_s \frac{R(s)}{\omega-s} \qquad R(s)=\frac{1}{\pi}\frac{E_2}{(s-E_1)^2+E_2^2}$$

$$G(z)=\frac{1}{z-(E_1+iE_2)} \qquad \Im(z)\neq 0$$

G. Onida, L. Reining, Lucia, A. Rubio, Rev. Mod. Phys. **74**, 601 (2002)
B. Farid, Phyl. Mag. B **79**, 1097 (1999) [arXiv 0004476 (2000)]
B. Farid, Phyl. Mag. B **82**, 1413 (2002) [arXiv 0110481 (2002)]

Images Adapted from
M. Gatti PhD thesis

The role of screening

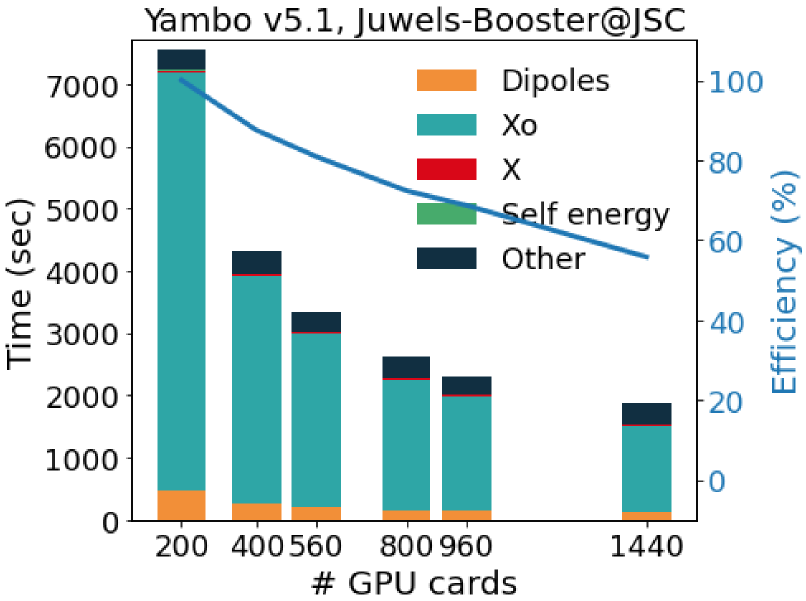
$$\Sigma^{xc}[G] = GW\Gamma$$

Screened
electron-hole interaction

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

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

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



Part III
Excitons:
The Bethe-Salpeter equation

Neutral excitations

1) Time ordered response function

$$L(1,2;3,4)=\langle \phi_0^N | T[\hat{\psi}(1)\hat{\psi}^+(2)\hat{\psi}(3)\hat{\psi}^+(4)] | \phi_0^N \rangle \qquad 1=(x,t)$$

Neutral excitations

1) Time ordered response function

$$L(1,2;3,4)=\langle \phi_0^N | T[\hat{\psi}(1)\hat{\psi}^+(2)\hat{\psi}(3)\hat{\psi}^+(4)] | \phi_0^N \rangle \qquad 1=(x,t)$$

2) Lehmann Representation

$$L(\omega)=\sum_\lambda \frac{[F_\lambda^N]^* F_\lambda^N}{\omega-(E_\lambda^N-E_0^N)+i\eta}-\frac{[F_\lambda^N]^* F_\lambda^N}{\omega+(E_\lambda^N-E_0^N)-i\eta} \qquad (t_1=t_2;t_3=t_4)$$

Neutral excitations

1) Time ordered response function

$$L(1,2;3,4)=\langle \phi_0^N | T[\hat{\psi}(1)\hat{\psi}^+(2)\hat{\psi}(3)\hat{\psi}^+(4)] | \phi_0^N \rangle \qquad 1=(x,t)$$

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$$L(\omega)=\sum_\lambda \frac{[F_\lambda^N]^* F_\lambda^N}{\omega-(E_\lambda^N-E_0^N)+i\eta}-\frac{[F_\lambda^N]^* F_\lambda^N}{\omega+(E_\lambda^N-E_0^N)-i\eta} \qquad (t_1=t_2;t_3=t_4)$$

3) Dyson like equation

$$L(\omega;\omega_1,\omega_2)=L^0(\omega;\omega_1,\omega_2)+L^0(\omega;\omega_1,\tilde{\omega}_1)K(\omega;\tilde{\omega}_1,\tilde{\omega}_2)L(\omega;\tilde{\omega}_2,\omega_2)$$

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

Bethe-Salpeter Equation

$$L^{s} = L^{qp} + L^{qp} K^{Hxc}(\omega = 0) L^{s}$$

$$K^{Hxc}(\omega = 0) = (v - W)$$

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

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

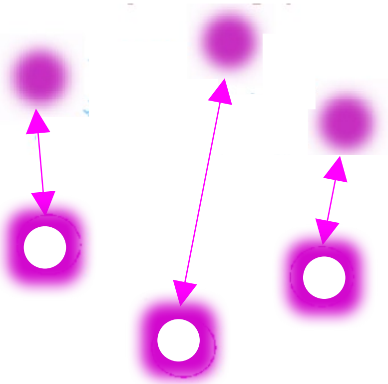
can be rewritten as an eigenvalue problem

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

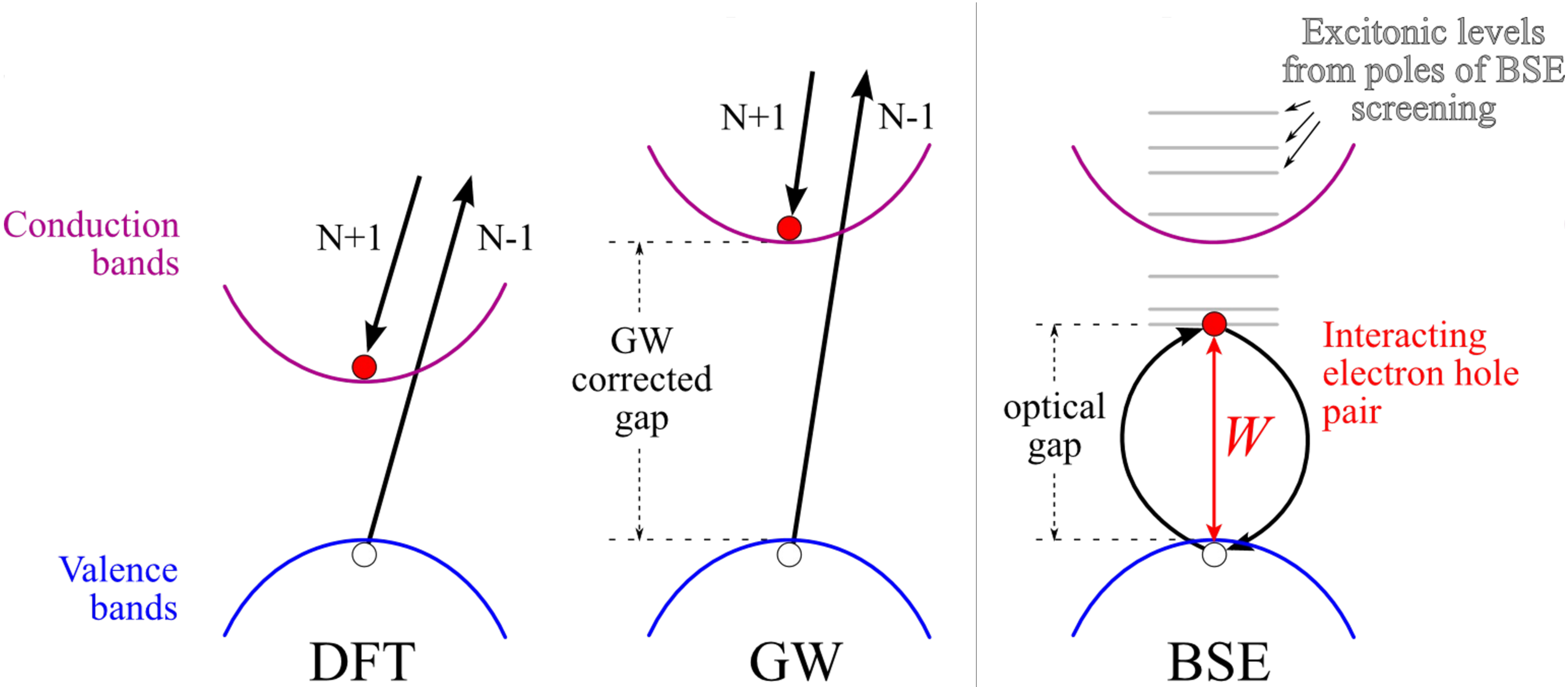
Excitation wave-function

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

Strongly interacting
(quasi)electron – (quasi)hole



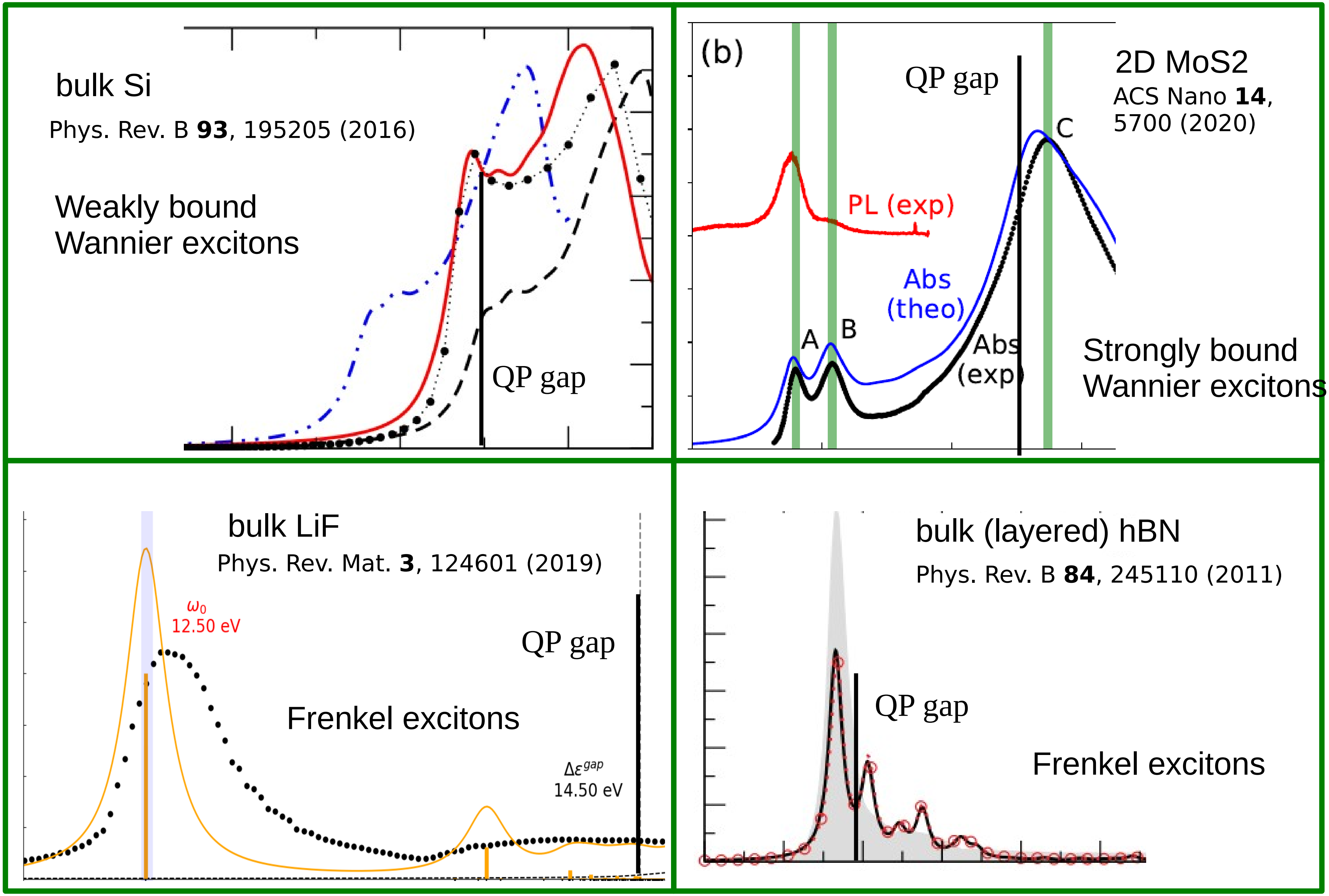
abinitio GW+BSE



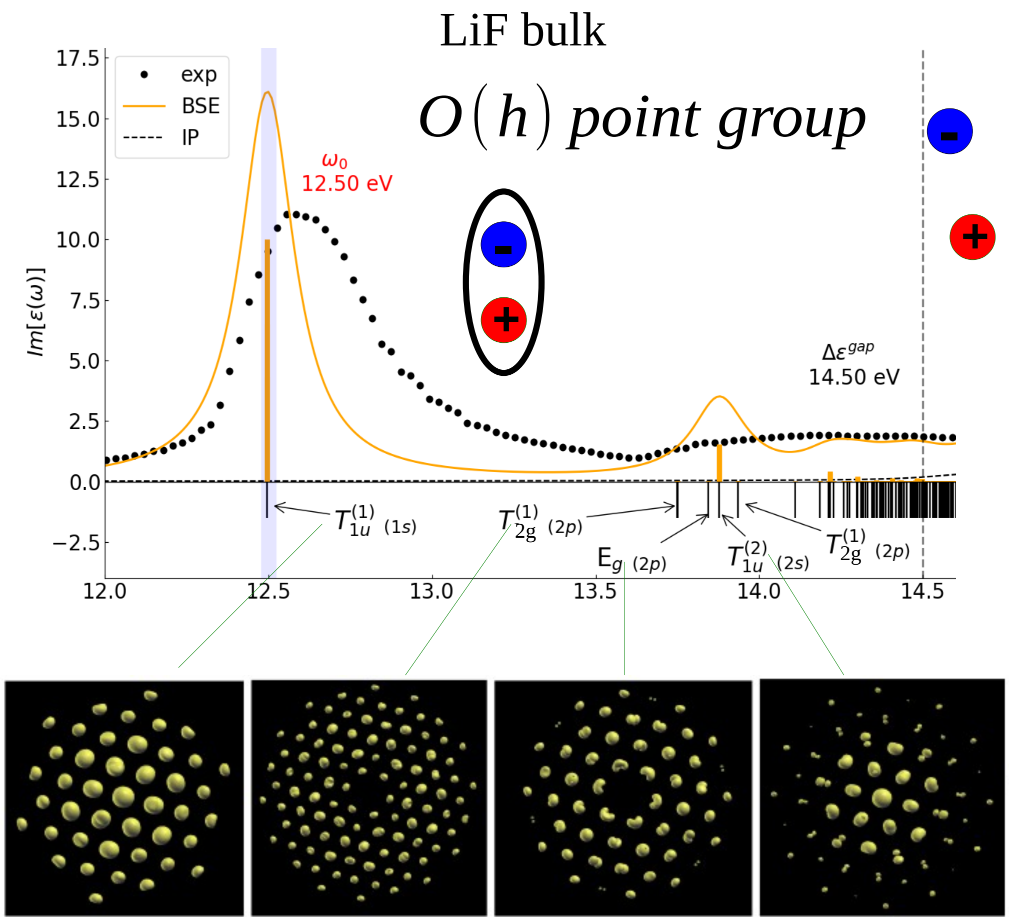
$$\epsilon_I = E_I(N \pm 1) - E_0(N)$$

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

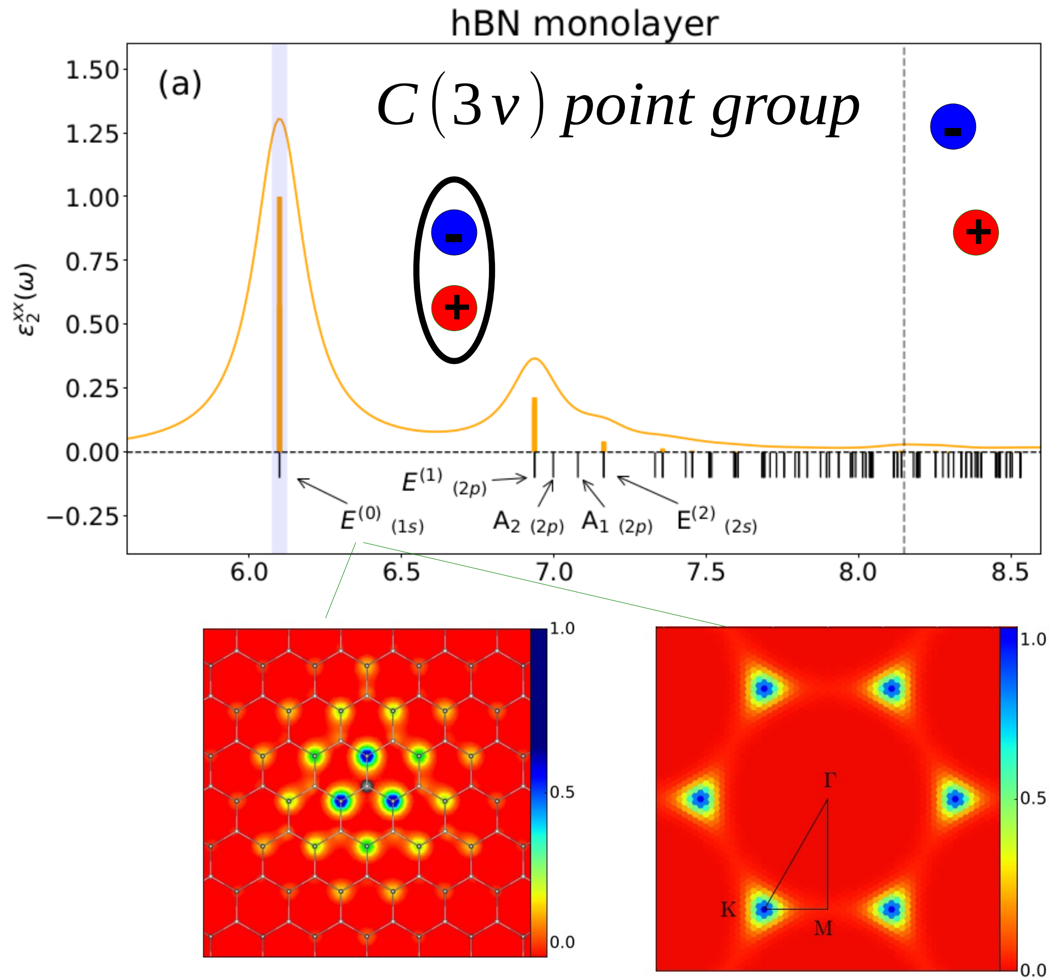
From Wannier to Frenkel excitons



Exciton wave-functions



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



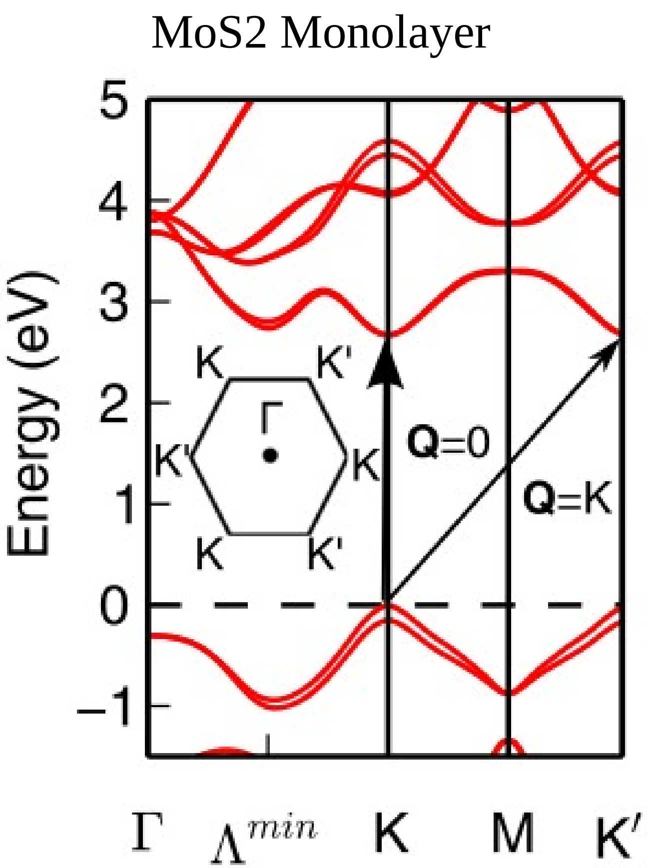
$$\left|\Psi^{\lambda q=0}(x_h^0, x)\right|^2 \qquad \left|\Psi^{\lambda q=0}(k)\right|^2$$

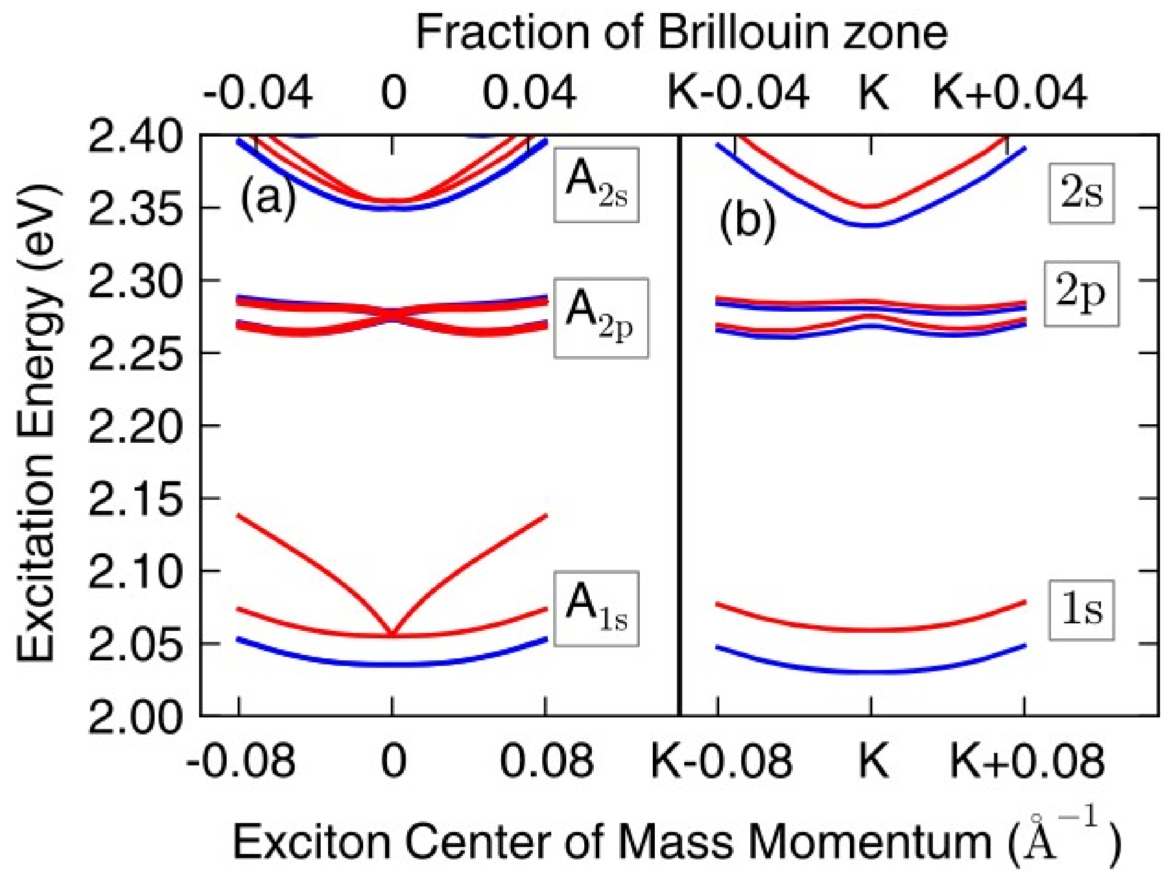
DS, M. D'Alessandro, C. Attaccalite, Phys. Rev. B **107**, 205203 (2023)

T. Galvani, F. Paleari, H. Miranda, Henrique A. Molina-Sanchez, L. Wirtz, S. Latil, H. Amara, F. Ducastelle, Phys. Rev. B **94**, 125303 (2016)

Exciton dispersion

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





D. Qiu, T. Cao, S. Louie, Steven,
Phys. Rev. Lett. **101**, 176801 (2015)

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* Miki Bonacci
* Elena Cannuccia
* Andrea Ferretti
* Myrta Gruening
* Alberto Guandalini
* Conor Hogan
* Dario Alejandro Leon-Valido
* Andrea Marini
* Alejandro Molina-Sánchez
* Fulvio Paleari
* Maurizia Palummo
* Davide Sangalli
* Nicola Spallanzani
* Daniele Varsano

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* Fabio Affinito
* David Kammerlader
* Ivan Marri
* Antimo Marrazzo
* Margherita Marsili
* Pedro Melo
* Henrique Miranda
* Ryan McMillan

Thank you
for your attention

MAX DRIVING THE EXASCALE TRANSITION

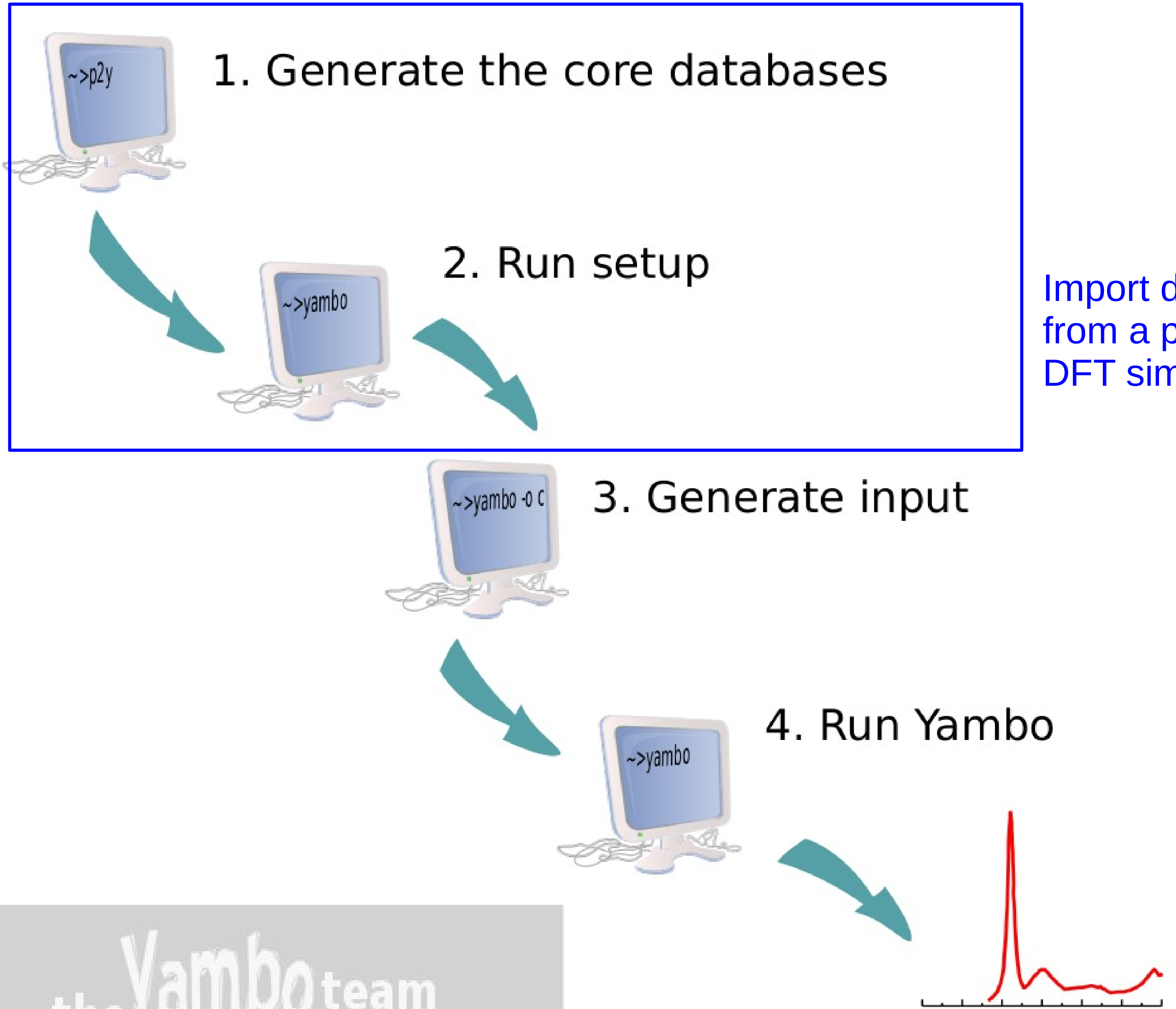
the Yambo team

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

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)

How the code works

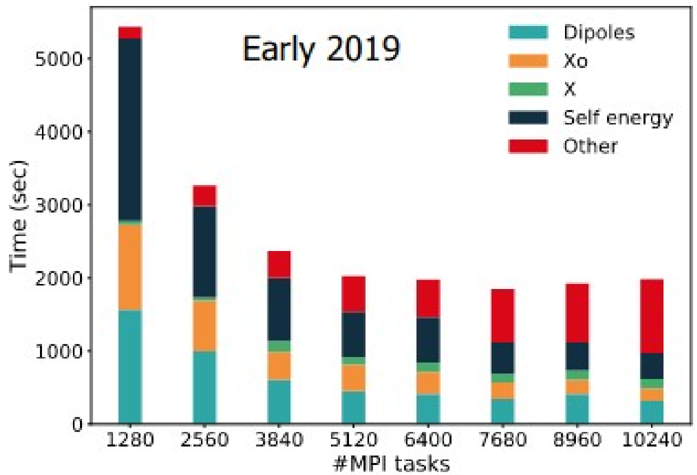


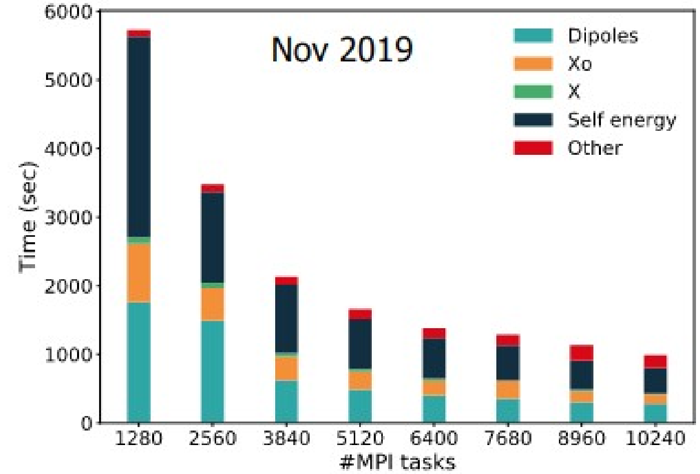
Import databases
from a previous
DFT simulation

the Yambo team

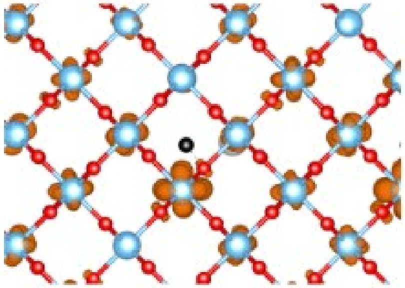
Yambo parallel performance

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

the Yambo team

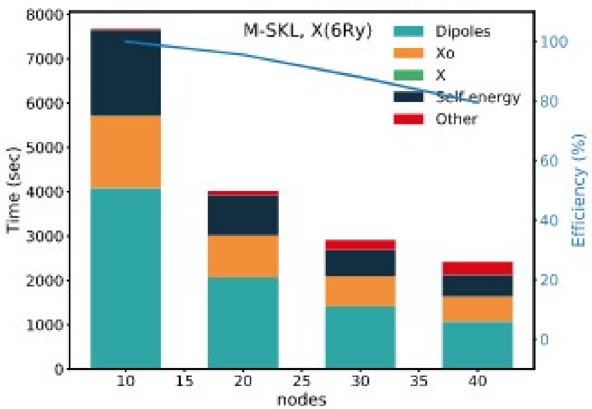
Yambo: performance (GPU)

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

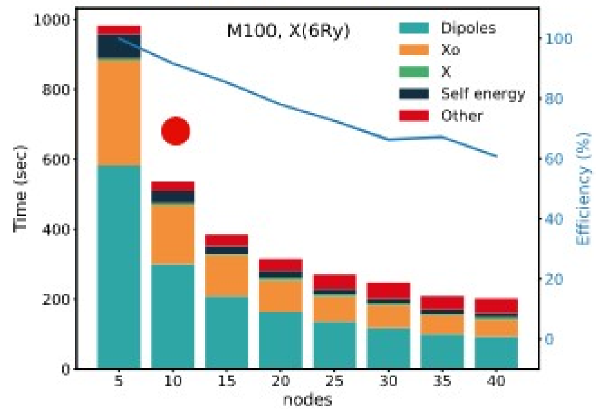
x14 wrt SKL (10 nodes)

x1.4 wrt V100 (2 nodes)

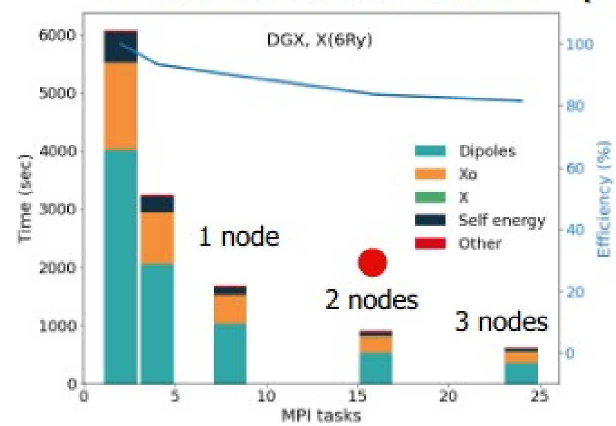
CPU: **Skylake**



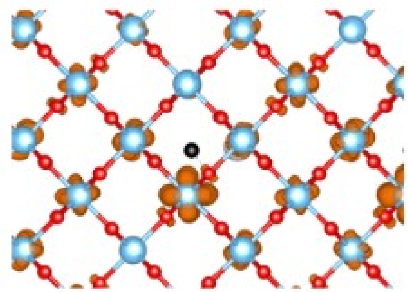
GPU: P9+**V100**



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



- complete **GW workflow** for defected TiO2 (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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the Yambo team