# Yambo à la carte

# Yambo

Yet Another Many

Body code

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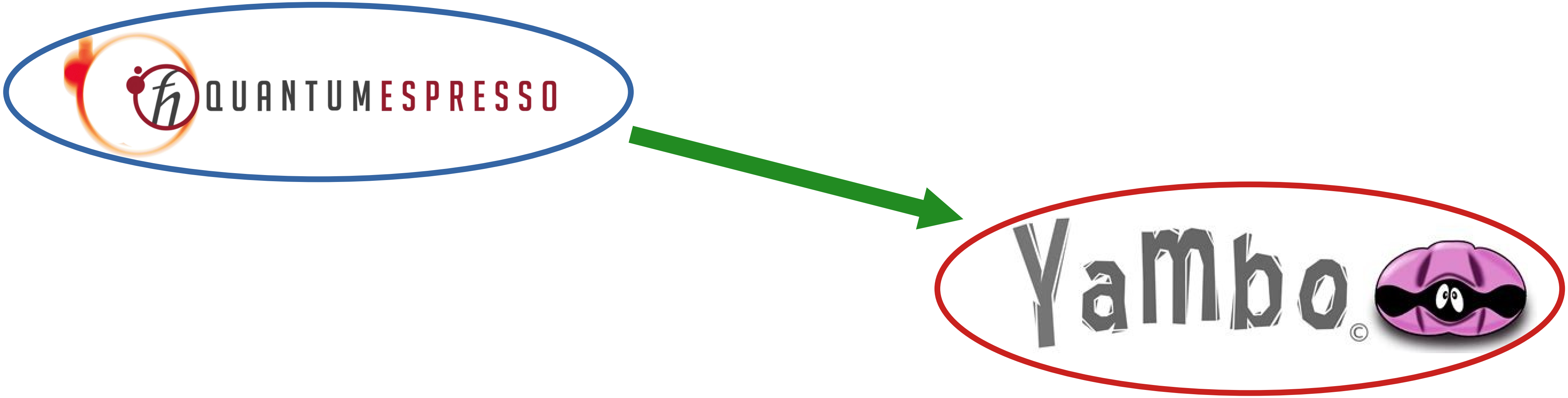
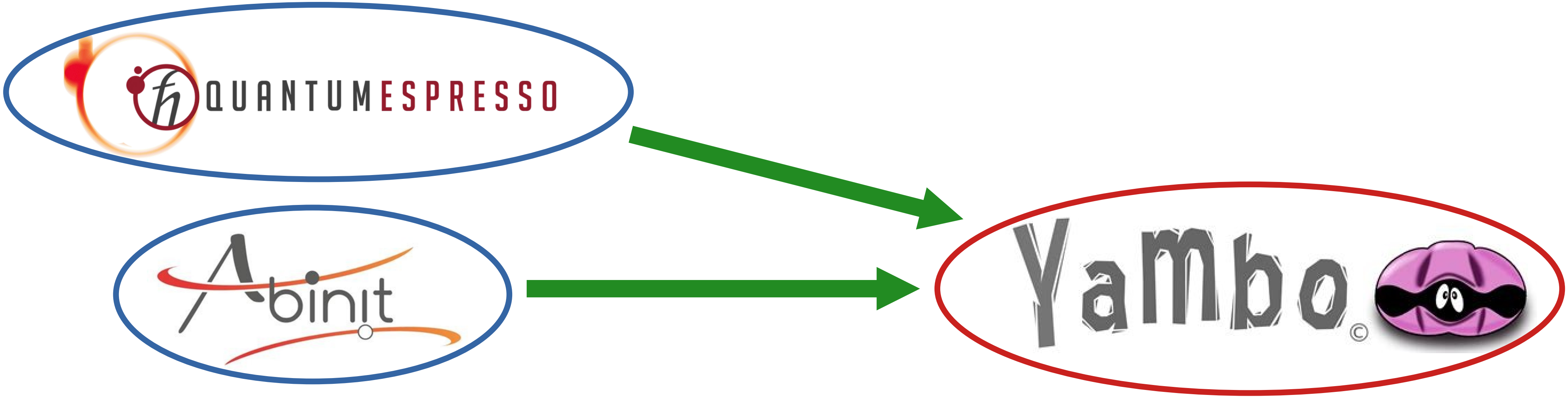
Yambo is a many-body code
in a Kohn-Sham basis

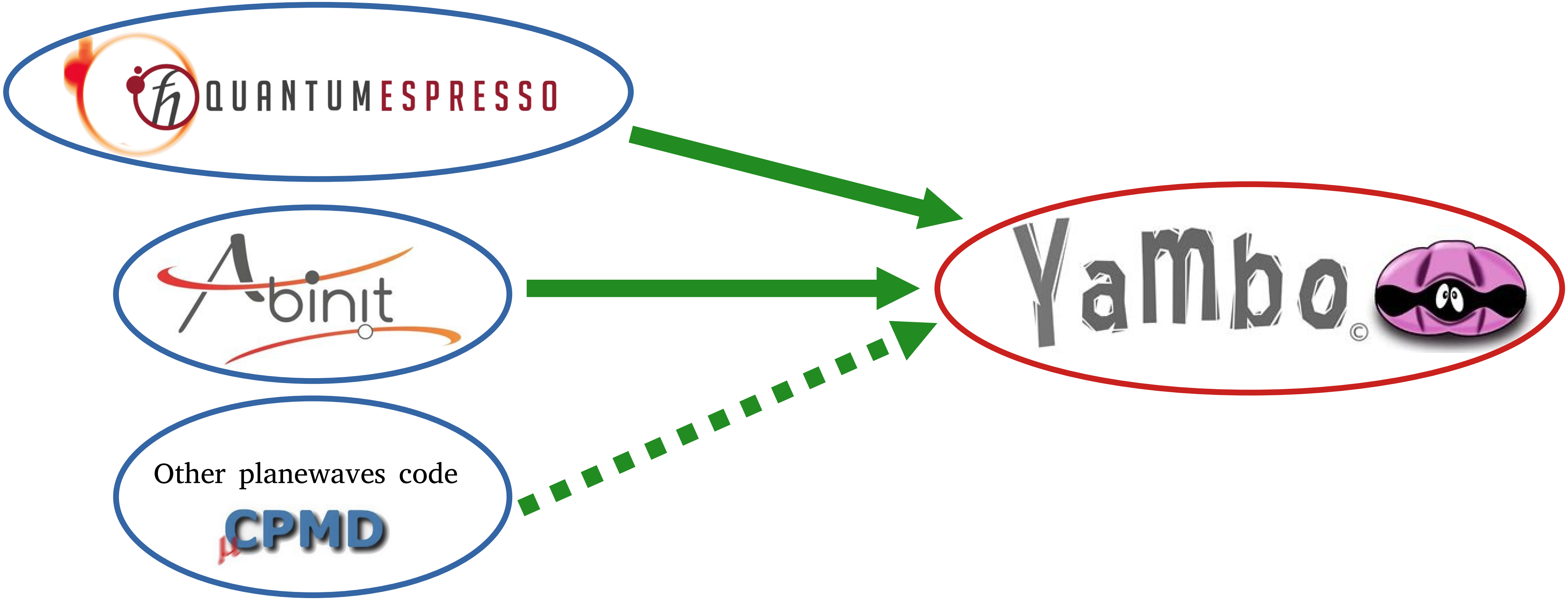
# Yambo is a many-body code in a Kohn-Sham basis



# Yambo is a many-body code in a Kohn-Sham basis



# Yambo is a many-body code in a Kohn-Sham basis



Other planewaves code

# What can you do with Yambo?

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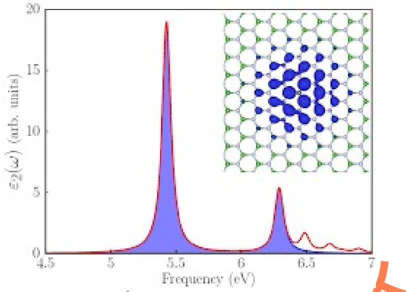
Optical properties



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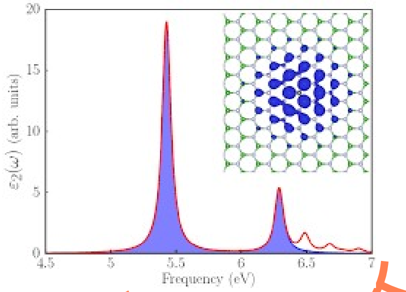
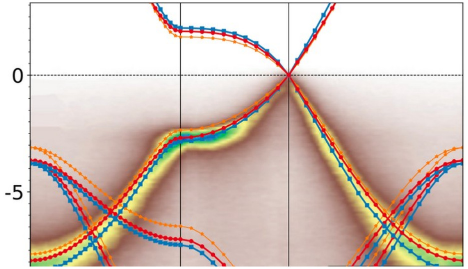


Quasi-particle band structure



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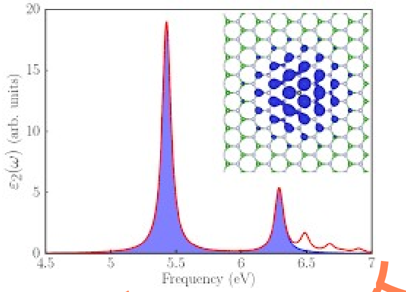

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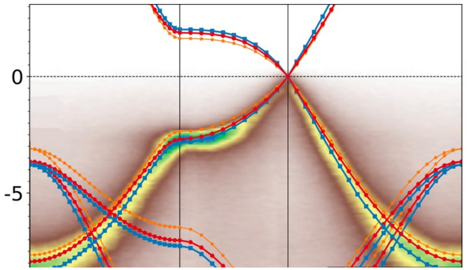
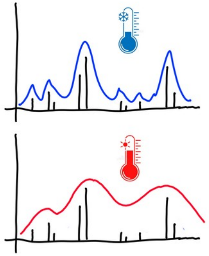
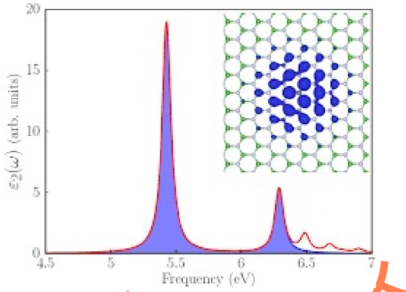


Electron-phonon coupling



# What can you do with Yambo?

## Optical properties



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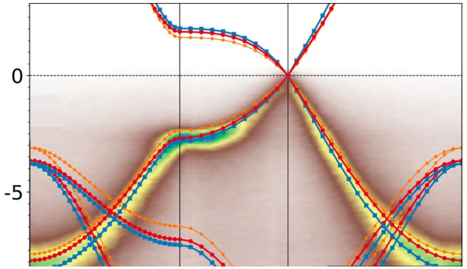
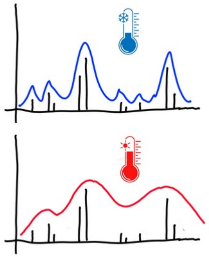
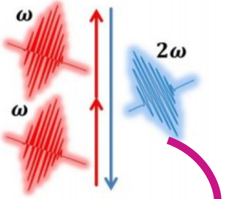


## Electron-phonon coupling



## Nonlinear optics



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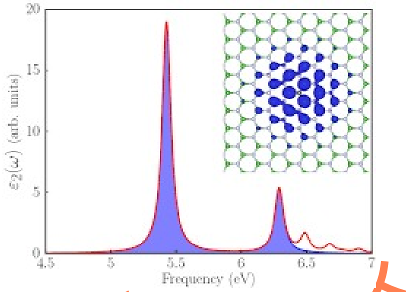

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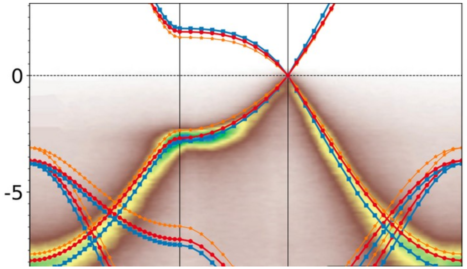

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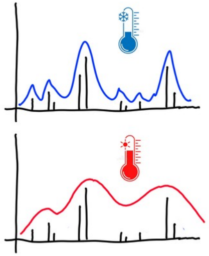

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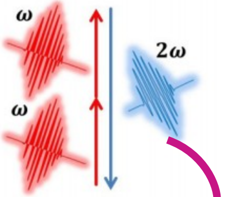
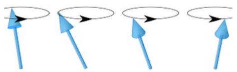
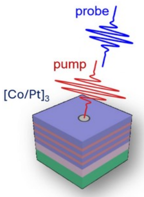
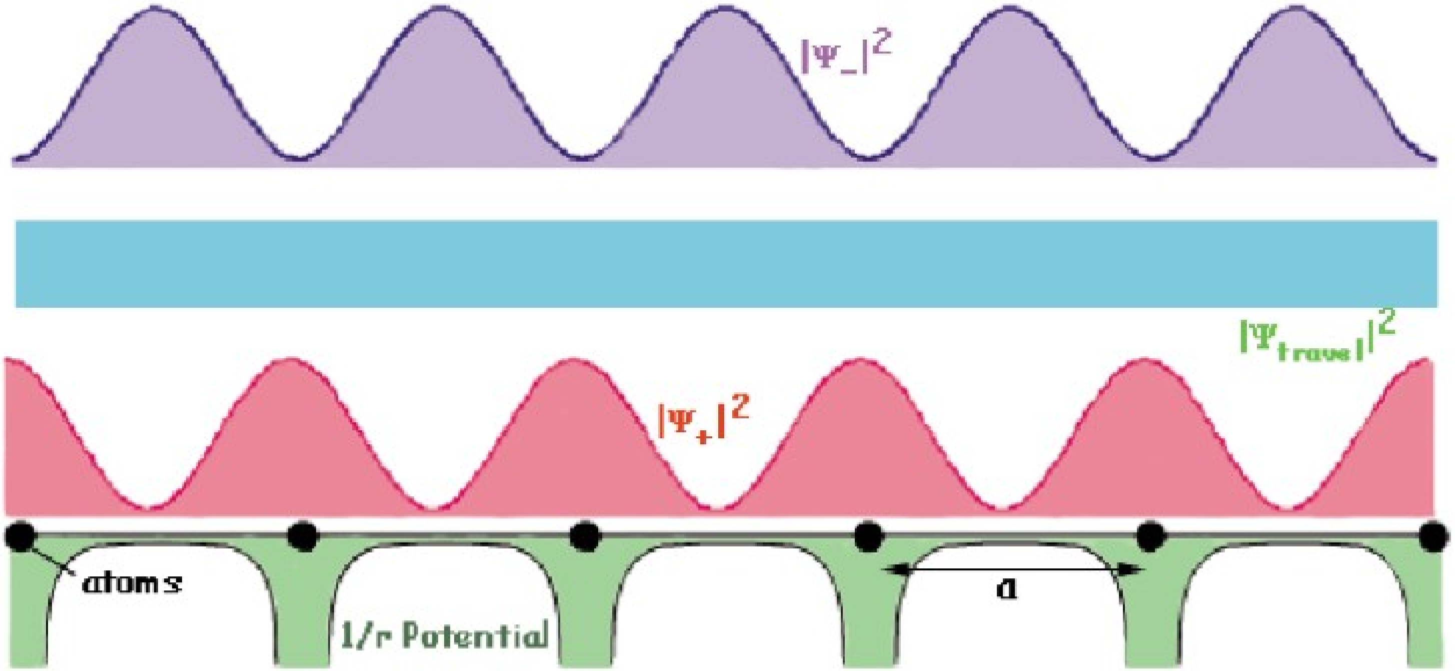


More...





# Basis set



# The basis: KS and plane-waves 1/2

KS Bloch functions

$$|\phi_{n\mathbf{k}}\rangle = e^{i\mathbf{k}r}|u_{n\mathbf{k}}(r)\rangle$$

$$\langle u_{n\mathbf{k}}(r)|u_{m\mathbf{k}}(r)\rangle = \delta_{n,m}$$

KS basis set

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KS basis set

$$H_{nm}(\mathbf{k}) = \langle u_{n\mathbf{k}}|\hat{H}(\mathbf{k})|u_{m\mathbf{k}}\rangle$$

# The basis: KS and plane-waves 1/2

KS Bloch functions

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$$H_{nm}(\mathbf{k}) = \langle u_{n\mathbf{k}}|\hat{H}(\mathbf{k})|u_{m\mathbf{k}}\rangle$$

$$A_{nm}(\mathbf{k},\mathbf{k}+\mathbf{q}) = \langle u_{n\mathbf{k}}|\hat{A}|u_{m\mathbf{k}+\mathbf{q}}\rangle$$

# The basis: KS and plane-waves 1/2

## KS Bloch functions

$$|\phi_{n\mathbf{k}}\rangle = e^{i\mathbf{k}r}|u_{n\mathbf{k}}(r)\rangle$$

$$\langle u_{n\mathbf{k}}(r)|u_{m\mathbf{k}}(r)\rangle = \delta_{n,m}$$

$$|u_{n\mathbf{k}}\rangle = \sum_{\mathbf{G}} C^{n\mathbf{k}}_{\mathbf{G}} e^{i\mathbf{G}r}$$

## KS basis set

$$H_{nm}(\mathbf{k}) = \langle u_{n\mathbf{k}}|\hat{H}(\mathbf{k})|u_{m\mathbf{k}}\rangle$$

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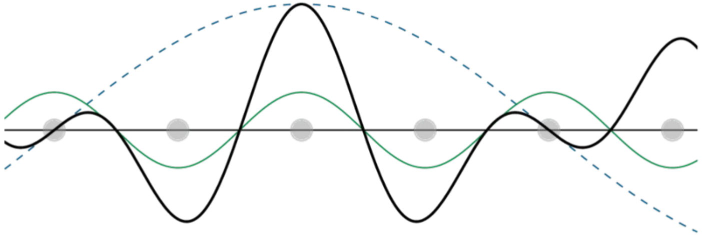
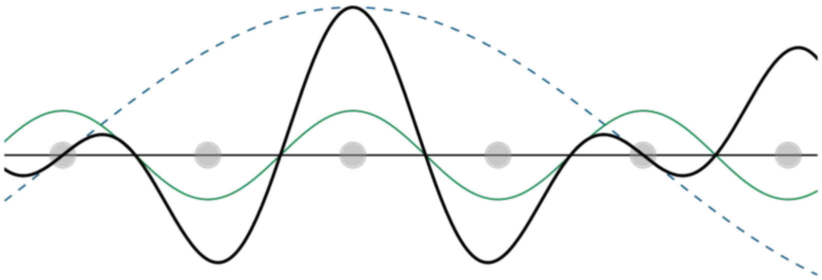
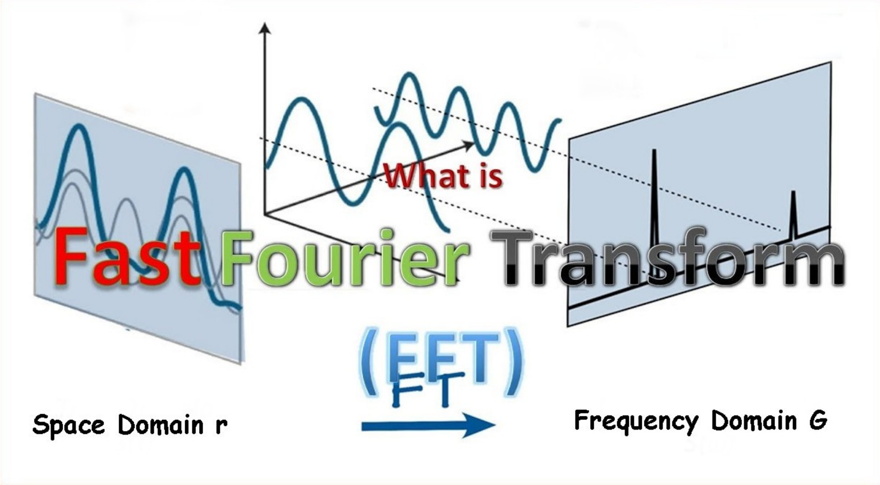


# The basis: KS and plane-waves 2/2

$$|u_{n\mathbf{k}}\rangle = \sum_{\mathbf{G}} C^{n\mathbf{k}}_{\mathbf{G}} e^{i\mathbf{G}r}$$





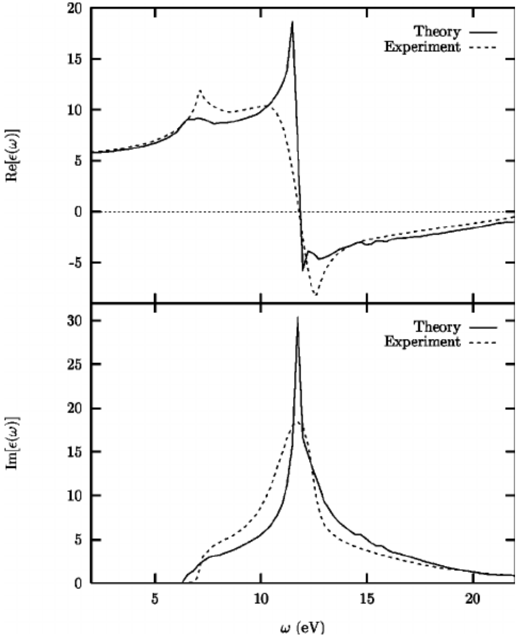
$$\langle A\rangle_{n,m} = \langle u_{n\mathbf{k}}(r)|\hat{A}(r)|u_{n\mathbf{k}}(r)\rangle$$

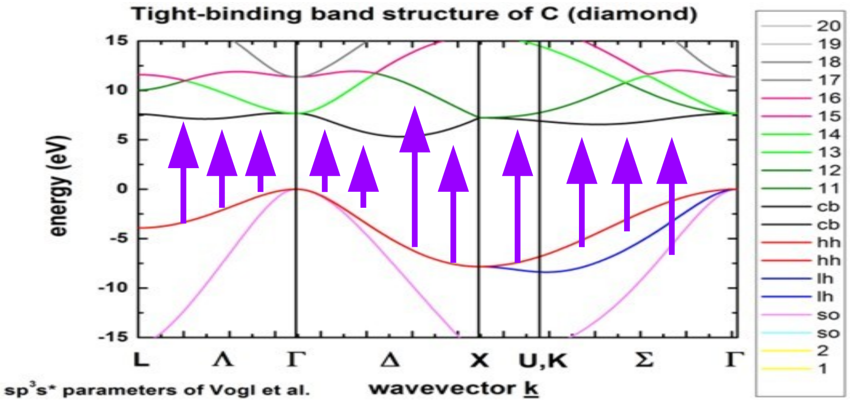
$$\langle B\rangle_{n,m} = \langle u_{n\mathbf{k}}(G)|\hat{B}(G)|u_{n\mathbf{k}}(G)\rangle$$

# Properties

# Linear optical response

$$\epsilon(\omega) = 1 - \frac{4\pi}{V} \sum_{\mathbf{k},v,c} \frac{|\langle \phi_{\mathbf{k},v} | r | \phi_{\mathbf{k},c} \rangle|^2}{\epsilon_{\mathbf{k},v} - \epsilon_{\mathbf{k},c} - \omega + i\eta}$$





Electrons are excited from valence
to conduction bands

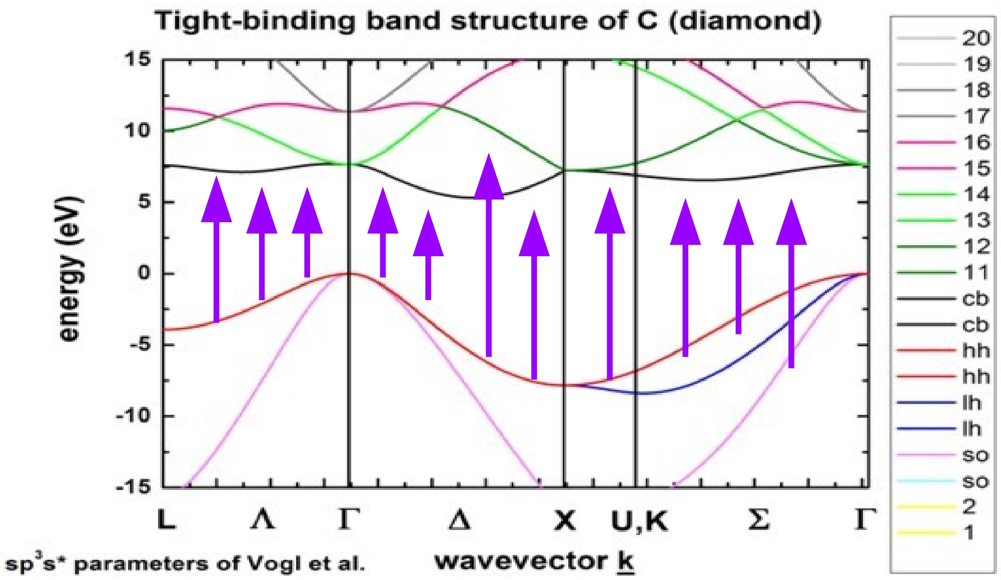
EELS

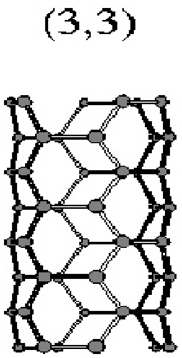
reflectivity

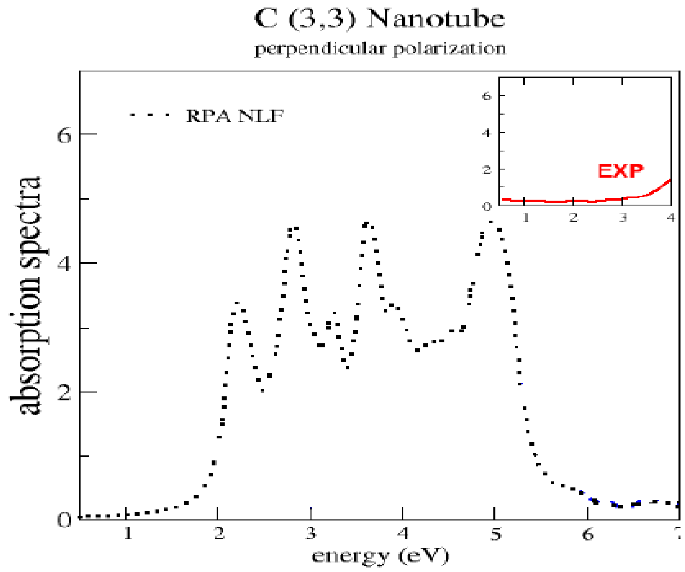
Dichroism

MOKE

# Local field effects 1/2



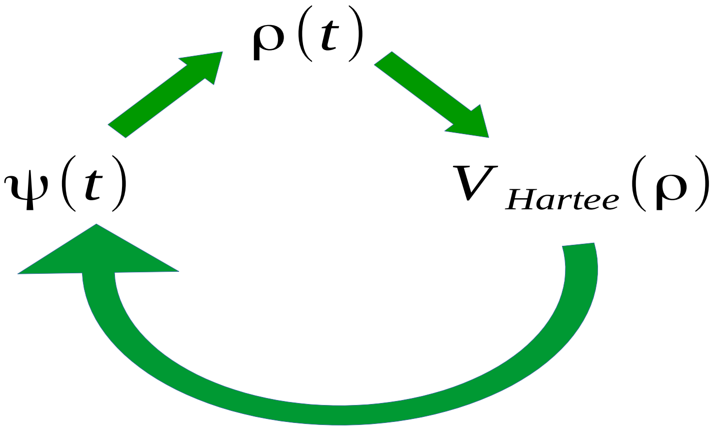




Electrons are excited from valence to conduction bands

Unfortunately these excitations are not independent

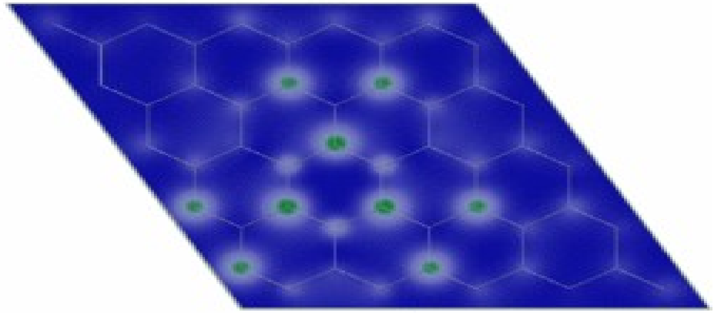
# Local field effects 2/2

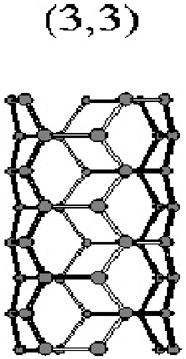


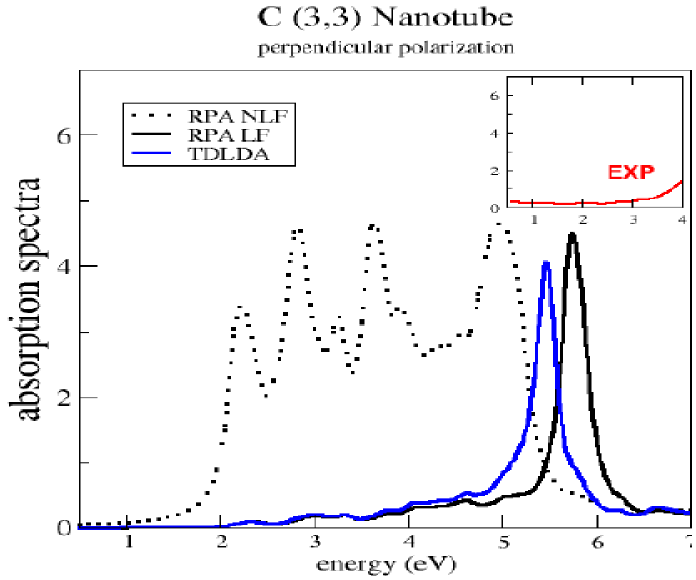
$\rho(t)$

$\psi(t)$

$V_{Hartee}(\rho)$







$$\chi_{g,g'} = \chi^0 + \chi^0 V \chi$$

# TDDFT

... in g-space...

$$\chi = \chi^0 + \chi^0(V + f_{xc})\chi$$

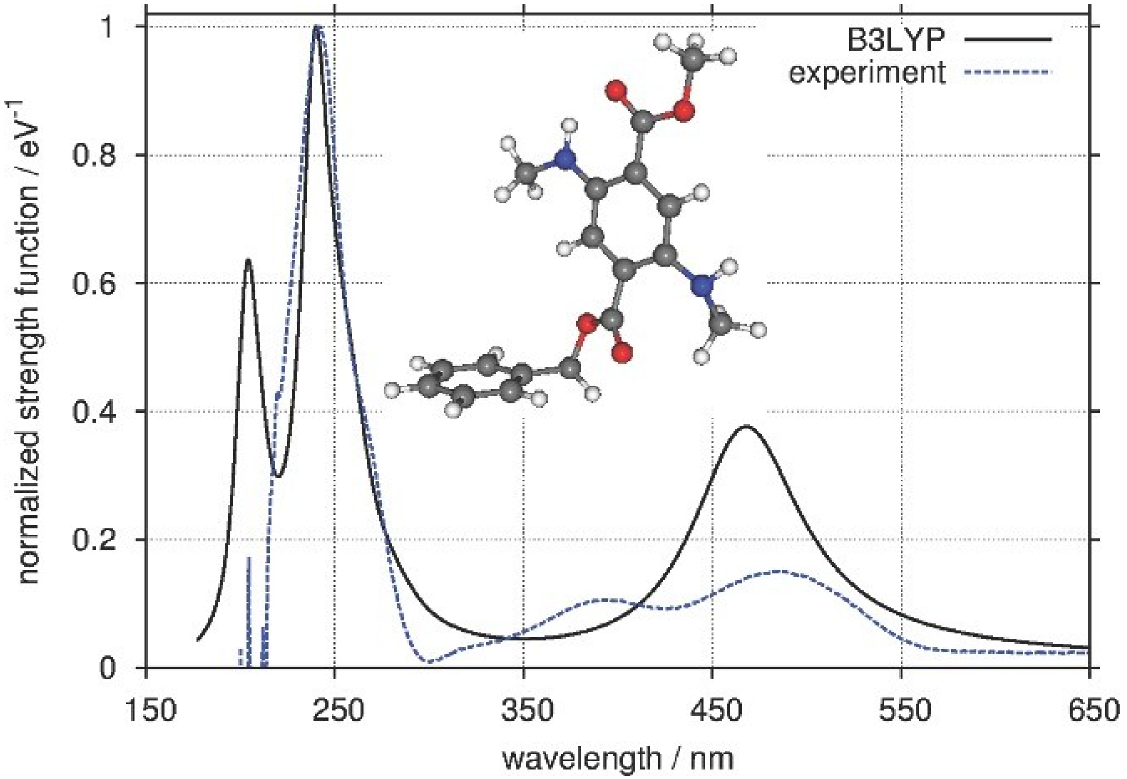
...or in e-h space (Casida eq.)...

$$\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \omega \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix}$$

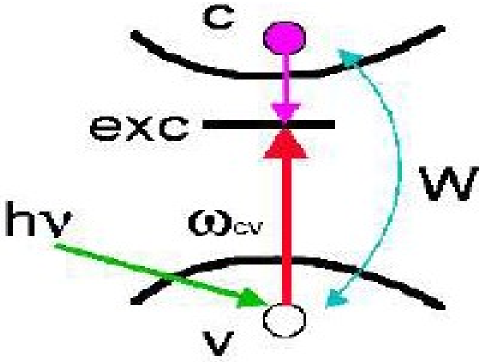
*Tamm – Dancoff Approximation reduces equations to* $AX = \omega X$

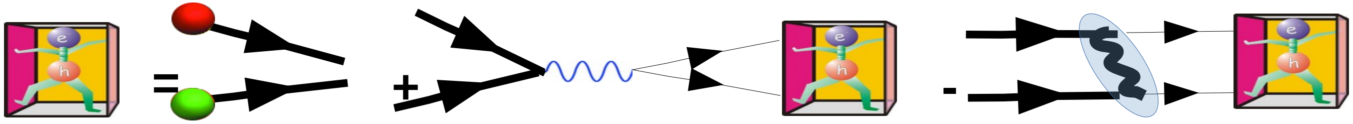
$$A = \delta_{ij}\delta_{ab}(\epsilon_a - \epsilon_i) + K_{ia,jb}$$

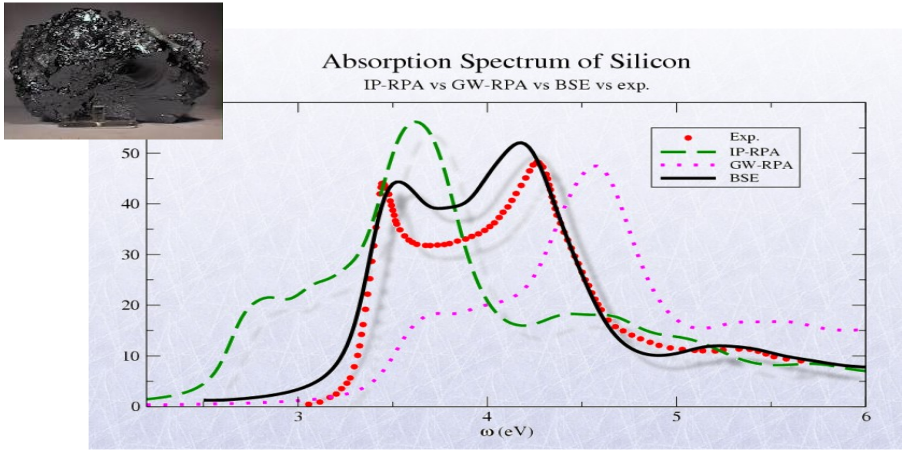
$$K_{ia,jb} = (pq|\frac{1}{r_{12}}|rs) + (pq|f_{xc}|rs)$$



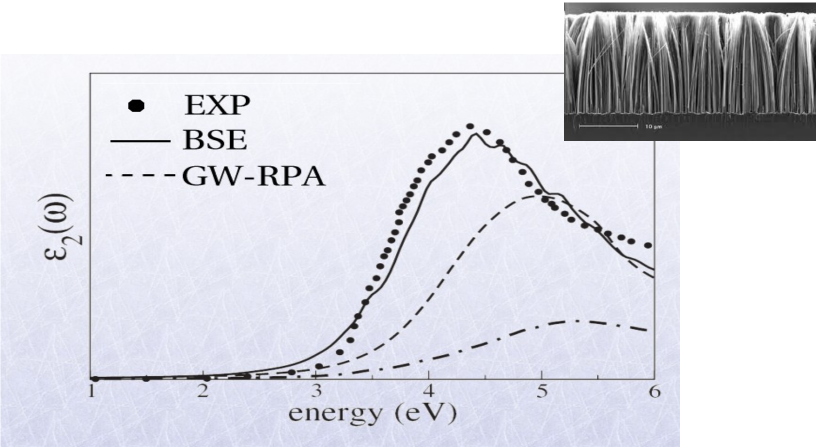
# Excitons



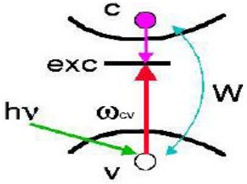



Absorption Spectrum of Silicon

IP-RPA vs GW-RPA vs BSE vs exp.



G. Strinati, Rivista del Nuovo Cimento, **11**, 1 (1988)

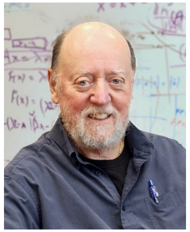


# Solving the Bethe-Salpeter equation

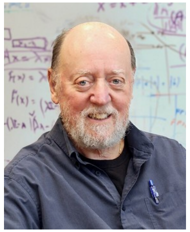
$$H^{BSE}_{cv\mathbf{k},c'v'\mathbf{k}} = H_0 + 2\bar{V} - W$$

Matrix size = $N_v$ x $N_c$ x N-kpoints

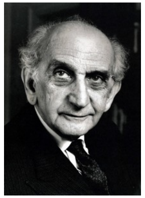
- Small size (Lapack)

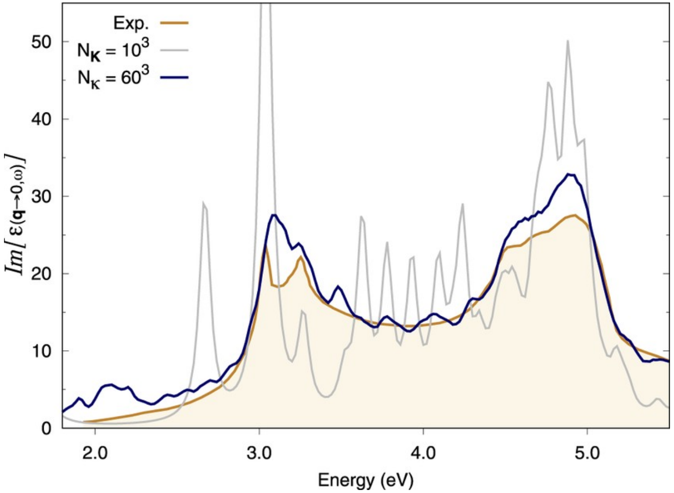


- Medium size (Scalpack, Magma,etc..)



- Big size (Haydock + Slepc)





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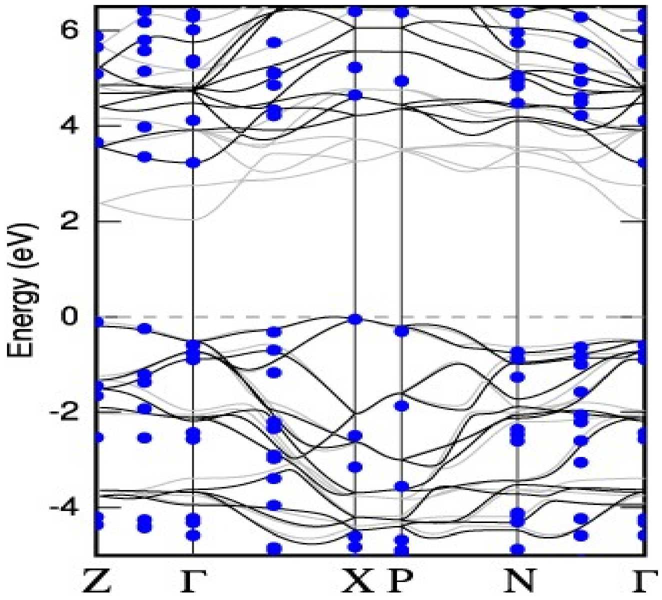
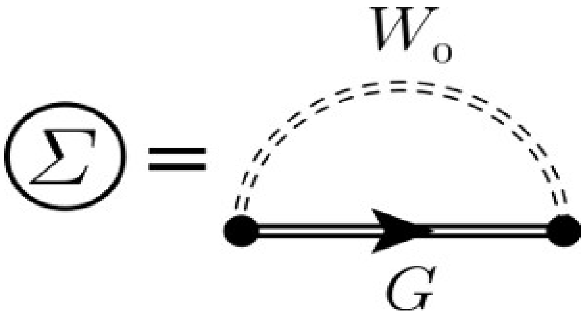
# Quasi-particle band structure 1/2



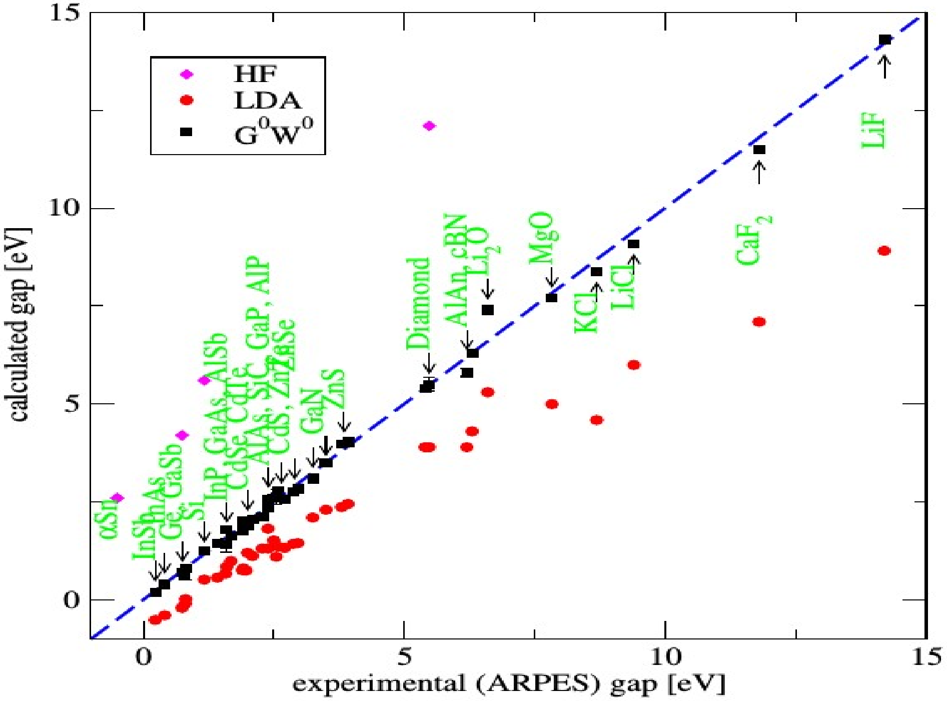
$$W(\omega) = \frac{V}{\epsilon(\omega)}$$



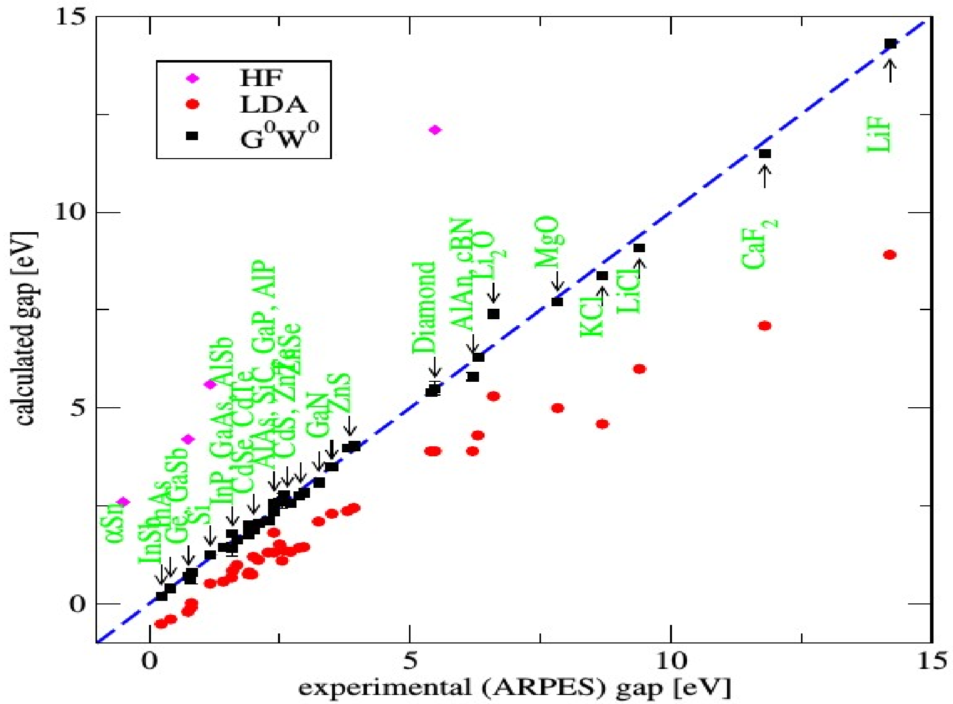
GW is the first order correction in terms of screened interaction

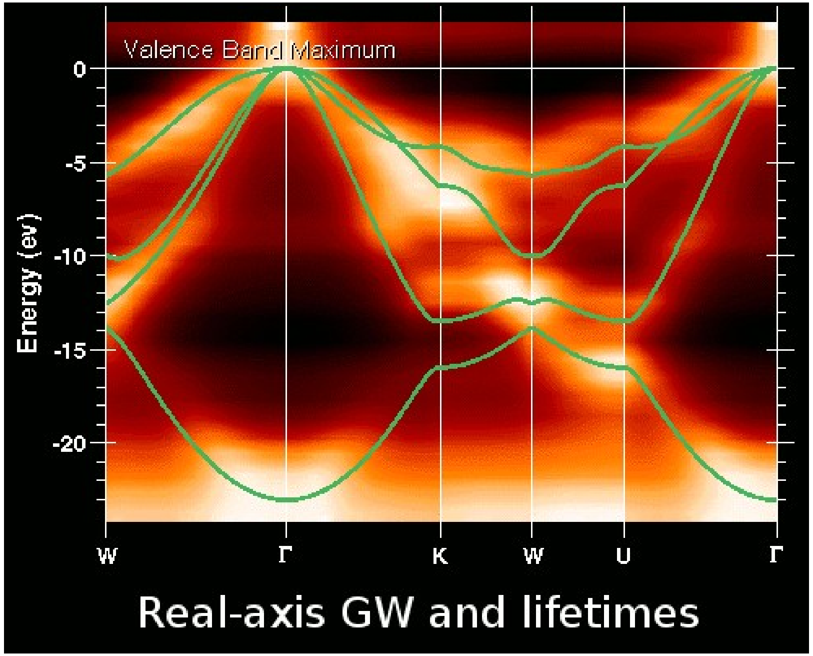
Aryasetiawan, F., & Gunnarsson, O. The GW method. Reports on Progress in Physics, **61**(3), 237.(1998).

# Quasi-particle band structure 2/2



# Quasi-particle band structure 2/2



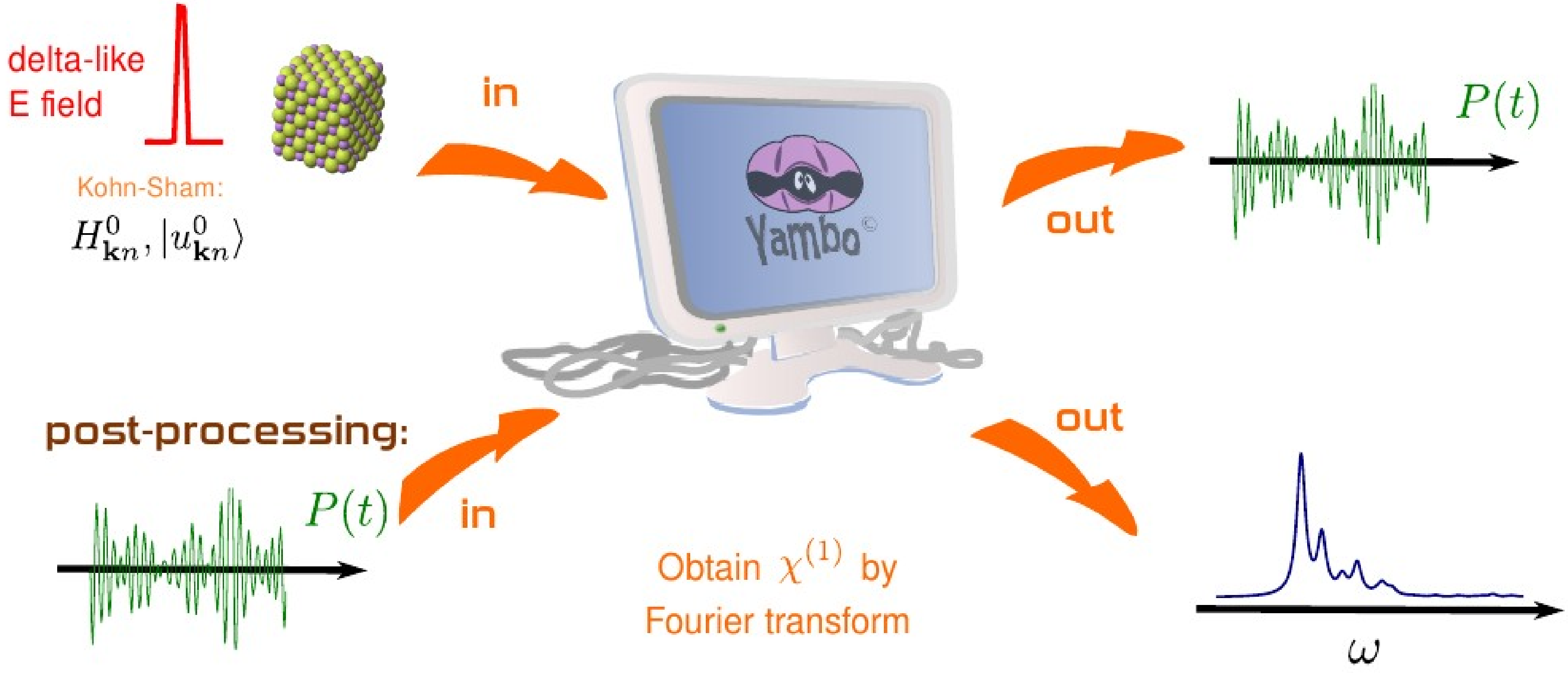


Real-axis GW and lifetimes

# Non-linear response

Solve Euler-Lagrange equations:

$$i|\dot{v}_{\mathbf{k},m}\rangle = \left(\hat{H}^0_{\mathbf{k}} + \hat{w}_{\mathbf{k}}(\boldsymbol{\mathcal{E}}) + \hat{w}^\dagger_{\mathbf{k}}(\boldsymbol{\mathcal{E}})\right)|v_{\mathbf{k},m}\rangle$$



delta-like
E field

Kohn-Sham:

$H^0_{\mathbf{k}n}, |u^0_{\mathbf{k}n}\rangle$

in

out

out

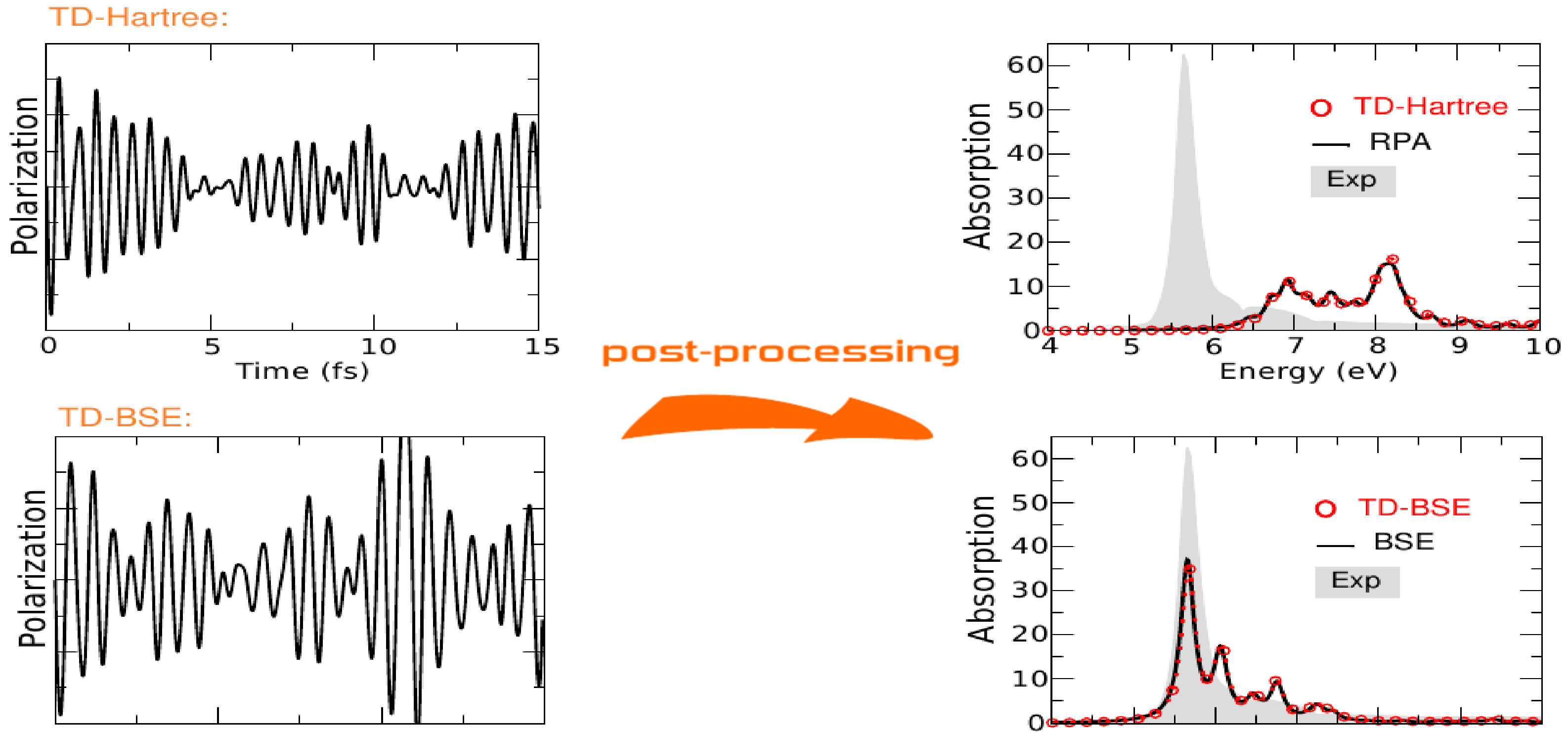
**post-processing:**

in

Obtain $\chi^{(1)}$ by
Fourier transform

# The Hamiltonian makes the difference

$$H^{eff} = h_k^0 + \Delta h_k + V_H[\Delta\rho] + \Sigma_{sex}[\Delta\gamma]$$



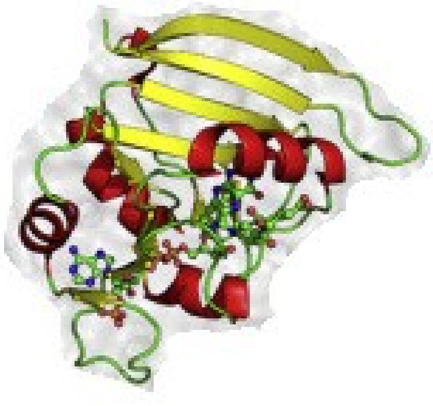
TD-Hartree:

TD-BSE:

post-processing

# Low dimensional systems

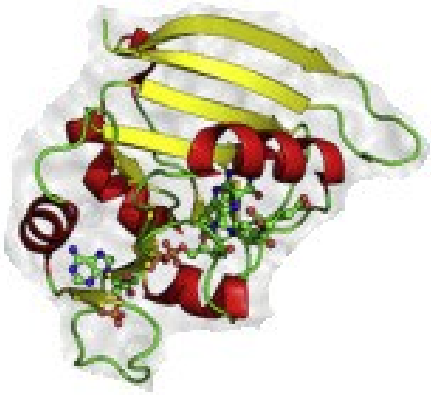
What you would like to simulate



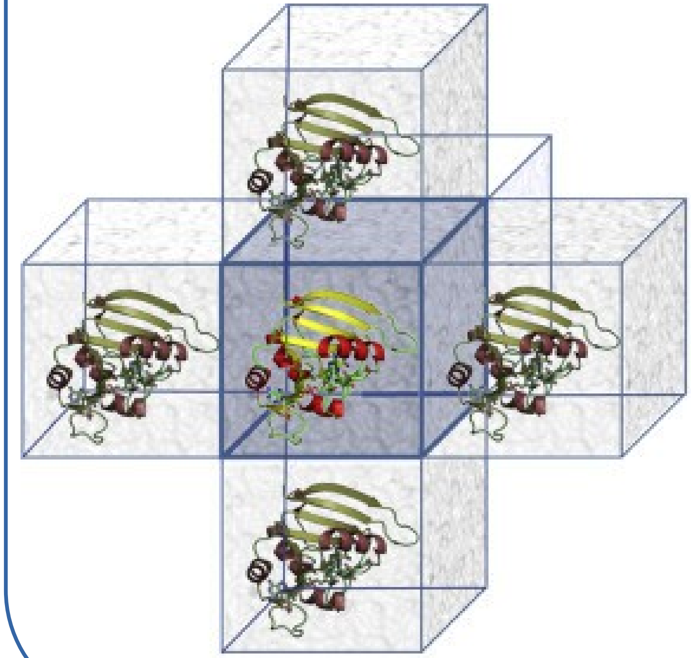
The image is for illustrative purposes only.

# Low dimensional systems

What you would like to simulate



What you really simulate



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# Low dimensional systems

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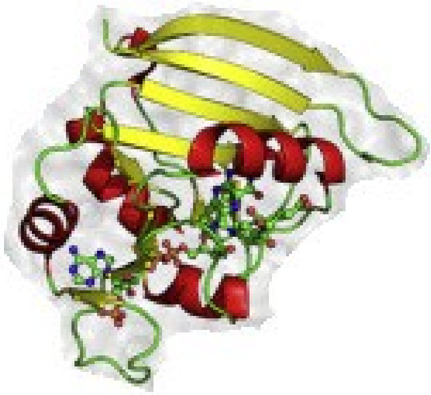

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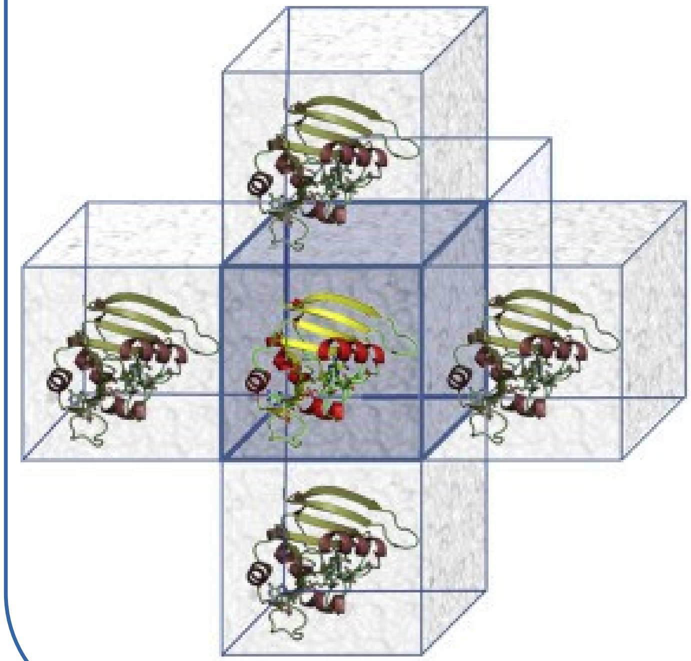
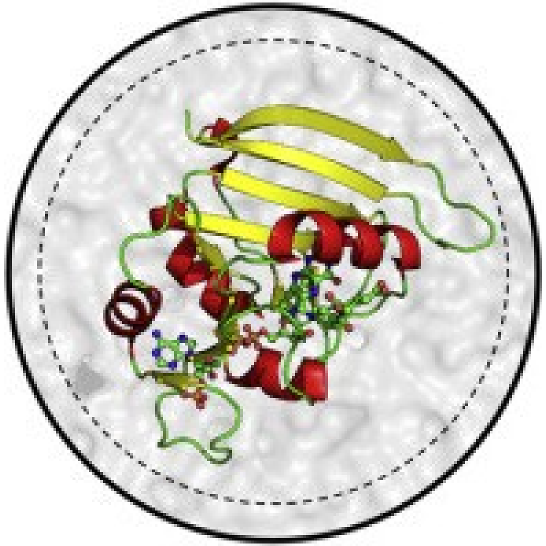


Solution:
Coulomb cutoff



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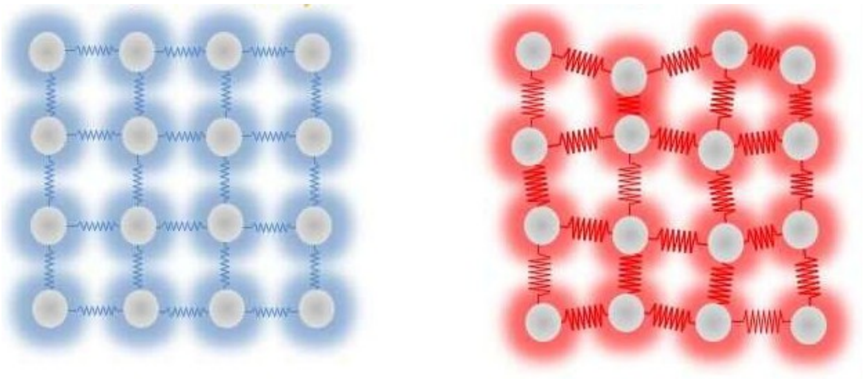
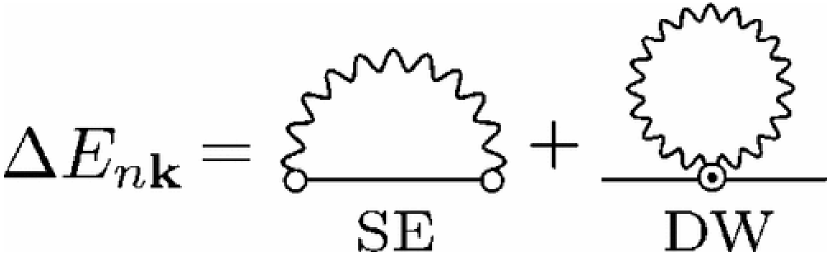
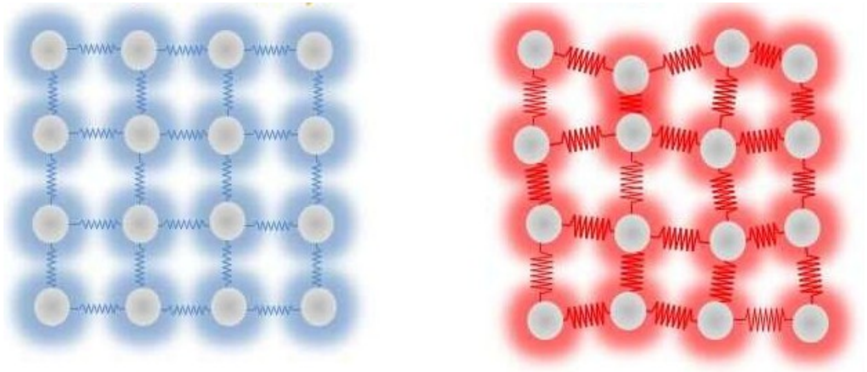
# Temperature

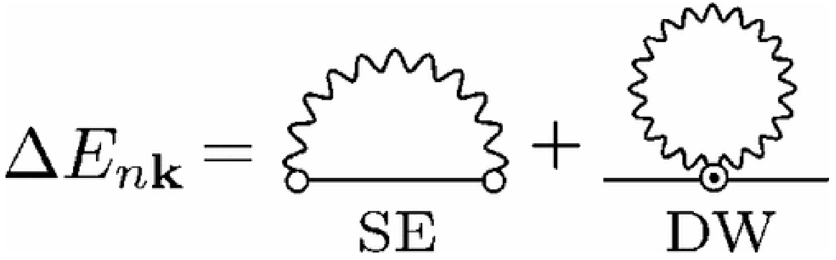


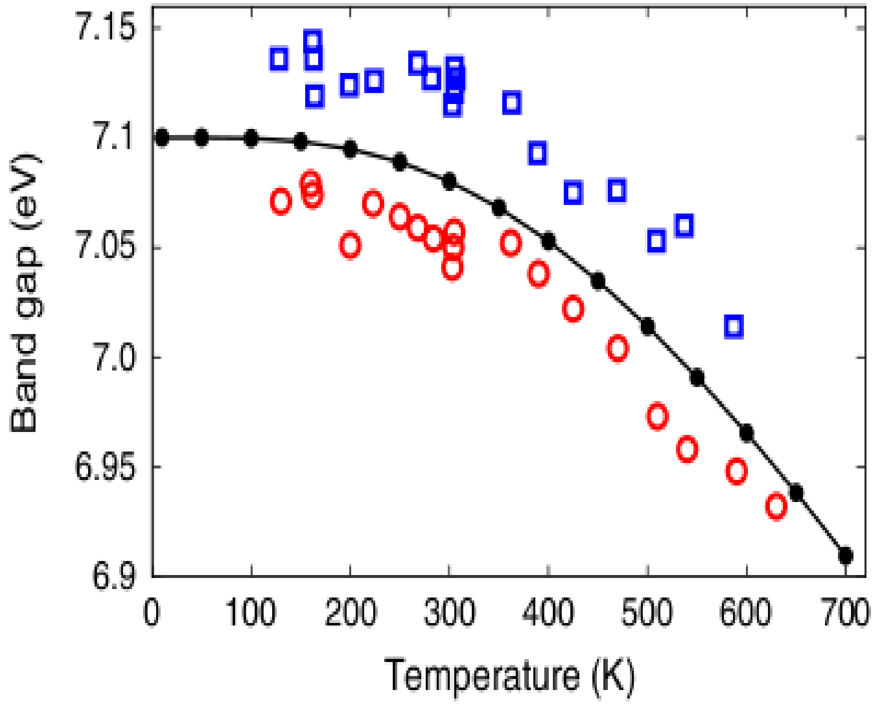


**Many-Body Effects on the Zero-Point Renormalization of the Band Structure**
G. Antonius, S. Poncé, P. Boulanger, M. Côté, and X. Gonze
Phys. Rev. Lett. **112,** 215501 (2014)

# Temperature 1/2

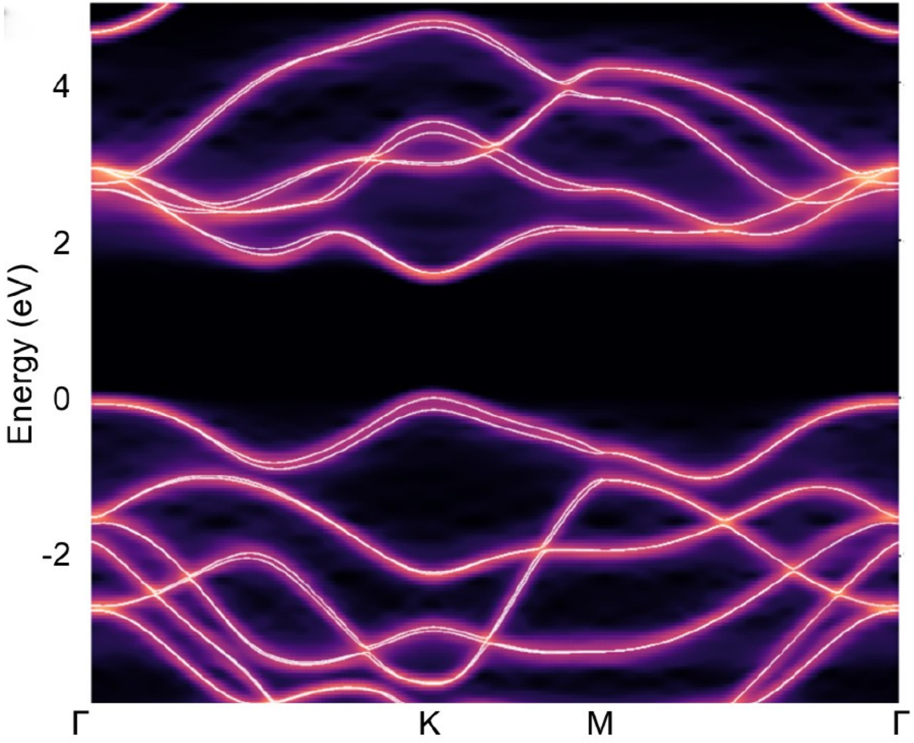




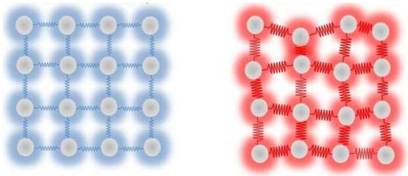


**Many-Body Effects on the Zero-Point Renormalization of the Band Structure**
G. Antonius, S. Poncé, P. Boulanger, M. Côté, and X. Gonze
Phys. Rev. Lett. **112,** 215501 (2014)

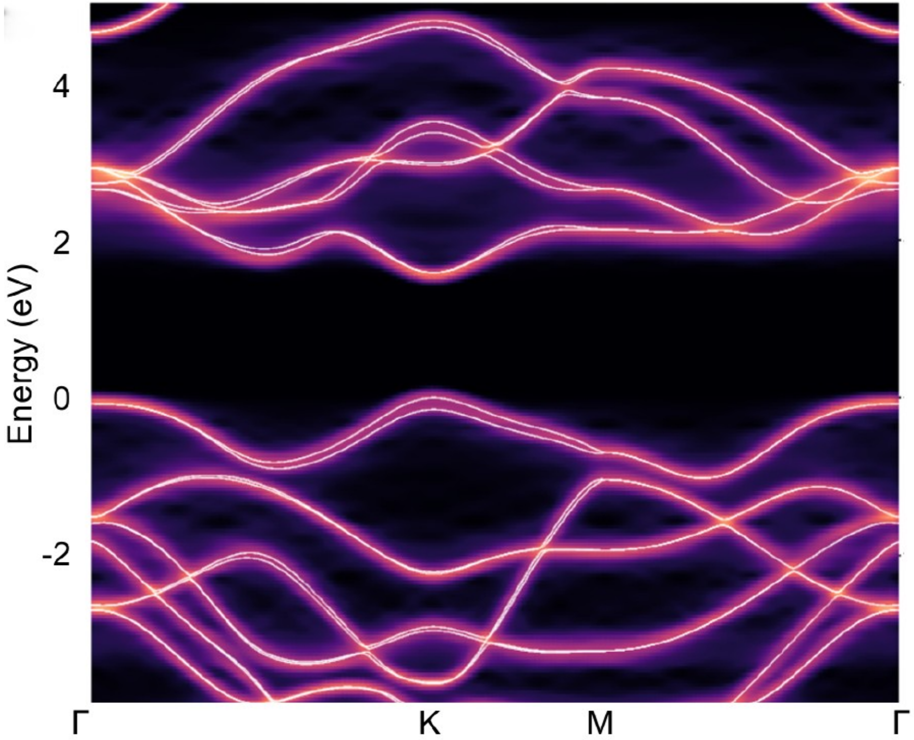
# Temperature 2/2



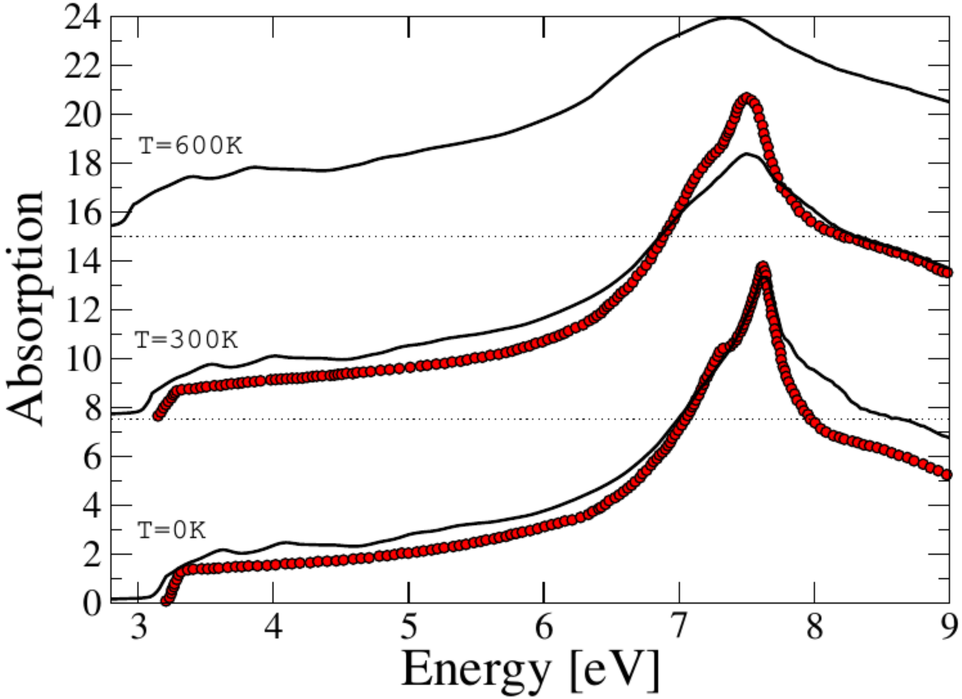
M. Zacharias, F. Giustino, Phys. Rev. Res. 2, 013357 (2020)



# Temperature 2/2

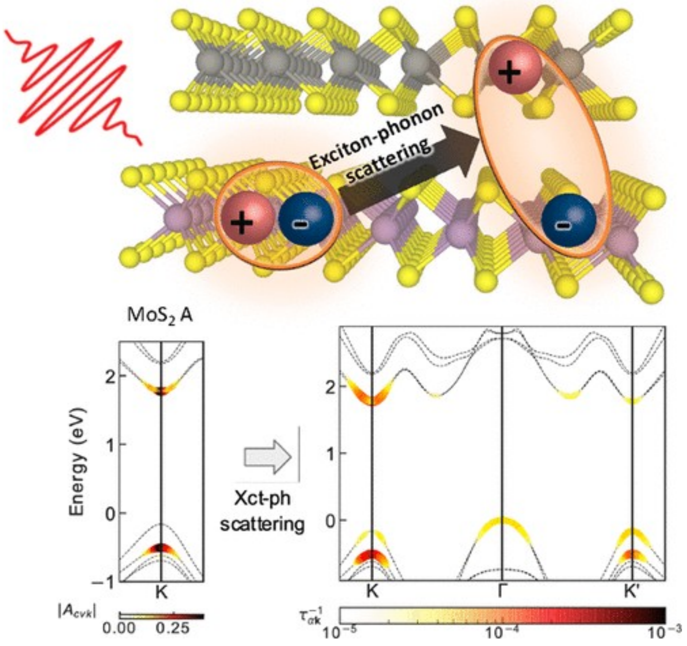


M. Zacharias, F. Giustino, Phys. Rev. Res. 2, 013357 (2020)

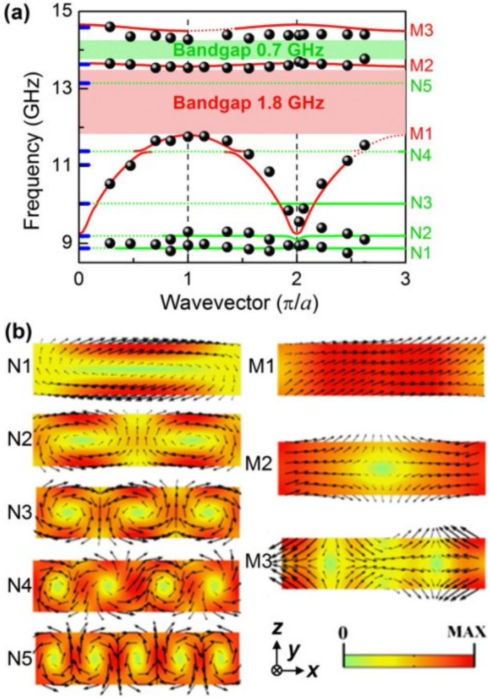


H Kawai, K Yamashita, E Cannuccia, A Marini
Physical Review B **89** (8), 085202 (2014)

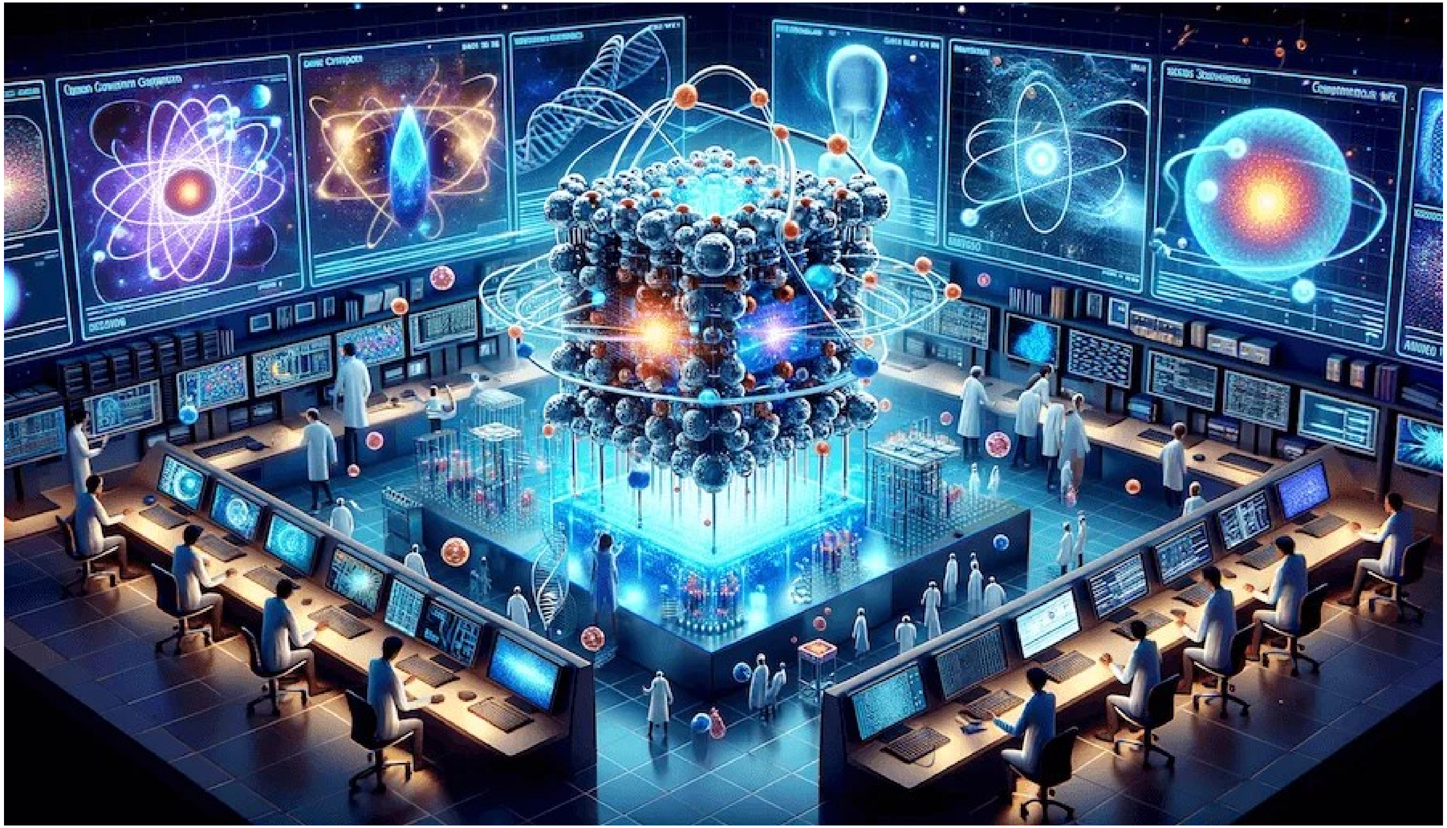
## Exciton-phonon (see Fulvio P. talk)



## Magnons (Alejandro M. S. et al.)

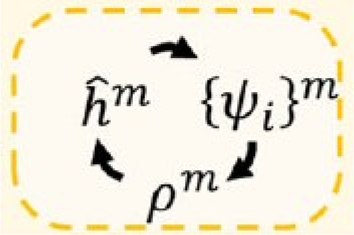


# Typical Yambo calculation



# Yambo calculation in 5 steps

Self-consistent DFT



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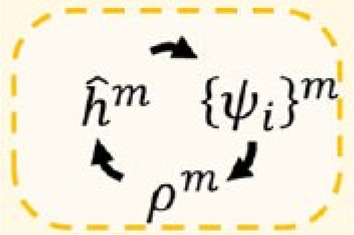
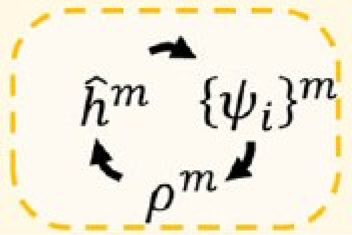


Non-Self-consistent

$$H^{KS}_{\mathbf{k}}|\phi_{n\mathbf{k}}\rangle = \epsilon_{n\mathbf{k}}|\phi_{n\mathbf{k}}\rangle$$

# Yambo calculation in 5 steps

Self-consistent DFT



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$$H^{KS}_{\mathbf{k}}|\phi_{n\mathbf{k}}\rangle = \epsilon_{n\mathbf{k}}|\phi_{n\mathbf{k}}\rangle$$

Import in Yambo

$p2y, a2y.....$

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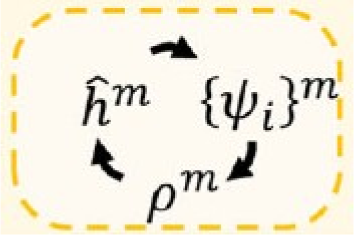

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$$p2y, a2y.....$$

Yambo setup

$$./yambo$$

r_setup

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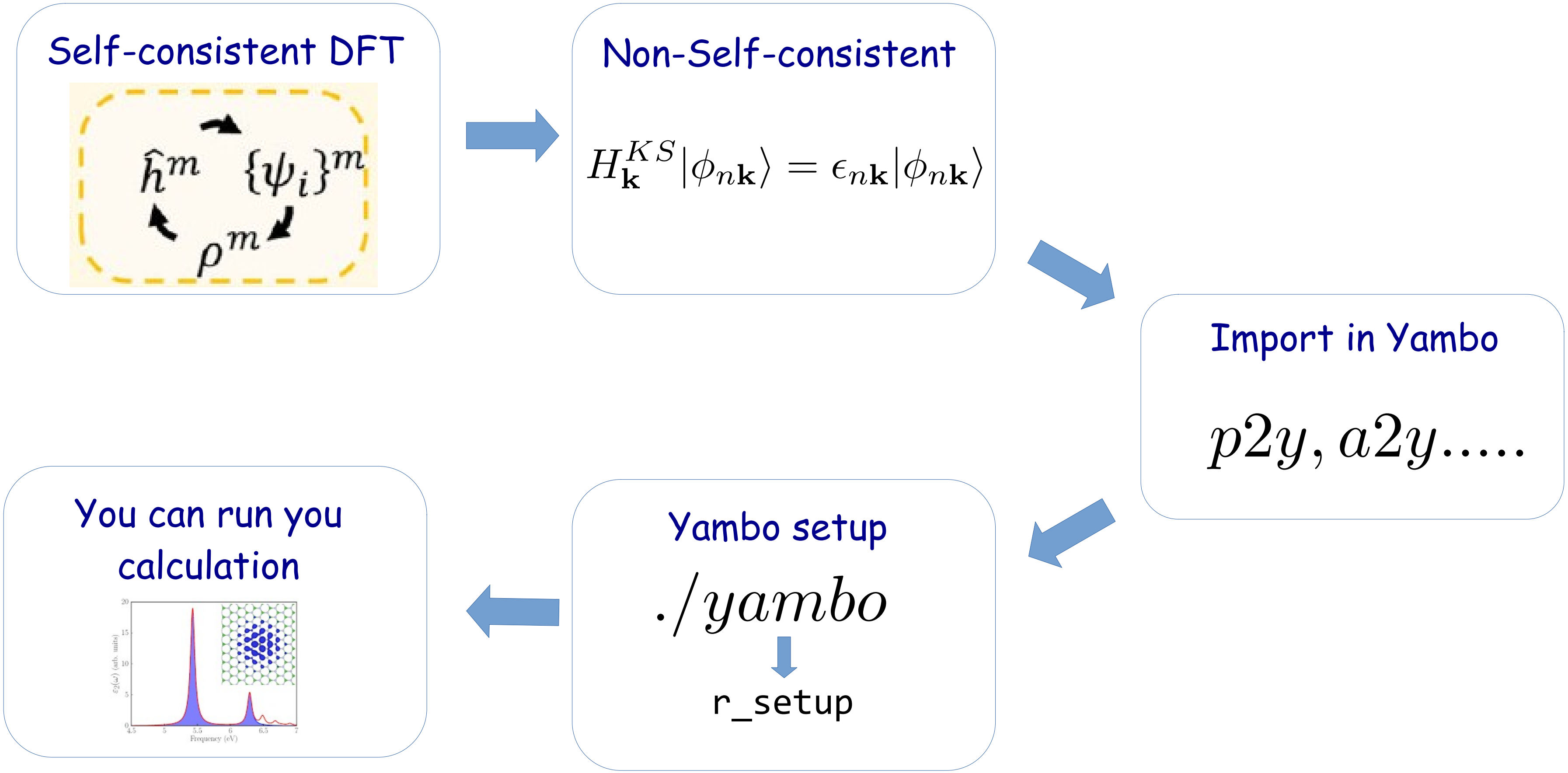

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Import in Yambo

$p2y, a2y.....$

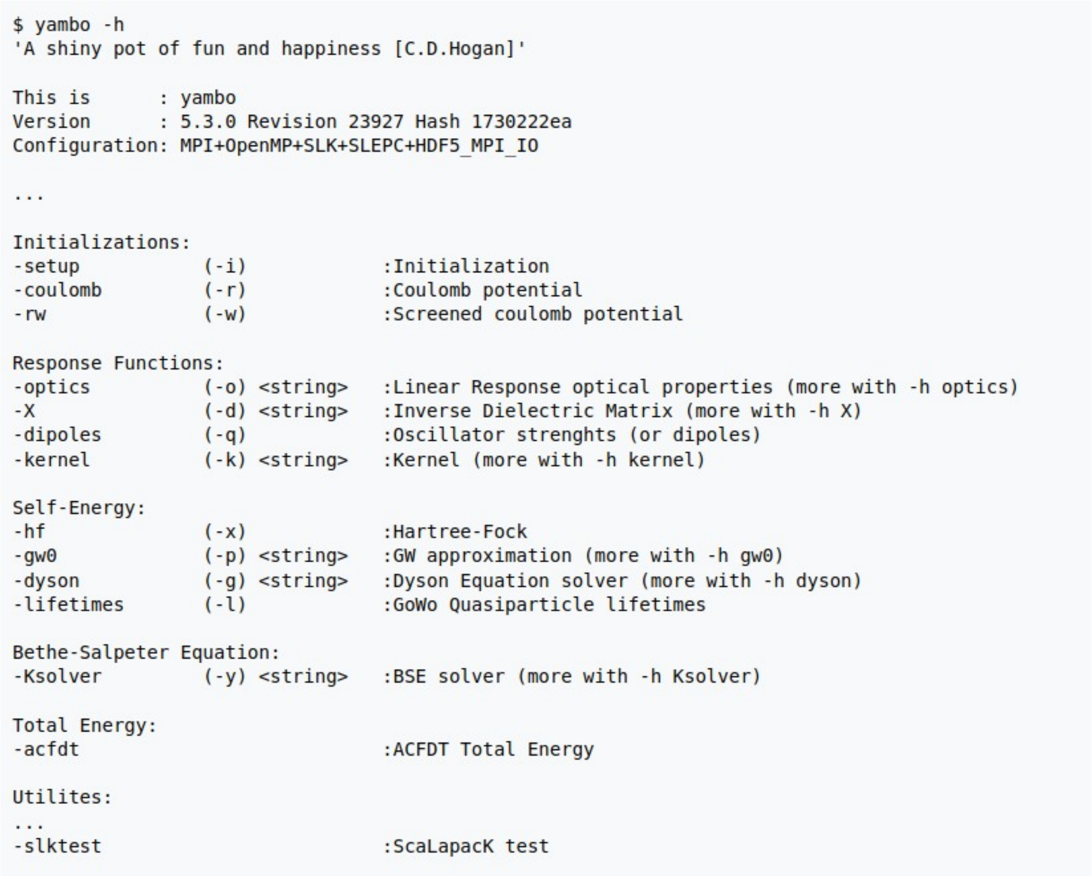
Yambo setup

$./yambo$

r_setup

You can run you calculation

# Input and command line



```
$ yambo -h
'A shiny pot of fun and happiness [C.D.Hogan]'

This is      : yambo
Version      : 5.3.0 Revision 23927 Hash 1730222ea
Configuration: MPI+OpenMP+SLK+SLEPC+HDF5_MPI_IO

...

Initializations:
-setup           (-i)            :Initialization
-coulomb         (-r)            :Coulomb potential
-rw              (-w)            :Screened coulomb potential

Response Functions:
-optics          (-o) <string>   :Linear Response optical properties (more with -h optics)
-X               (-d) <string>   :Inverse Dielectric Matrix (more with -h X)
-dipoles         (-q)            :Oscillator strenghts (or dipoles)
-kernel          (-k) <string>   :Kernel (more with -h kernel)

Self-Energy:
-hf              (-x)            :Hartree-Fock
-gw0             (-p) <string>   :GW approximation (more with -h gw0)
-dyson           (-g) <string>   :Dyson Equation solver (more with -h dyson)
-lifetimes       (-l)            :GoWo Quasiparticle lifetimes

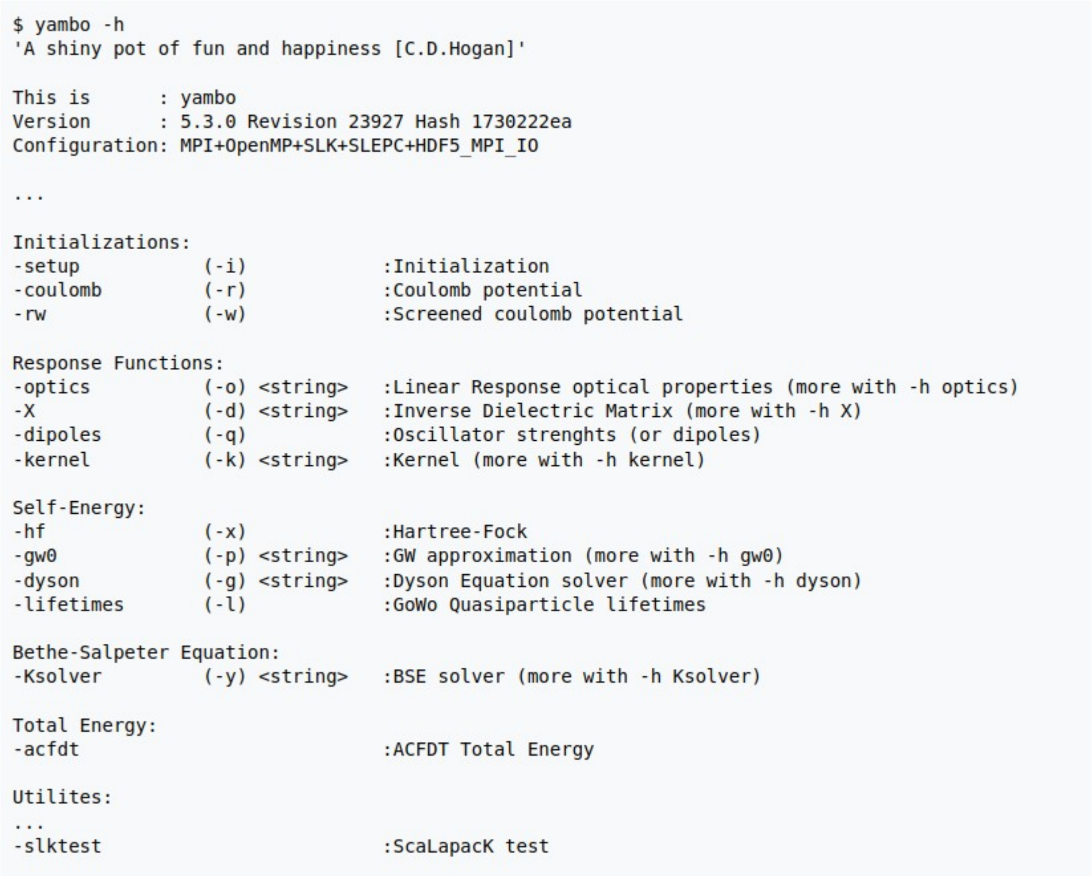
Bethe-Salpeter Equation:
-Ksolver         (-y) <string>   :BSE solver (more with -h Ksolver)

Total Energy:
-acfdt                           :ACFDT Total Energy

Utilites:
...
-slktest                         :ScaLapacK test
```

https://wiki.yambo-code.eu/wiki/index.php?title=First_steps:_walk_through_from_DFT(standalone)

# Input and command line



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Total Energy:
-acfdt                           :ACFDT Total Energy

Utilites:
...
-slktest                         :ScaLapacK test
```

## Linear optics  (IP) – Input generation

```
yambo -F yambo.in_IP -o c
```

## Linear optics  (IP) – Run calculation

```
yambo -F yambo.in_IP
```

https://wiki.yambo-code.eu/wiki/index.php?title=First_steps:_walk_through_from_DFT(standalone)

# Input and command line

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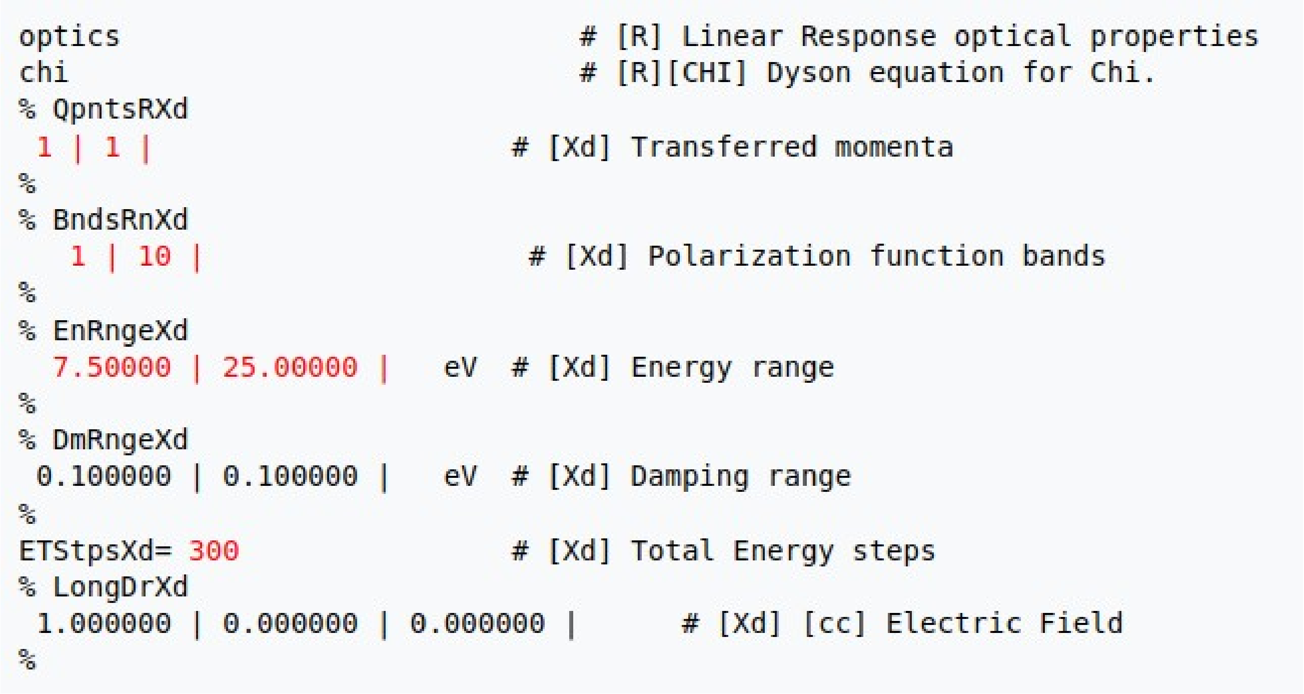
```



```
optics                           # [R] Linear Response optical properties
chi                              # [R][CHI] Dyson equation for Chi.
% QpntsRXd
 1 | 1 |                     # [Xd] Transferred momenta
%
% BndsRnXd
   1 | 10 |                   # [Xd] Polarization function bands
%
% EnRngeXd
  7.50000 | 25.00000 |   eV  # [Xd] Energy range
%
% DmRngeXd
 0.100000 | 0.100000 |   eV  # [Xd] Damping range
%
ETStpsXd= 300                # [Xd] Total Energy steps
% LongDrXd
 1.000000 | 0.000000 | 0.000000 |      # [Xd] [cc] Electric Field
%
```

## Linear optics  (IP) – Run calculation

```
yambo -F yambo.in_IP
```

# What you really calculate?

## (1) Linear response (IP/RPA-NLF): `yambo -optics c`

$$\epsilon_{\boxed{\alpha,\alpha}}(\omega) = 1 + \frac{16\pi}{\Omega}\boxed{\sum_{c,v}}\boxed{\sum_{\mathbf{k}}}\frac{1}{E_{c\mathbf{k}}-E_{v\mathbf{k}}}\frac{|\langle v\mathbf{k}|\overset{\text{See (2)}}{\mathbf{p}_\alpha + i[V^{\mathrm{NL}},\mathbf{r}_\alpha]}|c\mathbf{k}\rangle|^2}{(E_{c\mathbf{k}}-E_{v\mathbf{k}})^2-(\boxed{\omega}+\boxed{i\gamma})^2}$$

```
% LongDrXd
 1.000 | 0.000 | 0.000 |
%
```

**E-field direction (for q=0)**

*Vector (cartesian coordinate)*

Refers to first q-point (`QpntsRXd`)

**DFT k-grid**

```
% EnRngeXd
 0.000 | 10.000 | eV
%
ETStpsXd = 100
```

**Energy grid in output**

*Range from 0 to 10 in 100 steps*

```
% BndsRnXd
 1 | 100 |
```

**Bands used (empty & filled)**

*Range from 1 to nbnd*

Reduce range to lower memory. In metals, includes partially filled bands. See also `EhEngyXd (-V all)`

```
% DmRngeXd
 0.1000 | 0.100 | eV
%
```

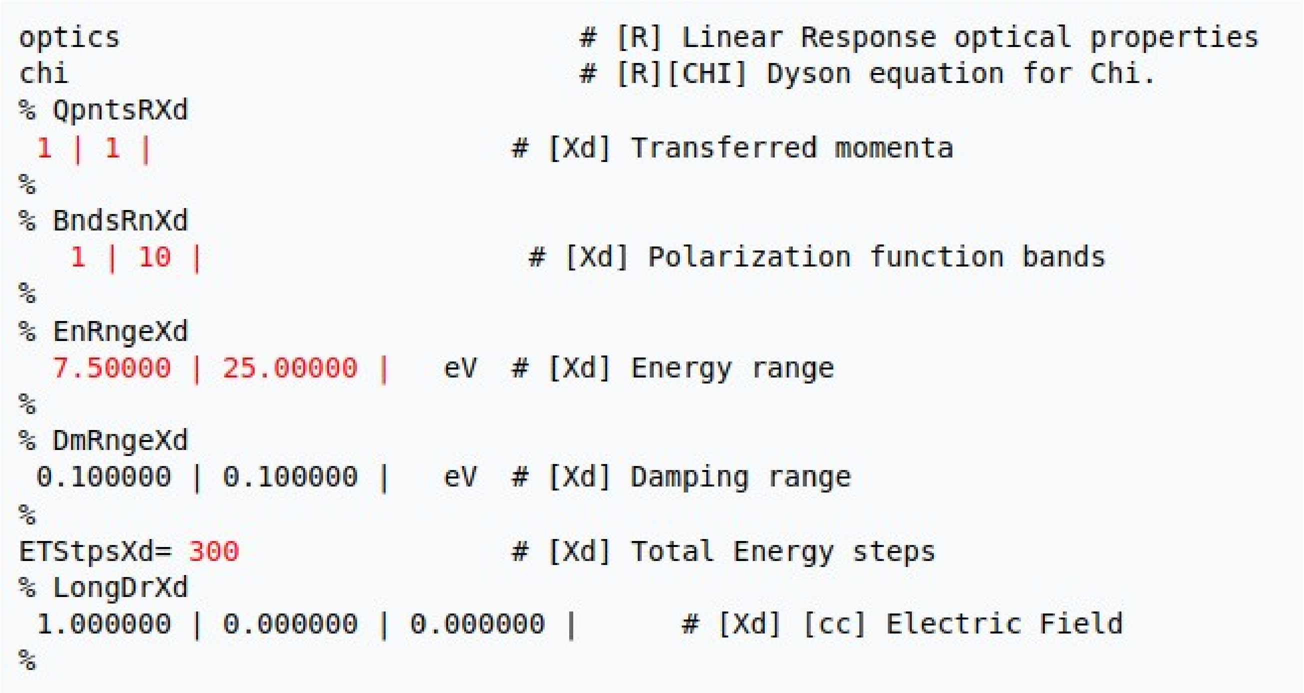
**Broadening of spectra**

*Either a fixed value, or linearly changing between 2 values*

# Input and command line

## Linear optics (IP) – Input generation

```
yambo -F yambo.in_IP -o c
```



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  7.50000 | 25.00000 |   eV  # [Xd] Energy range
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% DmRngeXd
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%
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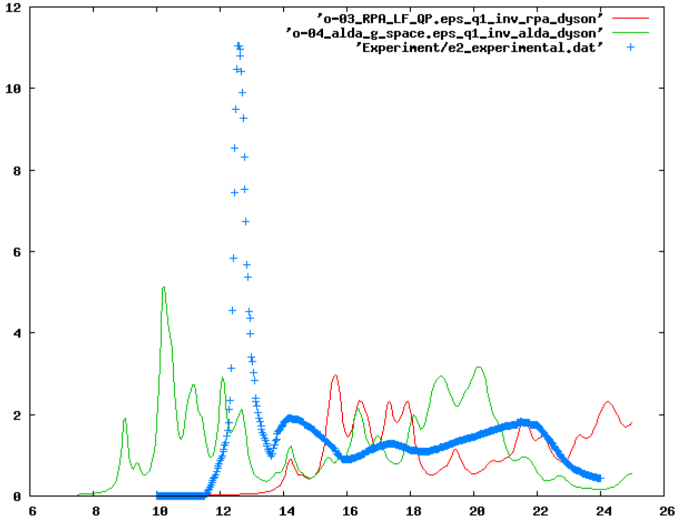
 1.000000 | 0.000000 | 0.000000 |      # [Xd] [cc] Electric Field
%
```

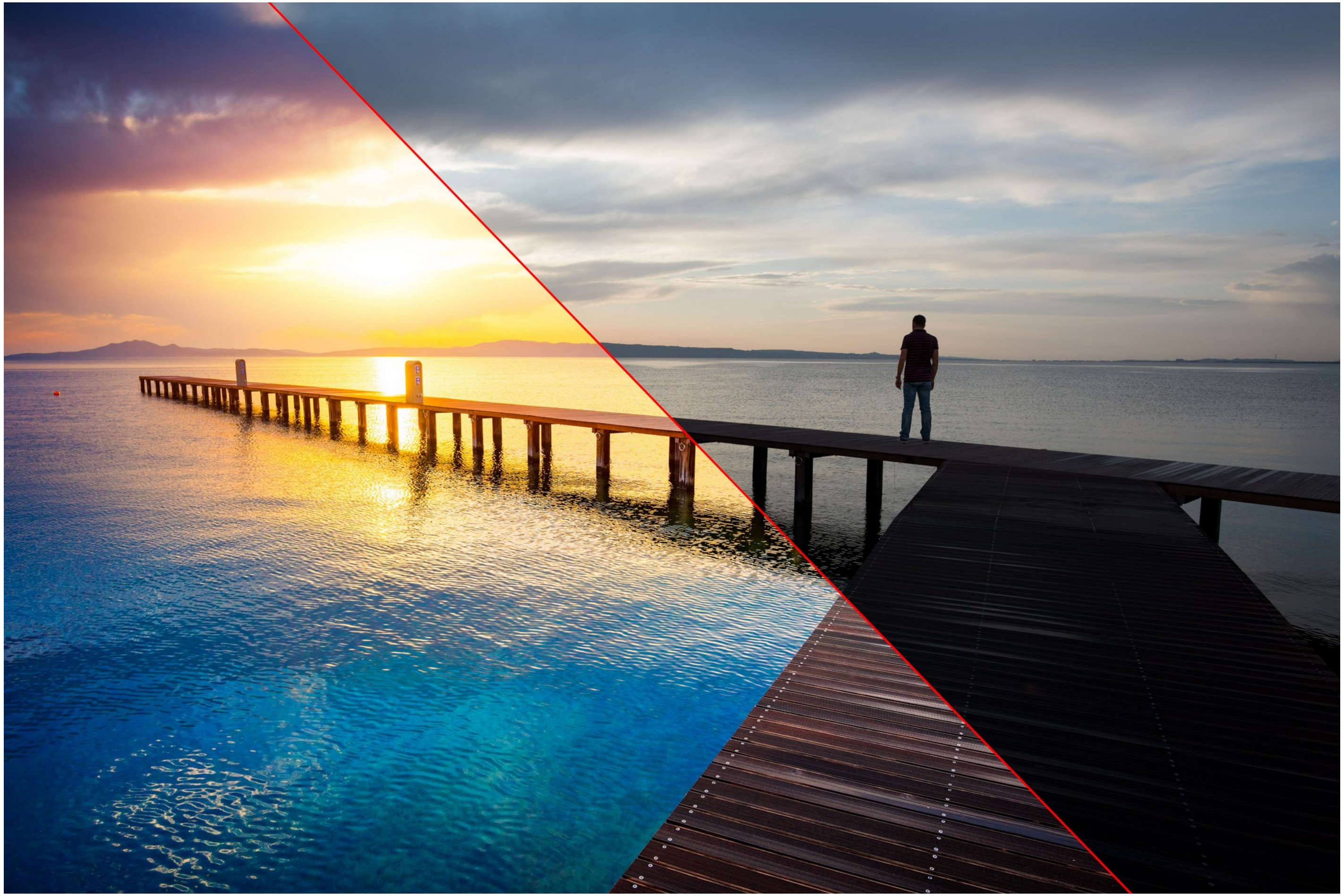


LiF

## Linear optics (IP) – Run calculation

```
yambo -F yambo.in_IP
```

# Post-processing



# YamboPy 1/4

*Yambopy goals:*

- ○ QE and Yambo interface
- ○ Access binary databases
- ○ Scripting
- ○ Pre/Postprocessing
- ○ Plotting
- ○ Workflows
- ○ Aiida plugin
- ○ Utilities
- ○ Quality-of-life tweaks
- ○ *Open to user tinkering*

# YamboPy 1/4

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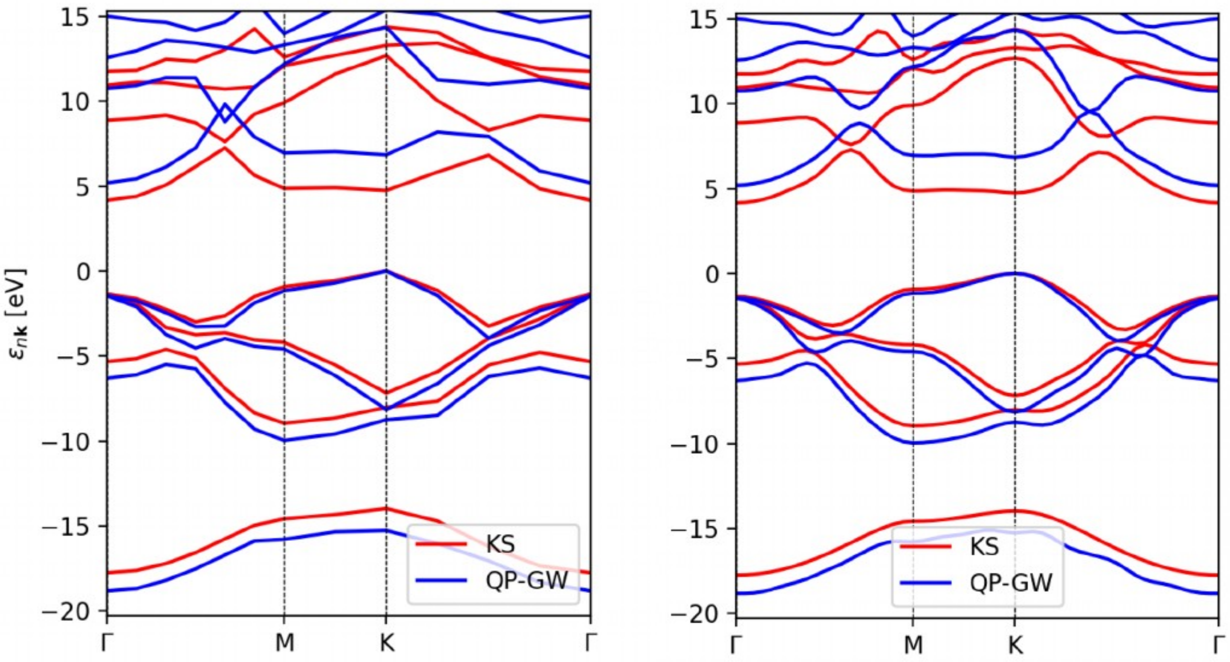
Smooth Fourier interpolation (SKW method) imported from *Abipy*



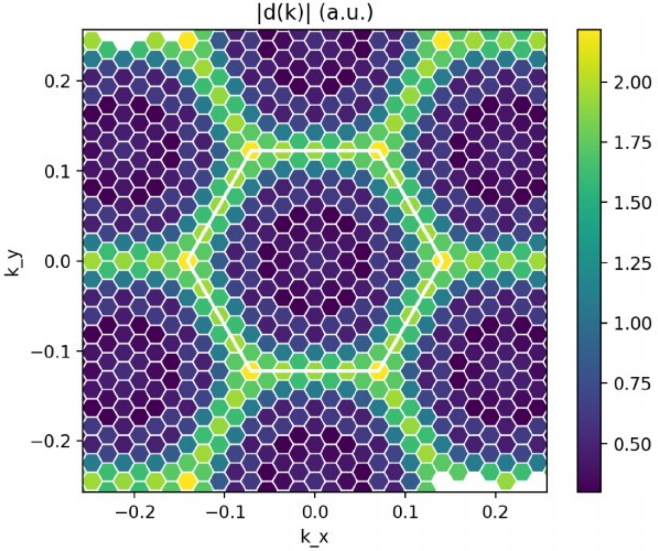
# YamboPy 2/4: visualization

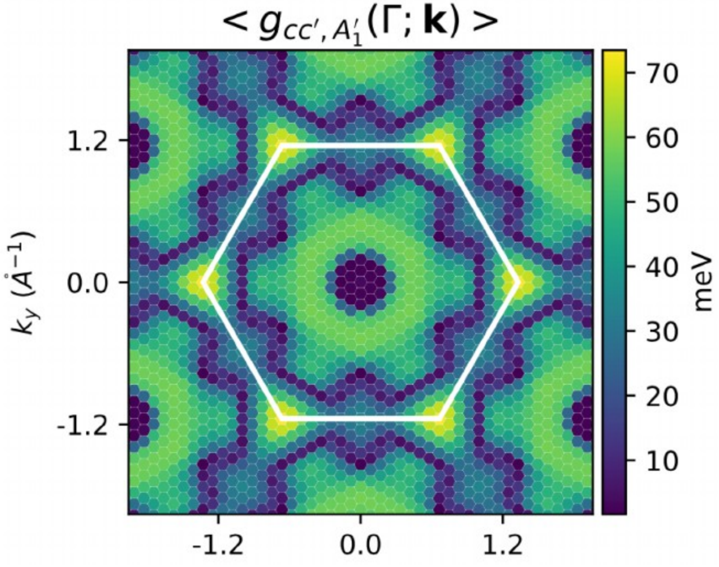
```
from yambopy import YamboDipolesDB
```

```
from yambopy import YamboElectronPhononDB
```

$$d_{cvk} = \langle ck|\epsilon\cdot\hat{\mathbf{r}}|vk\rangle$$

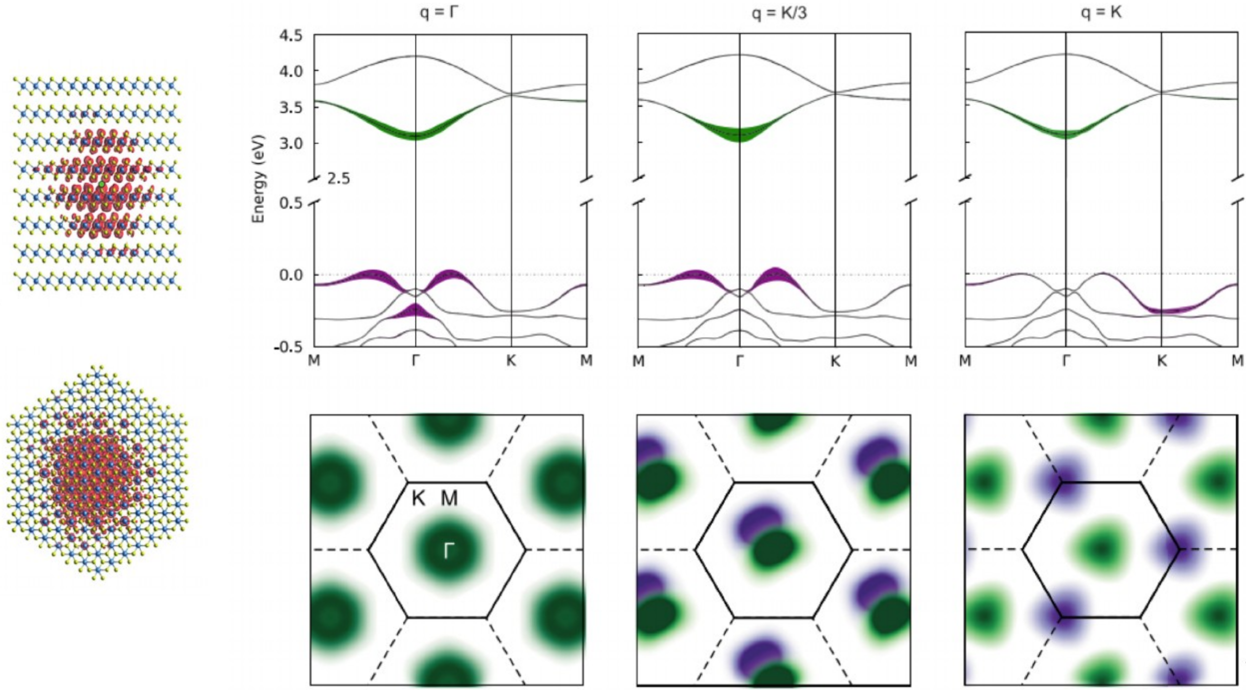
$$g^{\mu}_{cvk}(\mathbf{k},\mathbf{q}) = \frac{1}{\sqrt{2\Omega_{q\mu}}}\langle ck|\partial_{q\mu}V_{\mathrm{SCF}}(\mathbf{q})|vk-q\rangle$$





Monolayer MoS2

# YamboPy 3/4: exciton analysis

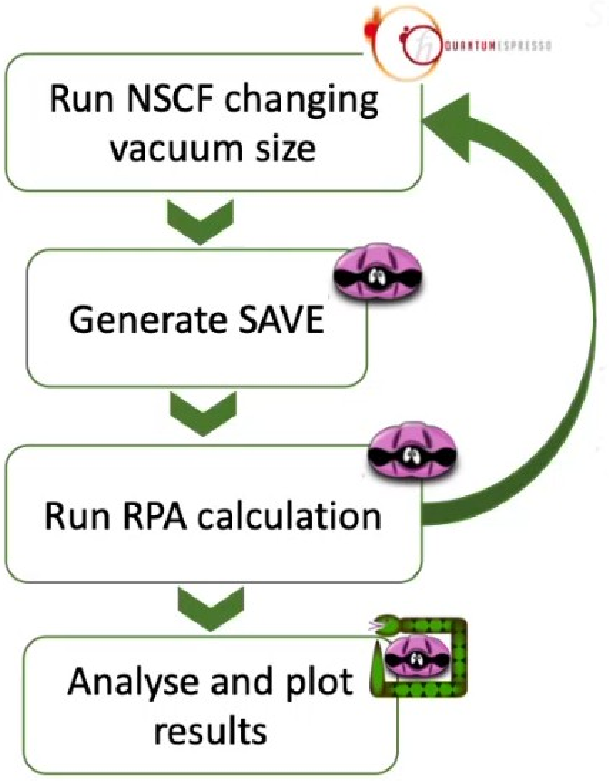


$$E_\alpha(\mathbf{q})$$

$$A_\alpha^{cvk}(\mathbf{q}) = \langle \alpha | (ck) \otimes (vk - q) \rangle$$

Figure on bulk BiI3 by Jorge Cervantes-Villanueva.
PRB **109** 155133 (2024)

# YamboPy 4/4: workflow

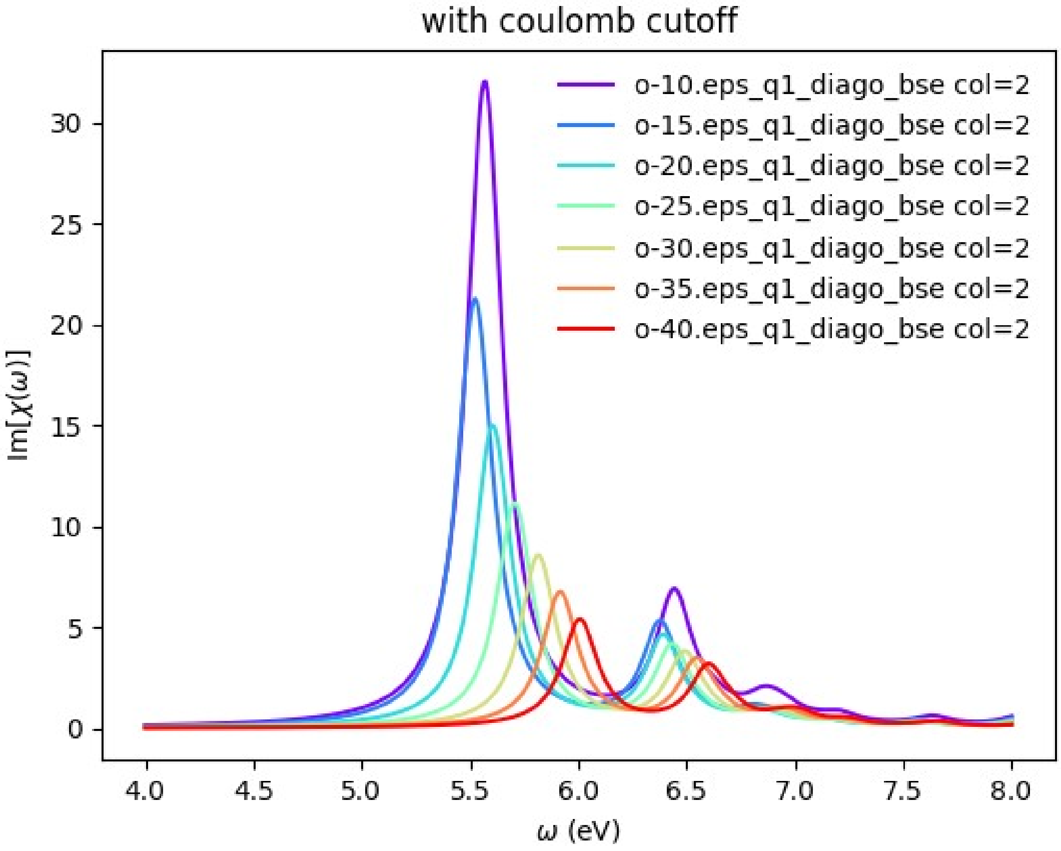


Run NSCF changing vacuum size

Generate SAVE

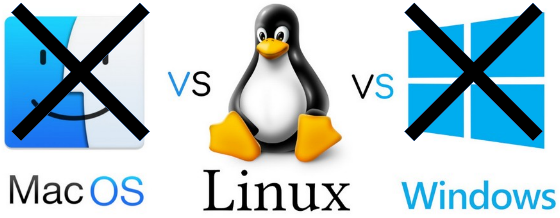
Run RPA calculation

Analyse and plot results



https://www.youtube.com/watch?v=gStCeigSXS0

# Installation



## Required libraries (included in Yambo)

- Lapack/Blas
- NetCDF (to be removed soon)
- HDF5

## Optional libraries

- Scalapack
- Slepc/Petsc
- Yaml/Magma etc….

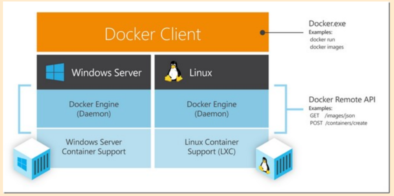
## Installation instructions

Spack

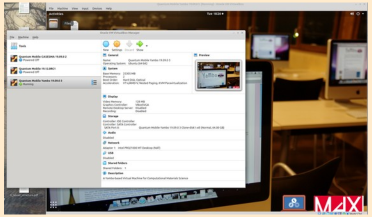
- Linux Ubuntu/LinuxMint
  (gfortran| intel | nvdia)
- MacOSX (ARM)
- Machine specific (Leonardo, Irene,..)

## Virtual Machines

Docker



VirtualBox



# Thank you for your attention

https://www.yambo-code.eu/

https://wiki.yambo-code.eu/wiki/index.php/Main_Page

https://www.youtube.com/@yambocode2721

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A short text to describe your forum

It is currently Tue Jan 15, 2013 3:54 pm

[ Moderator Control Panel ]

Last visit was: Mon Jan 14, 2013 8:00 pm

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|---|---|---|---|
| Your first forum<br>Description of your first forum. | 2 | 4 | by Bob<br>Mon Jan 14, 2013 3:48 pm |
| My New Forum | 2 | 1 | by Jane<br>Mon Jan 14, 2013 6:11 pm |

https://www.yambo-code.eu/forum/