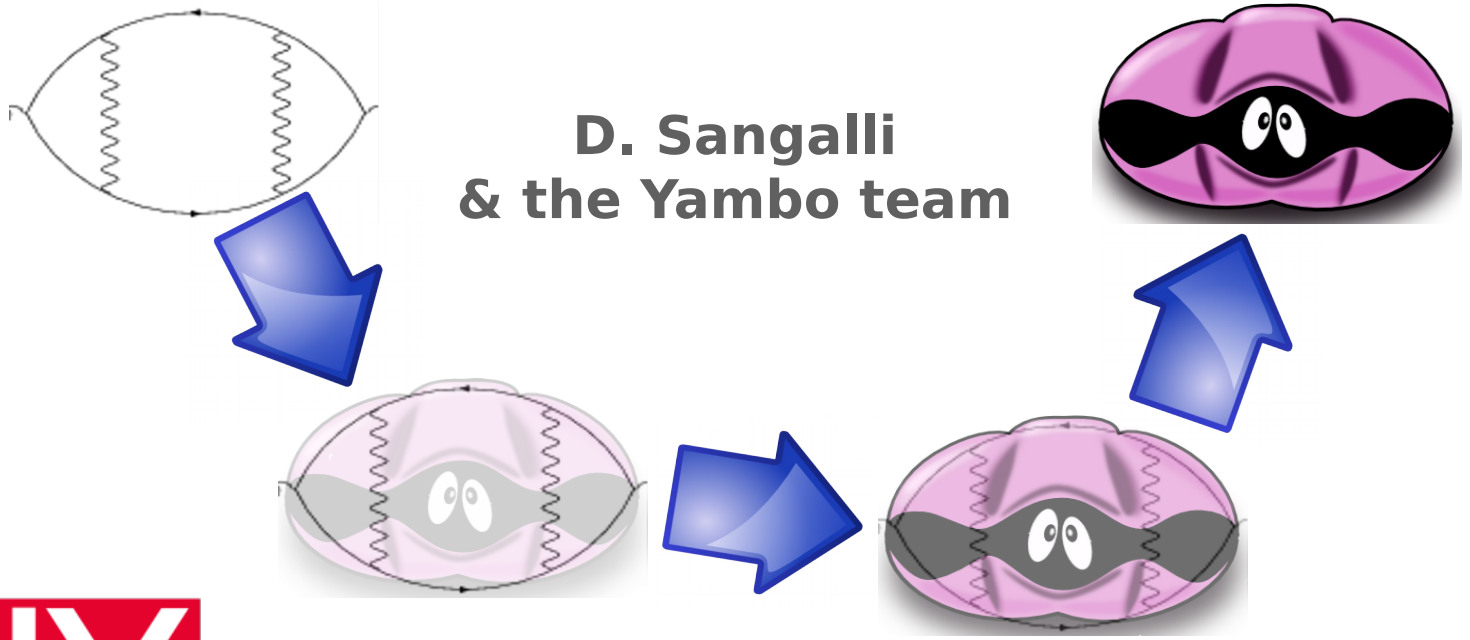
CNR
Istituto di Struttura
della Materia

CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy

Introduction to the Yambo code: Past, present and future

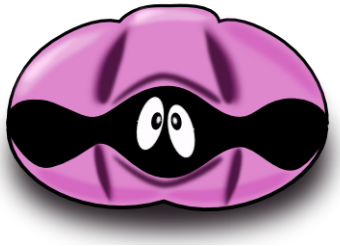


D. Sangalli
& the Yambo team

MAX

Bologna
4th Dec 2017

Yambo©



- 11.00-11.45 Introduction to the Yambo code: Past, Present and Future (D. Sangalli)
- [2] 11:45-12:30 Theoretical spectroscopy: GW and ARPES (A. Ferretti)
- [3] 14.00-14.45 Yambo parallelization: strategies & performances (Sangalli)
- [4] 14:45-15:30 HPC use cases: electronic and optical properties of gaphene nano-ribbons (A. Ferretti)

outline

- A bit of history
- The code: **the structure of yambo**
- Applications: **few examples**
- Users view: **how it works in practice**
- Future: **new developments and more**

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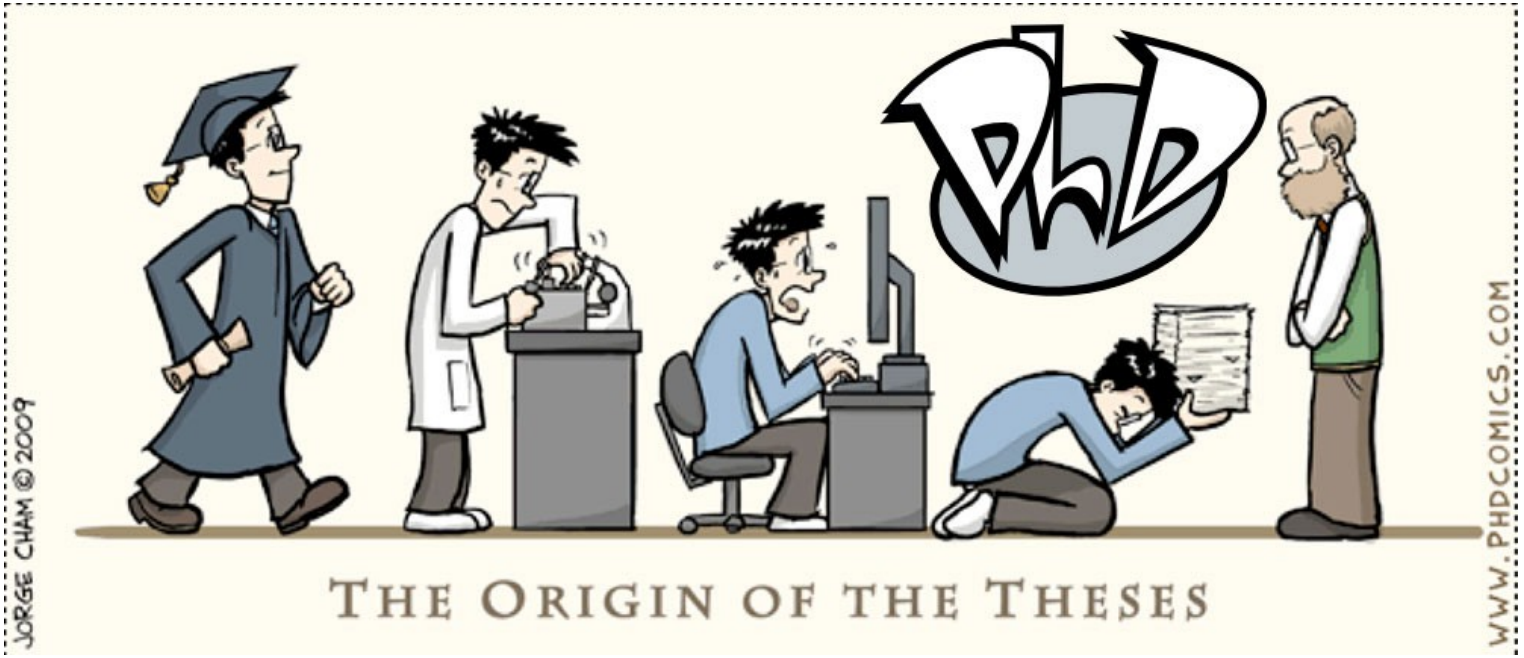
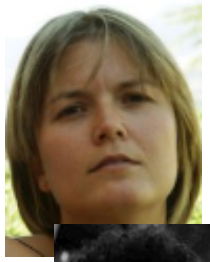
A bit of history



A bit of history

GW

Excitons



Lifetimes
TDDFT
DFT
(Orbital functionals)

Electron-Phonon

Iterative solvers

Magnetic properties
Time-Dependent phenomena
Total Energy
Collinear and non collinear spin support

.. and many more developers

Yambo: an ab initio tool for excited state calculations,
A. Marini, C. Hogan, M. Grüning, D. Varsano,
Comp. Phys. Comm. 180, 1392 (2009).

A new paper coming soon ...

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What is yambo ?

Interfaces

Planewave
Pseudopotential codes:

abinit.org

PWscf

www.yambo-code.org

What is yambo ?

Theory

Many-Body perturbation Theory

Time-dependent density functional theory

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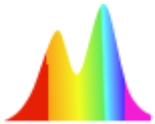
Different projects

Developers

What can yambo do ?

Properties

GPL



Quasi-particles
Optical absorption
Electron energy loss
Magneto optical properties
Electron-phonon coupling
Surface spectroscopy

DEVELOPMENT / PRE-GPL

Out of equilibrium dynamics
Multi-level parallelization

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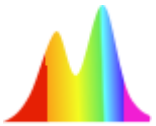

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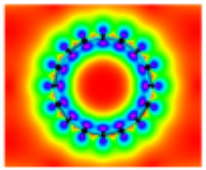

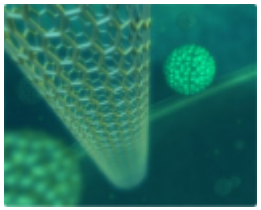

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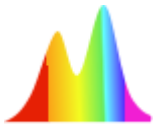

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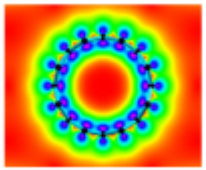
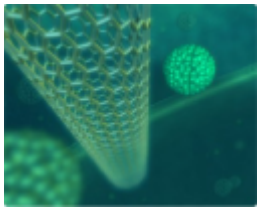
Community & Publications

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

www.yambo-code.org

Applications





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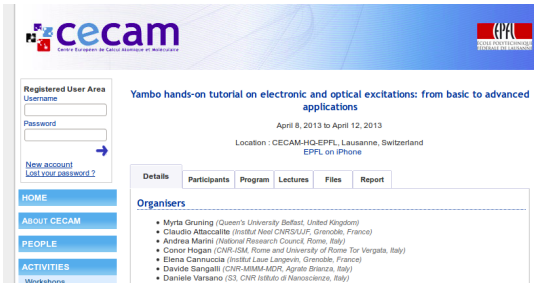
Schools



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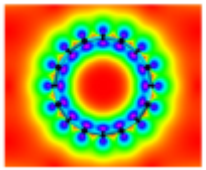
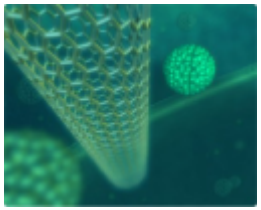
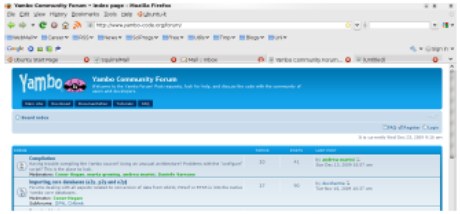


Support & reach out

Git repository

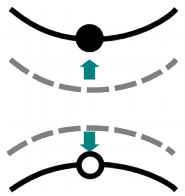


Dedicated User Forum

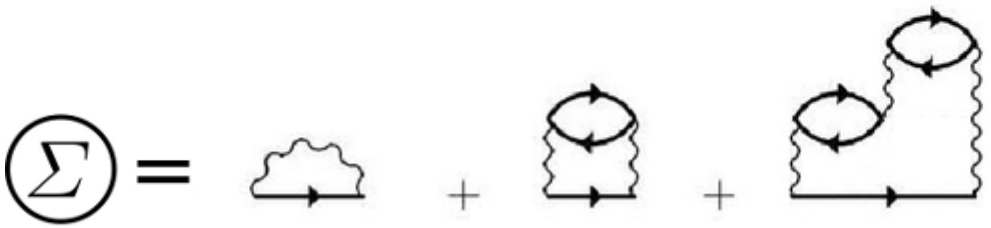
Online documentation and tutorials

Basic ingredients

Quasi-Particle energies (HF, Cohsex, GW)



$$\epsilon_{nk}^{QP} = \epsilon_{nk}^{KS} + \langle \psi_{nk} | \Sigma(\epsilon_{nk}^{QP}) - V_{xc} | \psi_{nk} \rangle$$



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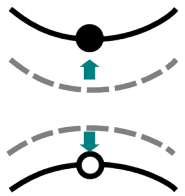
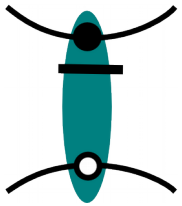


Absorption spectra (TDDFT, TDHF, BSE)

$$\epsilon(\omega) \propto \sum_I \sum_{nm,n'm'} \sum_{kk'} \frac{\left(x_{nmk} A^I_{nmk}\right)\left(A^I_{m'n'k'} x_{n'm'k'}\right)^*}{\omega - \omega_I + i\,\eta}$$



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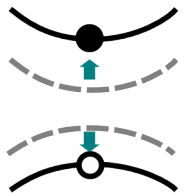

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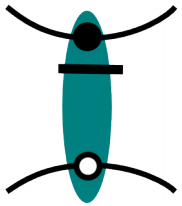
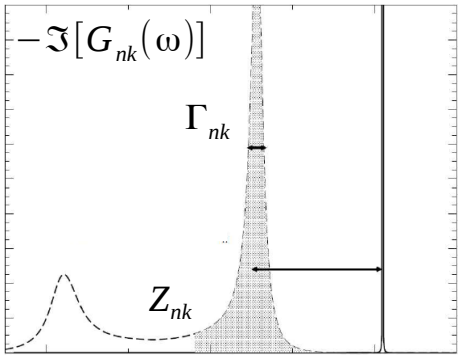


More: QP lifetimes and QP weights, Satellites

$$\Gamma_{nk} = \Im[\Sigma_{nk}] \qquad Z_{nk} = [1 - \frac{\partial \Sigma_{nk}(\omega)}{\partial \omega}]^{-1}$$

$$\Im[G_{nk}(\omega)] = \Im[G^0_{nk}(\omega) - \Sigma_{nk}(\omega)]^{-1}$$



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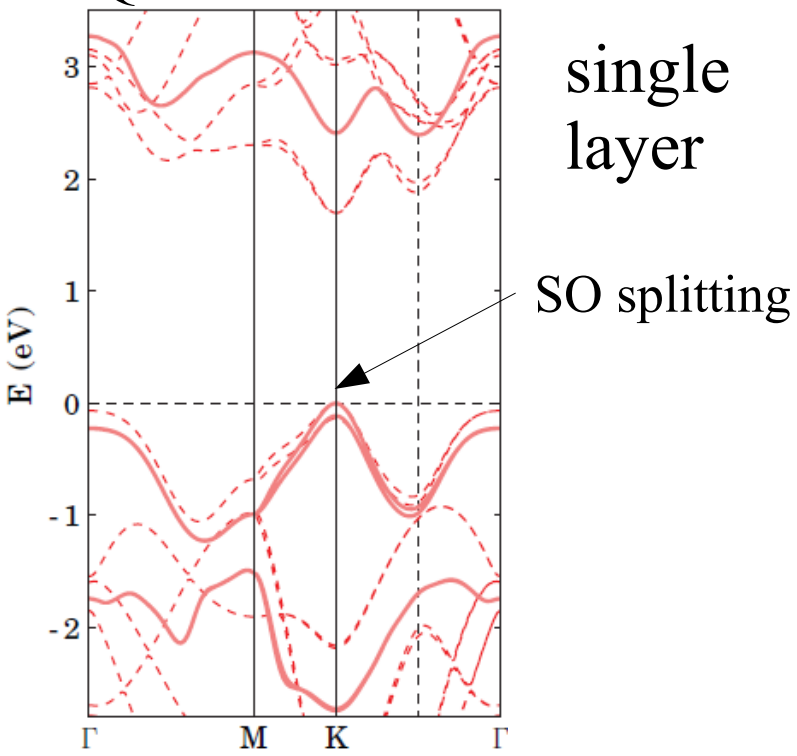
QP and BSE with SOC

PHYSICAL REVIEW B **88**, 045412 (2013)

Effect of spin-orbit interaction on the optical spectra of single-layer, double-layer, and bulk MoS_2

Alejandro Molina-Sánchez,[1,2] Davide Sangalli,[3] Kerstin Hummer,[4] Andrea Marini,[3] and Ludger Wirtz[1,2]

QP corrections



single layer

SO splitting

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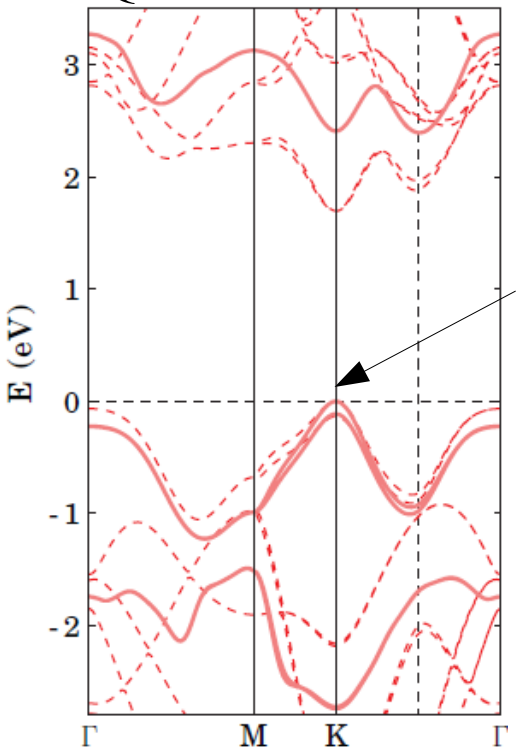
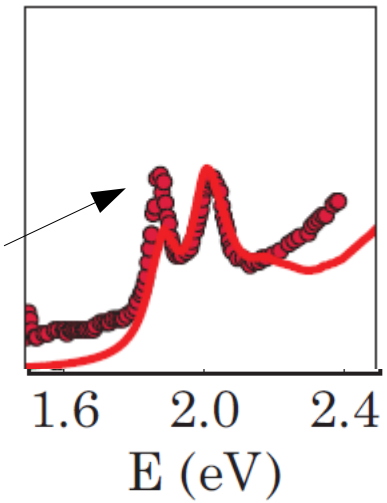


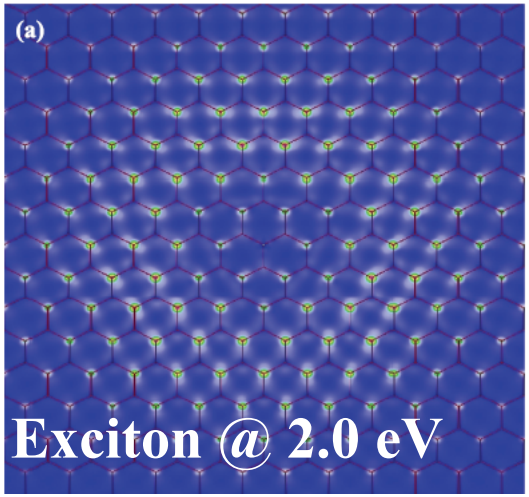
single layer

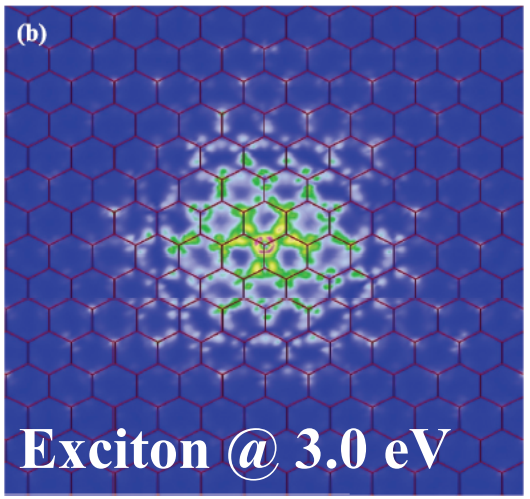
SO splitting ~ 0.15 eV

BSE spectrum



Only available code able to do MBPT with full SOC (i.e. non perturbative)





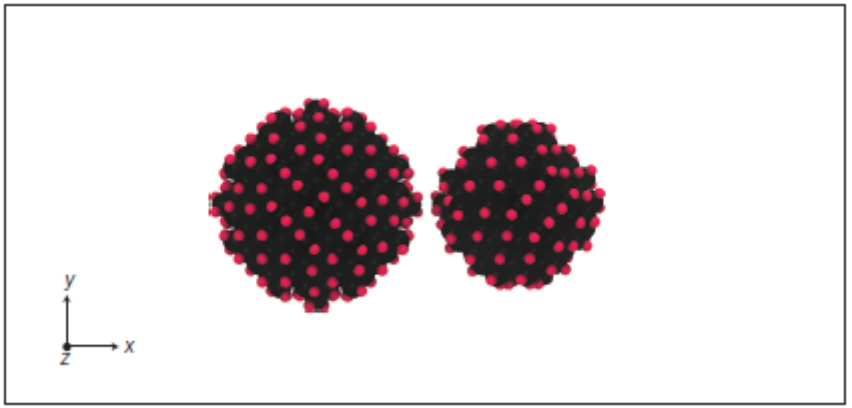
Lifetimes in nanostructures

ARTICLES
PUBLISHED ONLINE: 9 SEPTEMBER 2012 | DOI: 10.1038/NPHOTON.2012.206
nature photonics

Silicon Nano-Crystals
440 Si atoms + 272 H atomsc

Carrier multiplication between interacting nanocrystals for fostering silicon-based photovoltaics

Marco Govoni[1]*, Ivan Marri[2]* and Stefano Ossicini[2,3]



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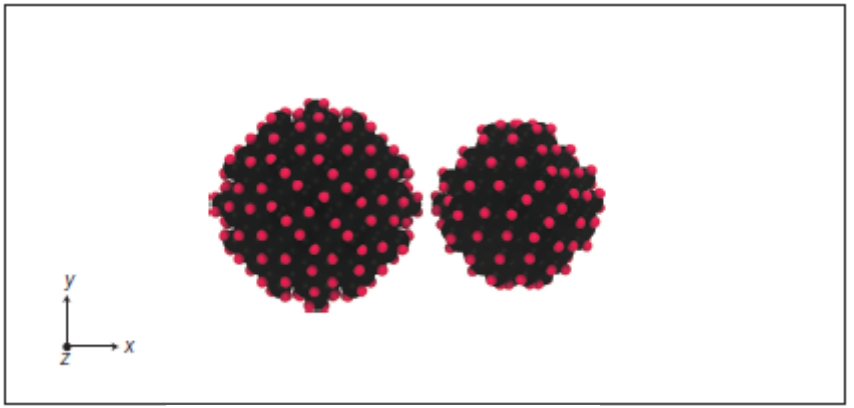

Carrier multiplication between interacting nanocrystals for fostering silicon-based photovoltaics

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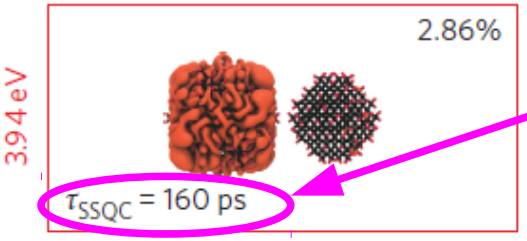
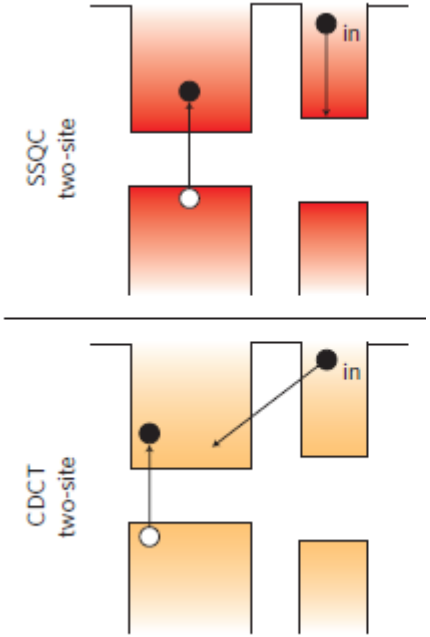


Carriers multiplications lifetimes



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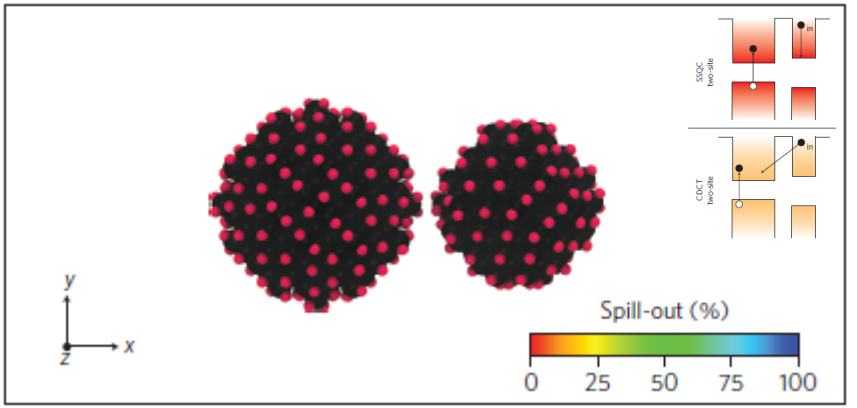

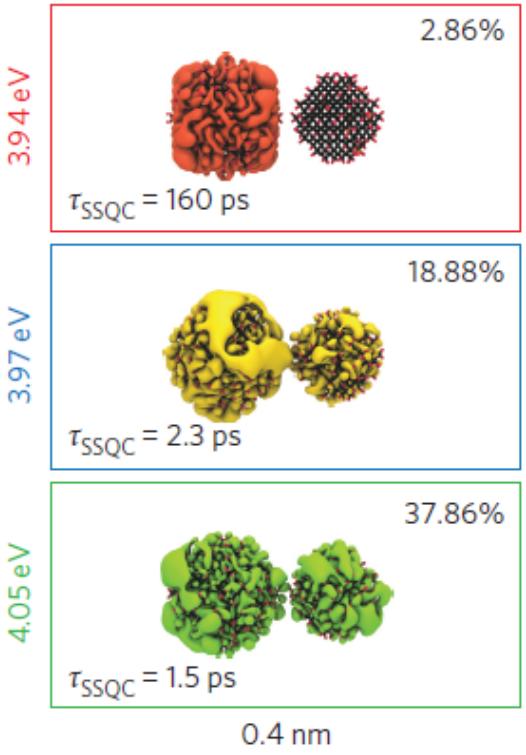

Carriers multiplications lifetimes

As a function of energy

Lifetimes in nanostructures

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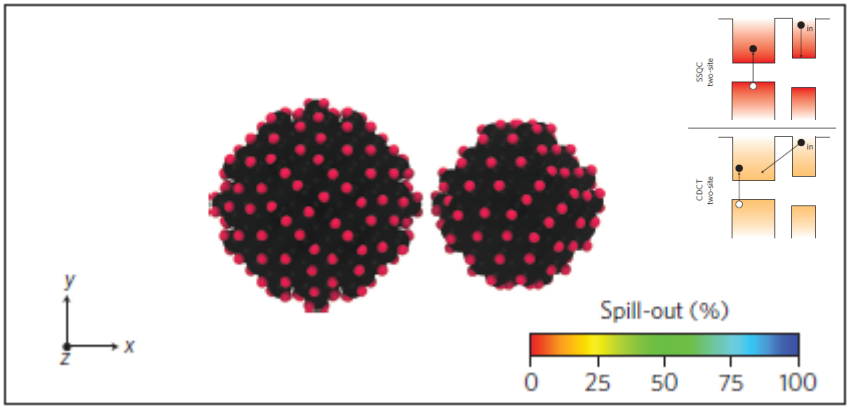
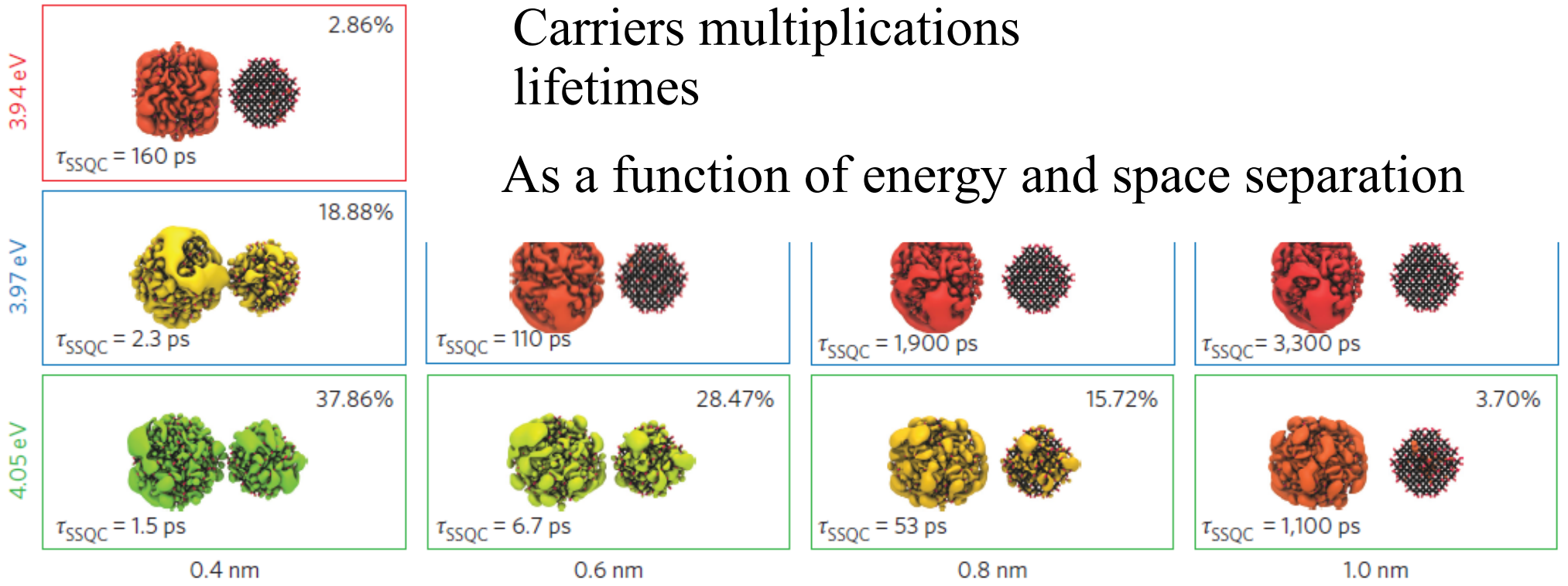
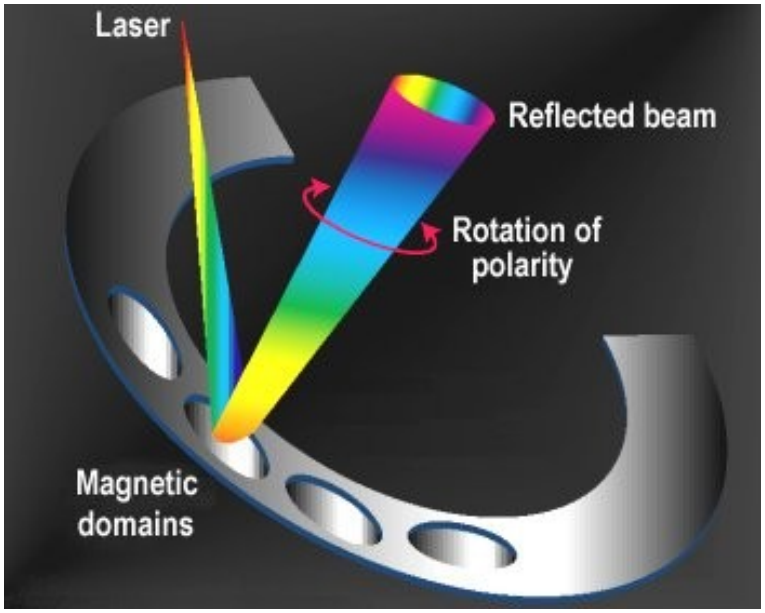


Carriers multiplications
lifetimes

As a function of energy and space separation



More: magneto-optics

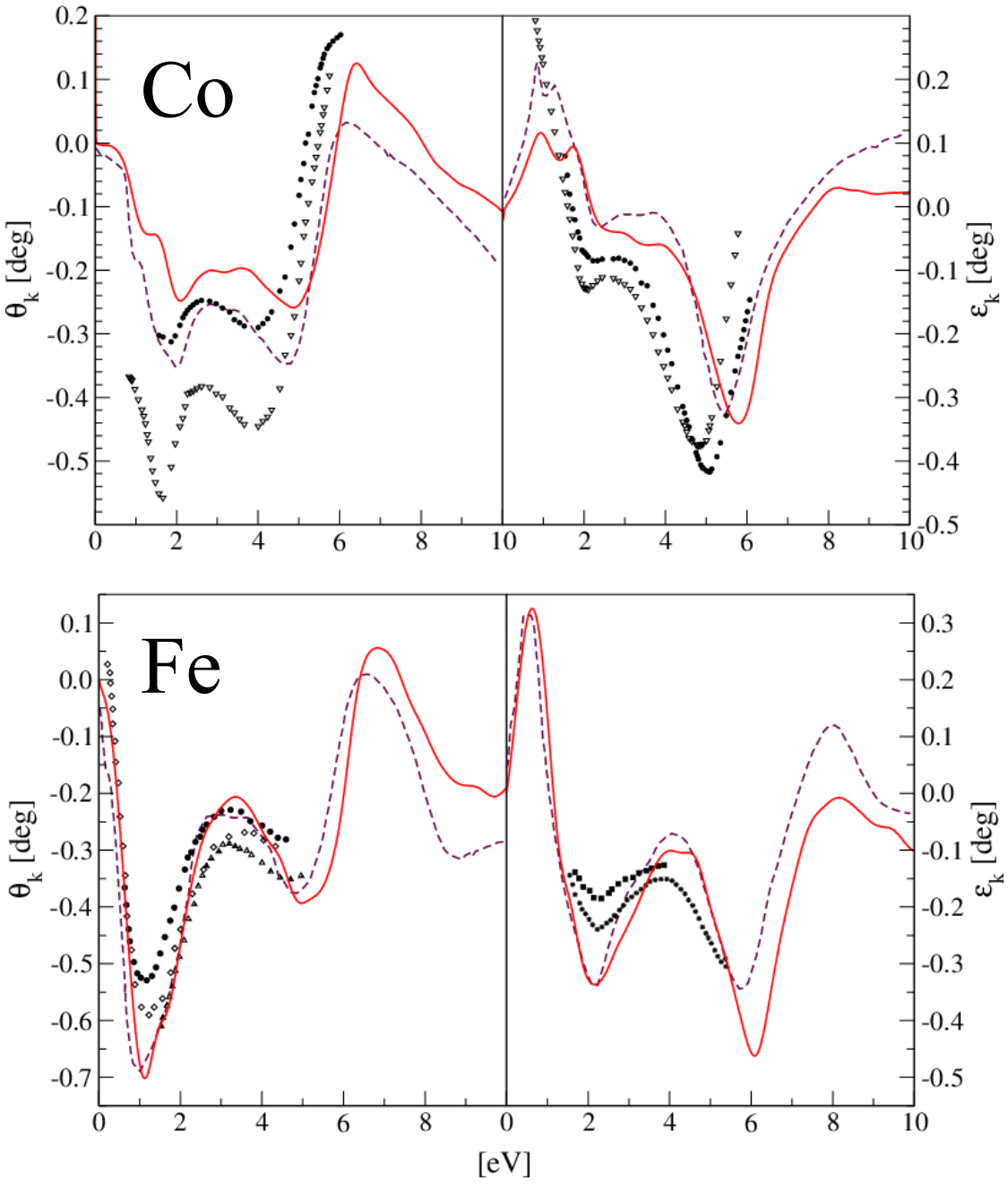


D. Sangalli et al. Phys. Rev. **B 86**, 125139 (2012)

Need the off-diagonal dielectric function

$$\epsilon_{\pm}(\omega) = \epsilon_{xx}(\omega) \pm i\epsilon_{xy}(\omega)$$

Needs to fully account for the spinorial wave-functions



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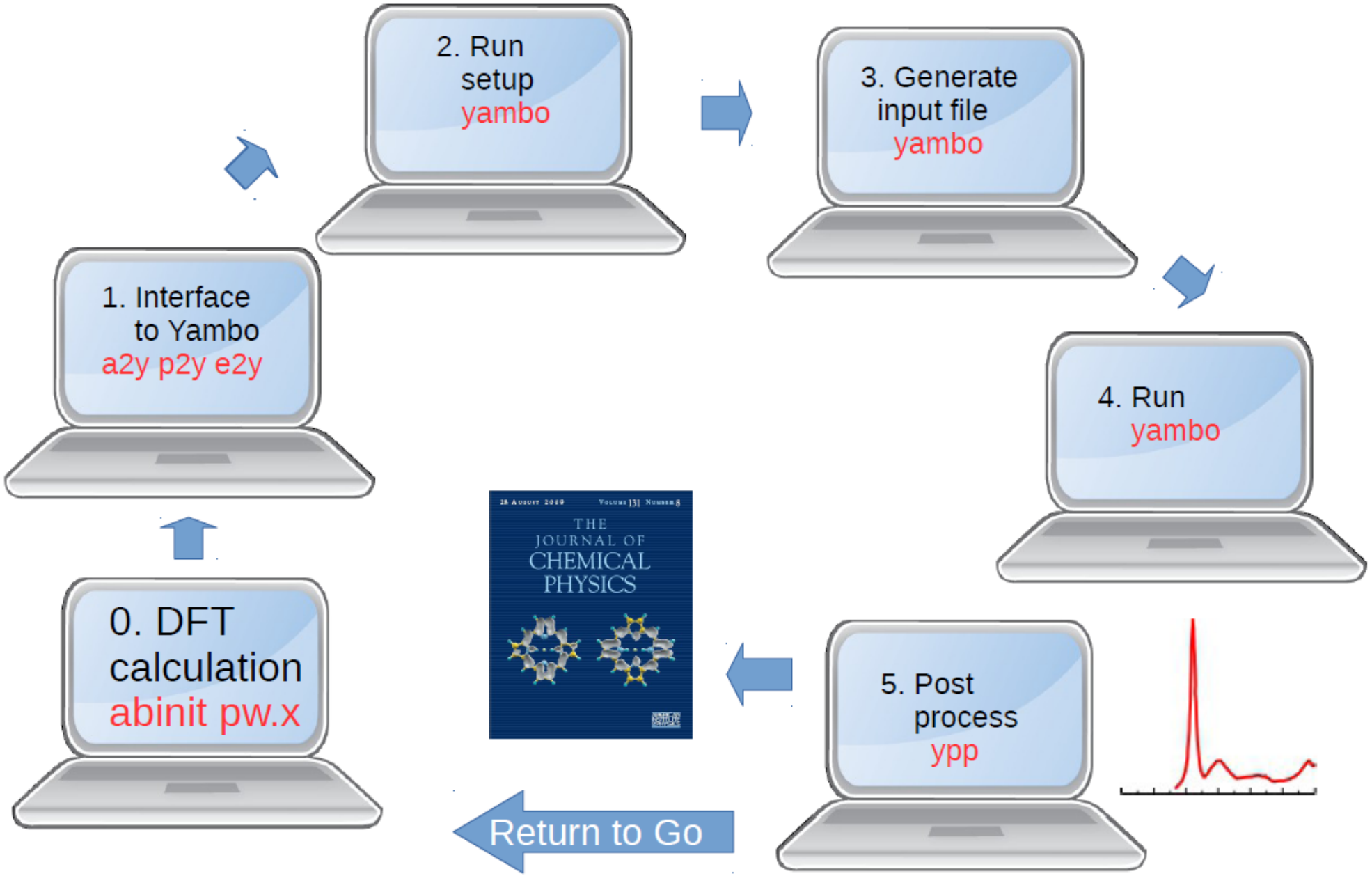
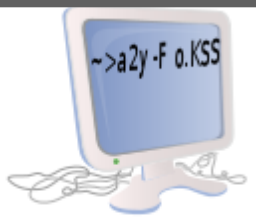
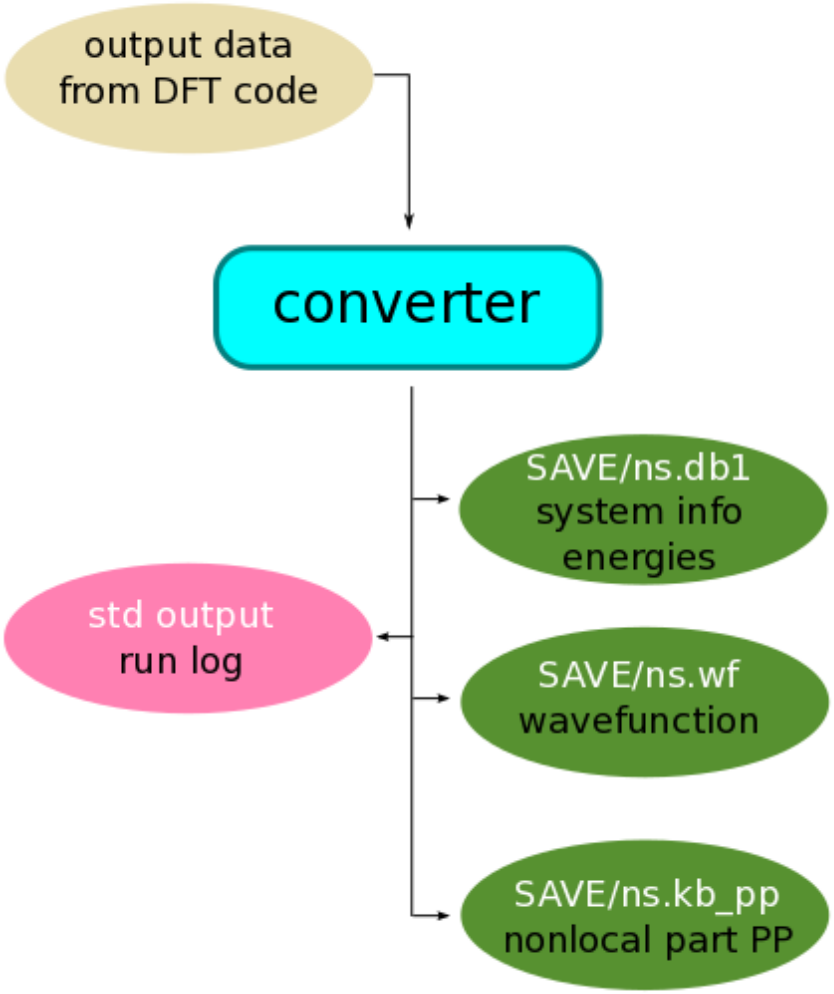
How it works


2. Run
setup
yambo
3. Generate
input file
yambo
1. Interface
to Yambo
a2y p2y e2y
4. Run
yambo
THE
JOURNAL OF
CHEMICAL
PHYSICS
0. DFT
calculation
abinit pw.x
5. Post
process
ypp
Return to Go

How it works



1. Generate the core databases



example: convert abinit KSS file with a2y

```
% ls
3D_LiF_o_DS2_KSS
```

```
% a2y -F 3D_LiF_o_DS2_KSS

 <---> [01] A(binit) 2 Y(ambo)
 <---> Checking input file ...3D_LiF_o_DS2_KSS
 <---> DBs path set to :.
 <---> KSS Header...abinit version 5.8.4
 <---> :: Atoms positions...done
 <---> Symmetries...[ID yes]...[INV no]...[TR yes]...[SI yes]
 <---> RL vectors...done
 <---> Energies...done
 <---> Report:
 <--->  :: Electrons            : 8.000000
 <--->  :: Temperature      [ev]: 0.000000
 <--->  :: Lattice factors [a.u.]: 7.703475  7.703475  7.703475
 <--->  :: K-points             : 10
 <--->  :: Bands                : 10
 <--->  :: Spinor components    : 1
 <--->  :: Spin polarizations   : 1
 <--->  :: Spin orbit coupling  : no
 <--->  :: Symmetries   [spatial]: 24
 <--->  ::              [T-rev]: yes
 <--->  :: Max WF components    : 1885
 <--->  :: RL vectors       (WF): 1885
 <--->  :: RL vectors    (CHARGE): 1885
 <--->  :: XC potential         : Perdew & Wang (xc)
 <--->  :: Atomic species       : 2
 <--->  :: Max atoms/species    : 1
 <---> == DB1 ...done ==
 <---> == DB2 + nlPP ...done ==
```

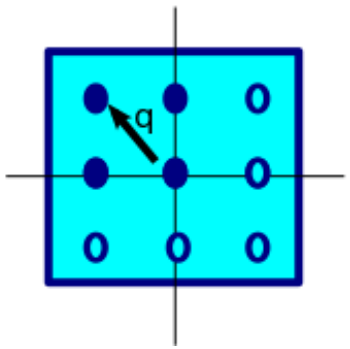
```
% ls SAVE
ns.db1        ns.kb_pp      ns.wf
```

How it works

2. Run setup

= prepare general purpose databases for later use

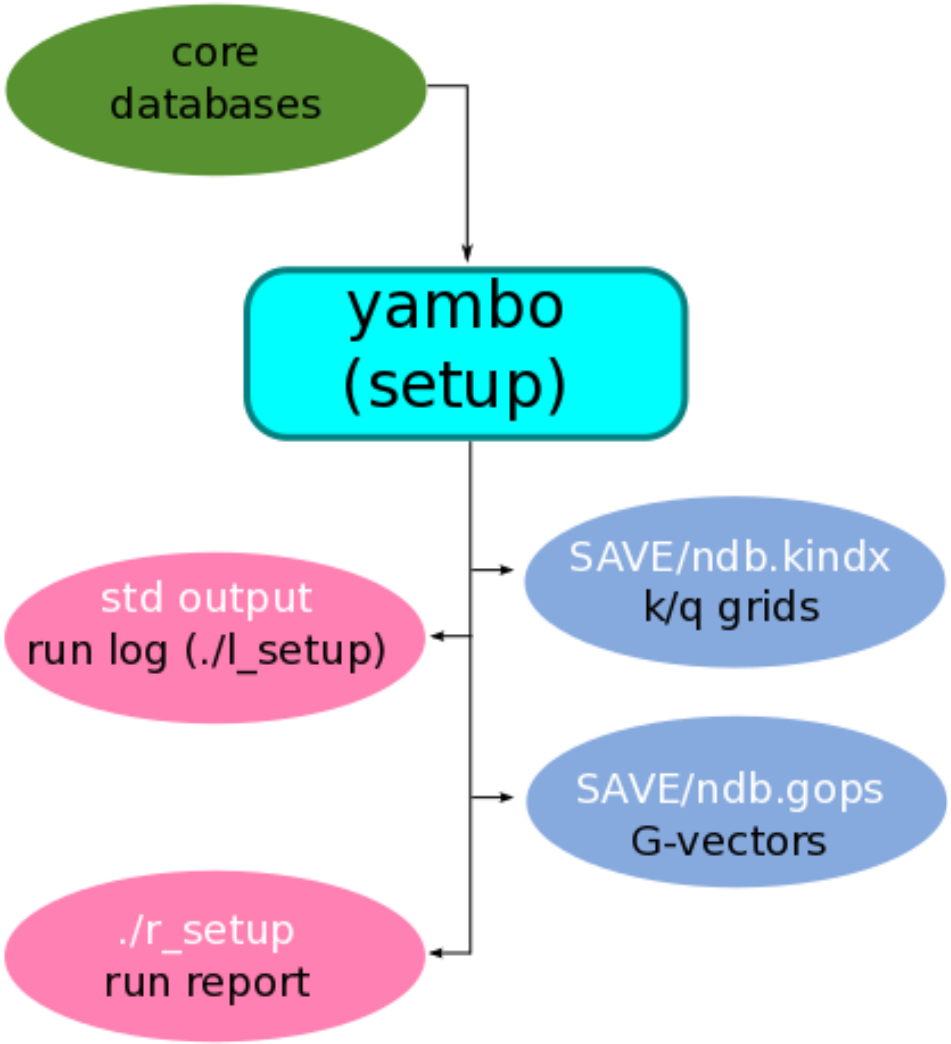
* **Data initialization:**
reorders G-vectors into spherical shells
calculates Fermi level and electronic occupations
sets up energy grids



* **Brillouin-zone sampling:**
expands k-points to full BZ
generates q-point meshes
checks on uniformity of grids

How it works

2. Run setup



example: setup run

```
% ls SAVE/
ns.db1  ns.kb_pp  ns.wf
```

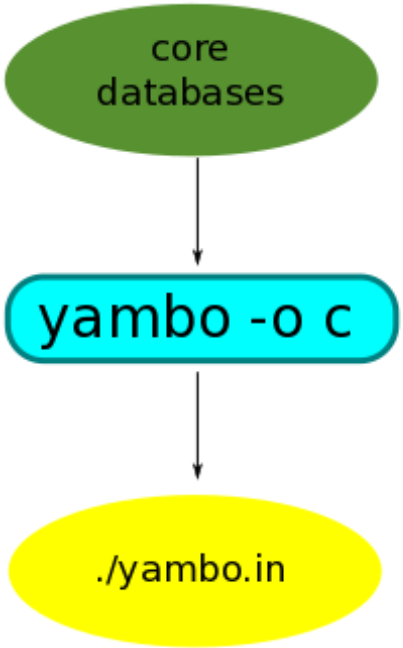
```
% yambo

 <---> [01] Job Setup
 <---> [02] Input variables setup
 <---> [02.01] Unit cells
 <---> [02.02] Symmetries
 <---> [02.03] RL shells
 <---> Shells finder |####################| [100%] --(E) --(X)
 <---> [02.04] K-grid lattice
 <---> [02.05] Energies [ev] & Occupations
 <---> [03] Transferred momenta grid
 <---> X indexes |####################| [100%] --(E) --(X)
 <---> SE indexes |####################| [100%] --(E) --(X)
 <---> [04] Game Over & Game summary
```

```
% ls
r_setup  SAVE
% ls SAVE
ndb.gops  ndb.kindx  ns.db1  ns.kb_pp  ns.wf
```

How it works

3. Generate input file

example: linear response (rpa level)



directly open in editor

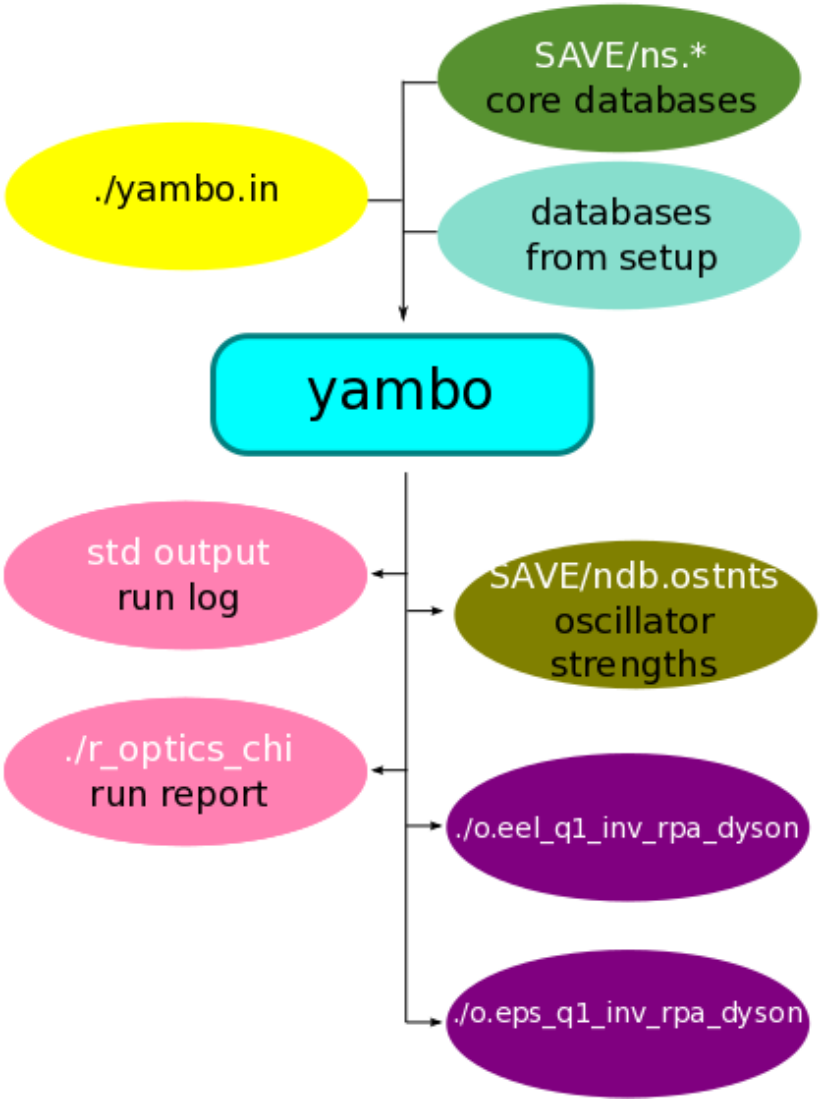
```
optics                  # [R OPT] Optics
chi                     # [R CHI] Dyson equation for Chi.
% QpntsRXd
 1 | 19 |               # [Xd] Transferred momenta
%
% BndsRnXd
 1 | 10 |               # [Xd] Polarization function bands
%
NGsBlkXd= 1             RL  # [Xd] Response block size
% EnRngeXd
 0.00000 | 10.00000 |   eV  # [Xd] Energy range
%
% DmRngeXd
 0.10000 |  0.10000 |   eV  # [Xd] Damping range
%
ETStpsXd= 100               # [Xd] Total Energy steps
% LongDrXd
 1.000000 | 0.000000 | 0.000000 |     # [Xd] [cc] Electric Field
%
```

runlevels

default values from existing databases (compatibility)

How it works

4. Run yambo



example: linear response (RPA)

```
% ls
r_setup  SAVE  yambo.in
```

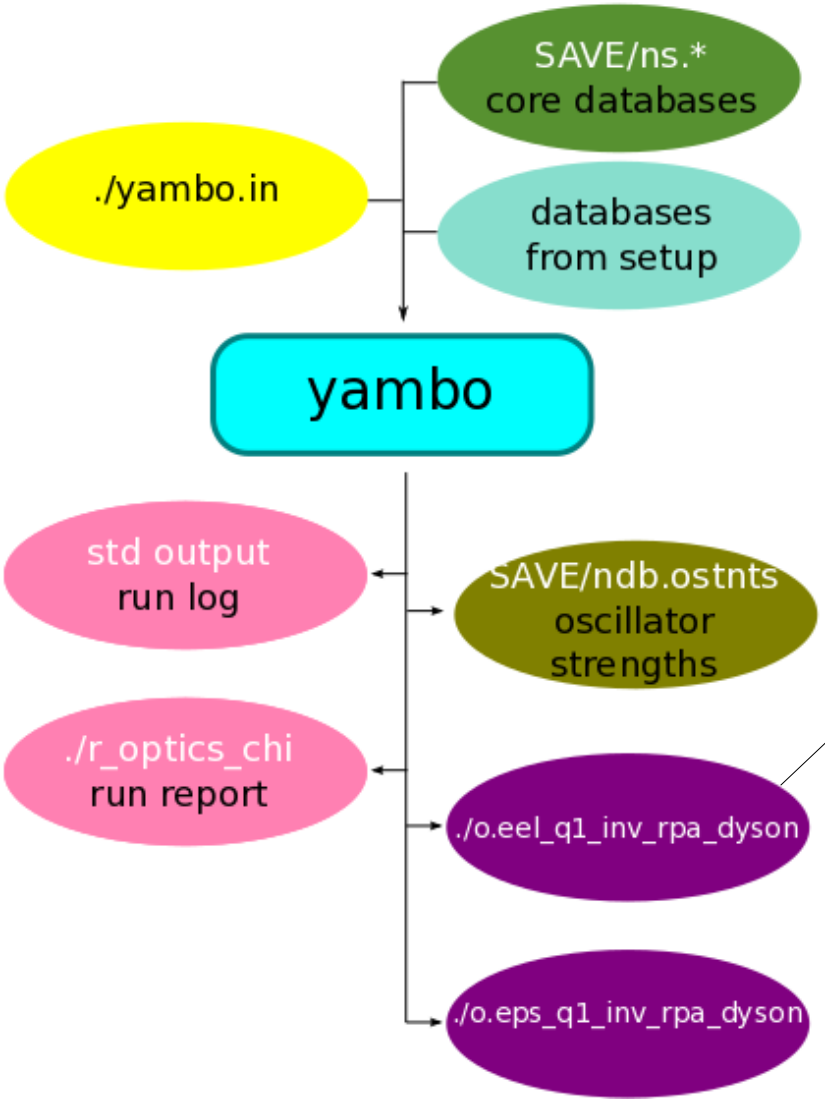
```
% yambo

 <---> [01] Job Setup
 <---> [02] CORE Variables Setup
 <---> [02.01] Unit cells
 <---> [02.02] Symmetries
 <---> [02.03] RL shells
 <---> [02.04] K-grid lattice
 <---> [02.05] Energies [ev] & Occupations
 <---> [03] Transferred momenta grid
 <---> [04] Optics
 <---> [WF-Oscillators/G space loader] Wfs (re)loading | [...]
 <---> Dipole (T): |####################| [100%] --(E) --(X)
 <---> [FFT-X] Mesh size: 18  18  18
 <---> [WF-X loader] Wfs (re)loading |#####| [100%] --(E) --(X)
 <---> [X-CG] R(p) Tot o/o(of R)  :   222   6144    100
 <---> [X] Upper matrix triangle filled
 <---> Xo@q[1] 1-100 |####################| [100%] --(E) --(X)
 <---> X @q[1] 1-100 |####################| [100%] --(E) --(X)
 <---> [05] Game Over & Game summary
```

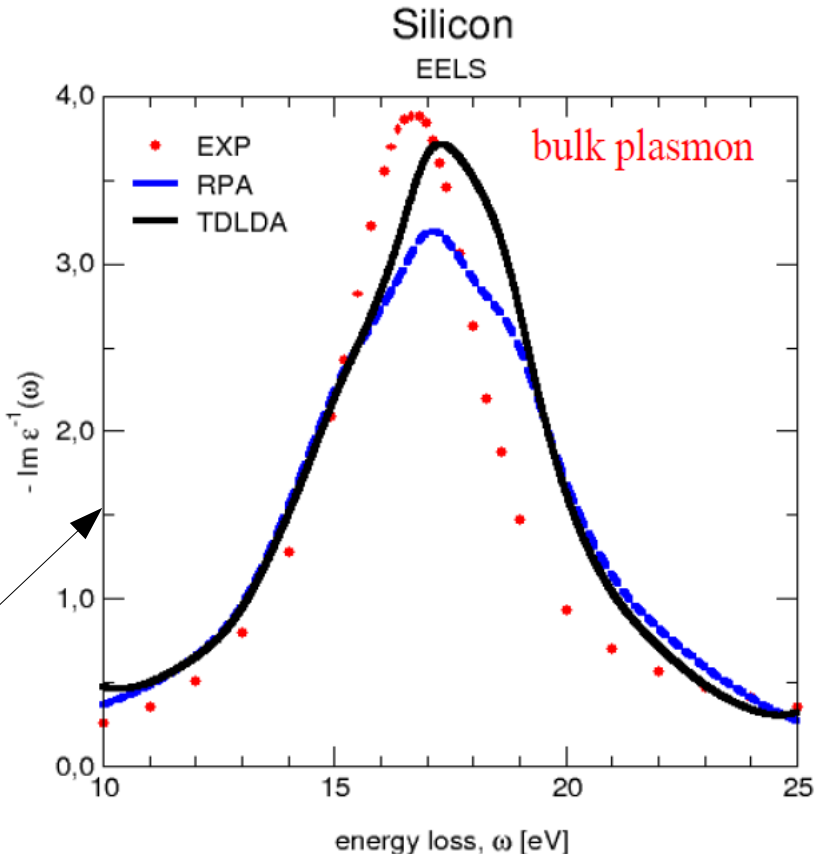
```
% ls
o.eel_q1_inv_rpa_dyson  o.eps_q1_inv_rpa_dyson
r_optics_chi  r_setup  SAVE  yambo.in
```

```
% ls SAVE
ndb.gops  ndb.kindx  ndb.ostnts  ns.db1  ns.kb_pp  ns.wf
```

How it works

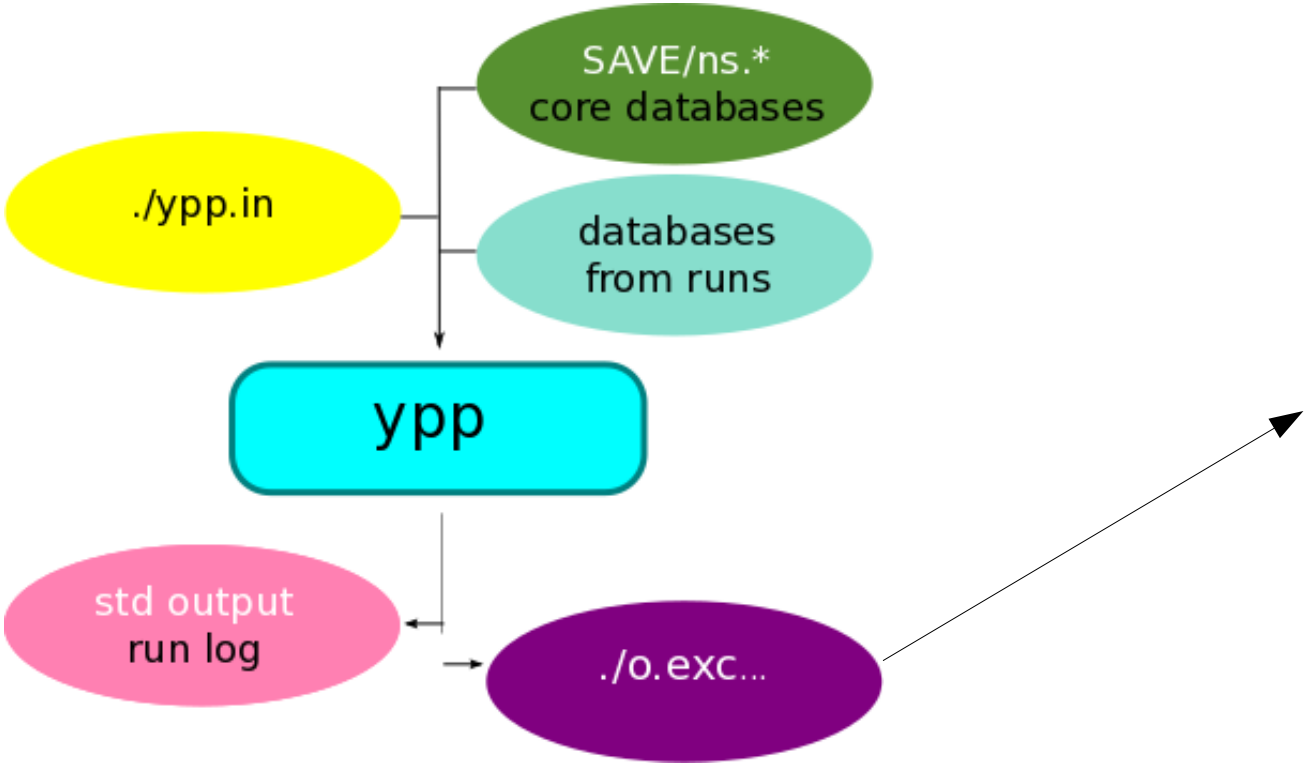
4. Run yambo

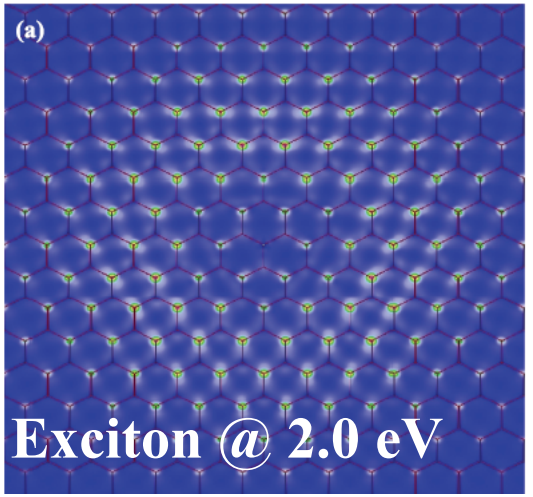


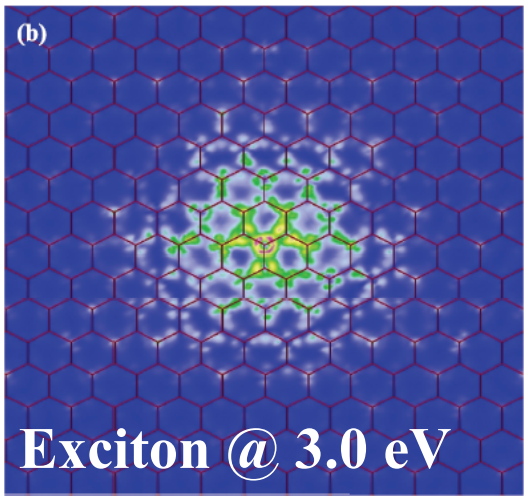


How it works

5. Post-processing with ypp





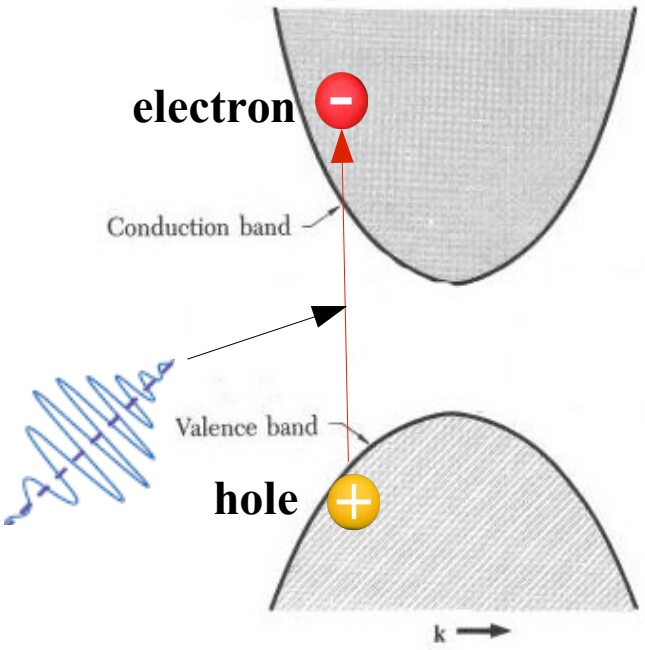


outline

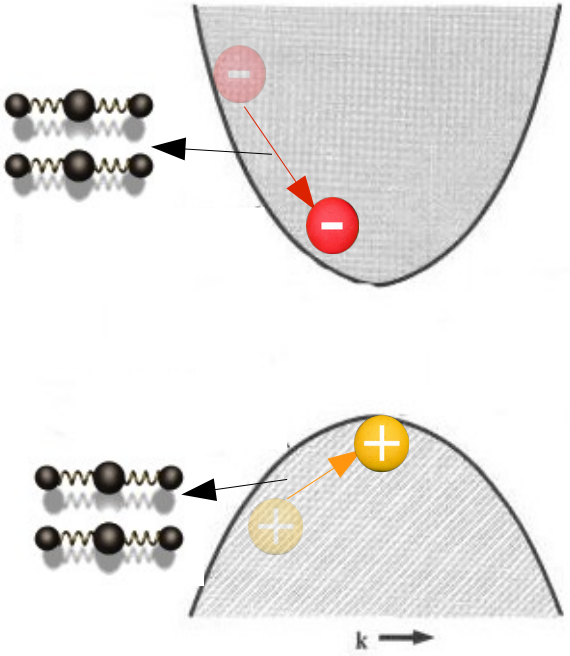
- Motivations and history
- The code: **the structure of yambo**
- Applications: **few examples**
- Users view: **how it works in practice**
- Future: **new developments and more**

Not yet GPL

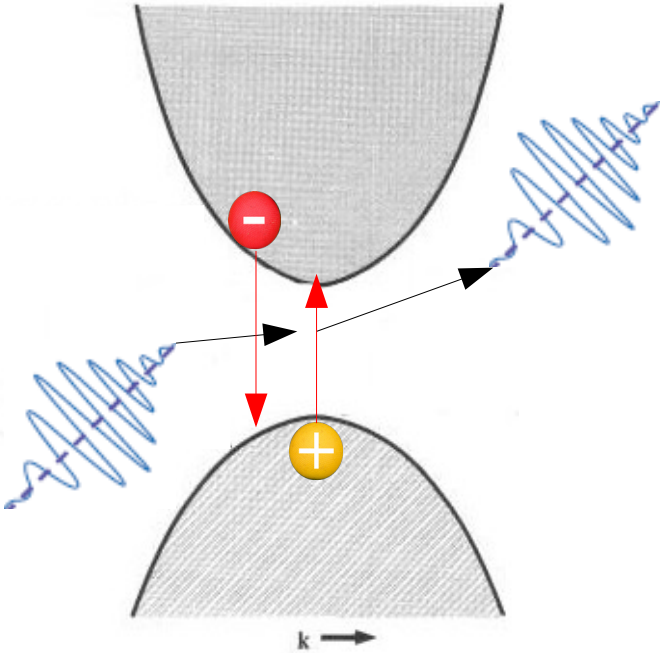
Non-equilibium physics



1 – Photo-excitation process



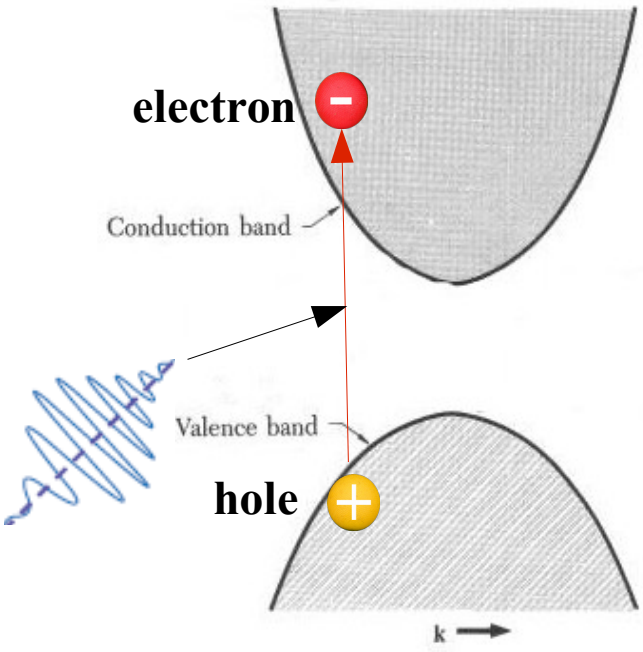
2 – relaxation



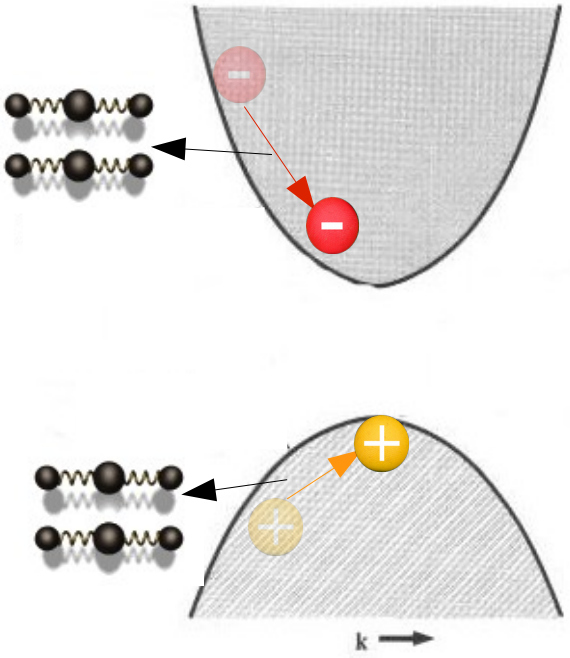
3 – Probing
(Transient aborption)

Not yet GPL

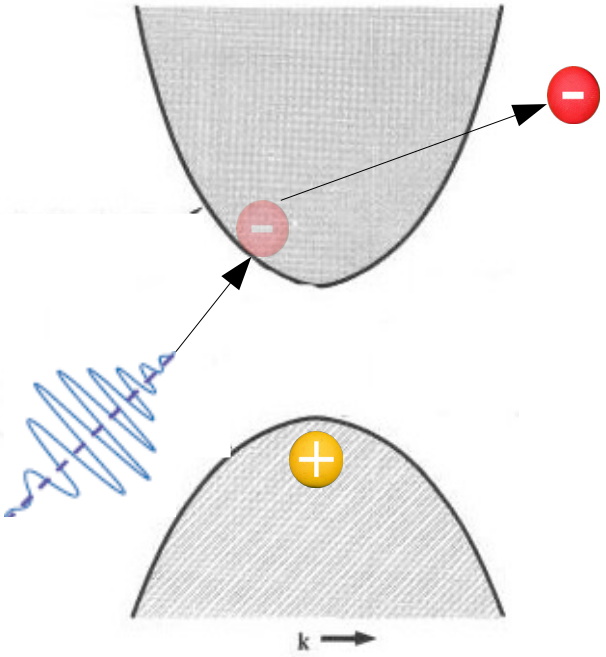
Non-equilibium physics



1 – Photo-excitation process



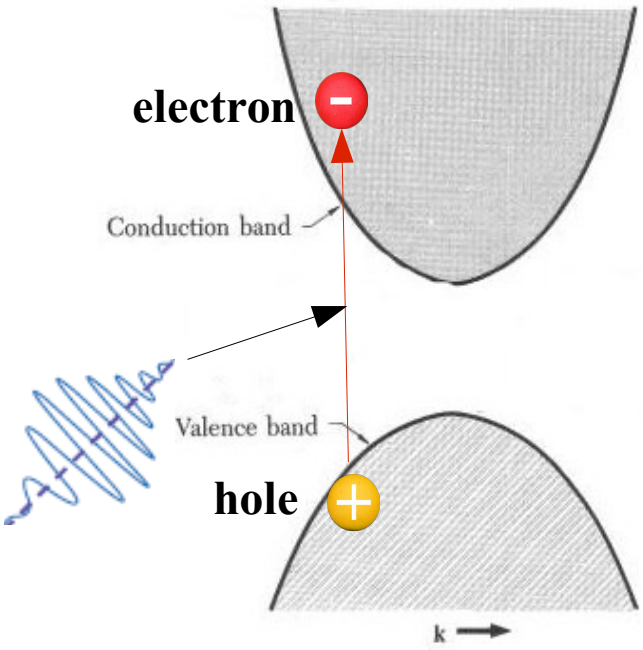
2 – relaxation



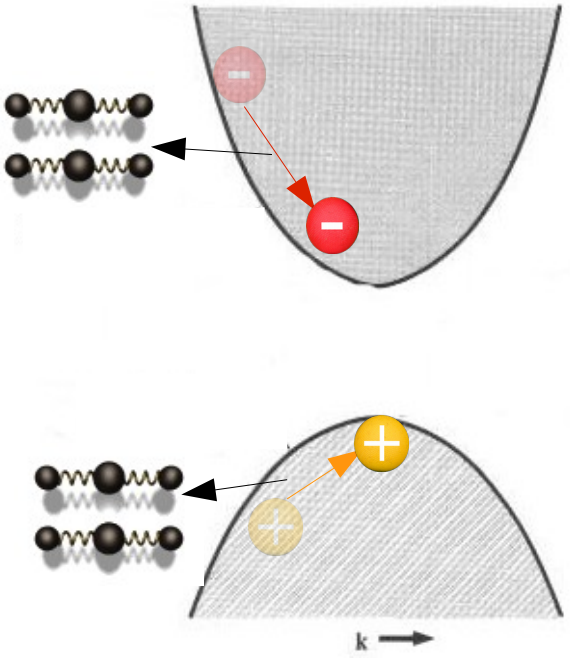
3 – Probing
(photo-emission)

Not yet GPL

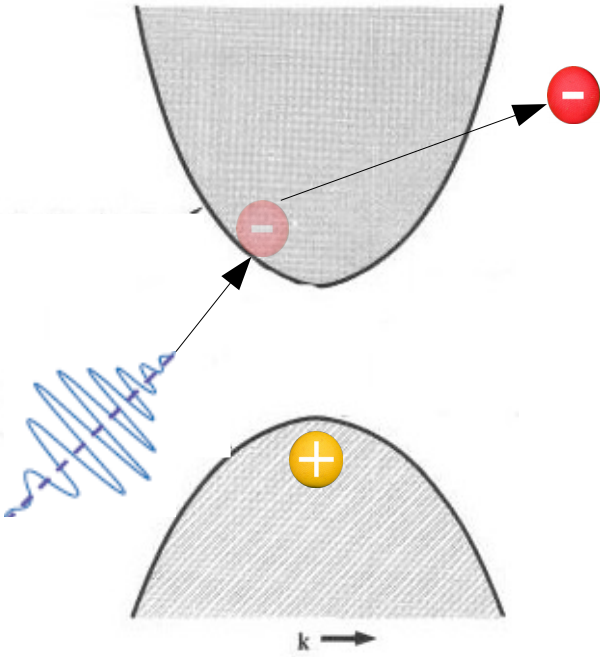
Non-equilibium physics



1 – Photo-excitation process



2 – relaxation



3 – Probing (photo-emission)

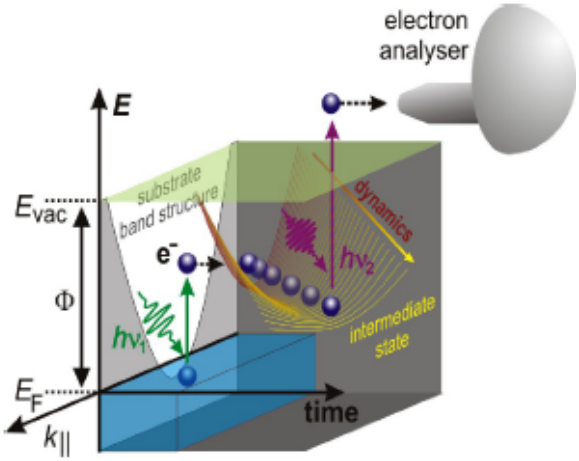
Propagate the equation of motion of the NEQ Green function

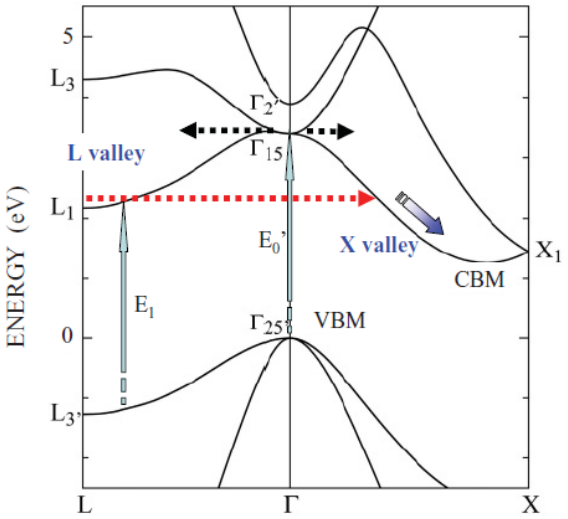
$$i\,\partial_t G^{<}_{nmk}(t,t) - [\,H^{eq}_{QP} + \Delta V^{H} + \Delta \Sigma^{st}_{xc} + U^{ext}(t), G^{<}(t,t)\,]_{nmk} = S_{nmk}(t)$$

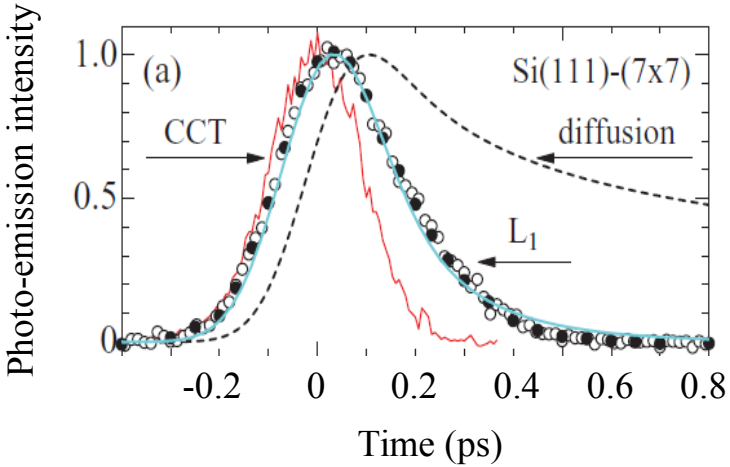
GKBA approximation and more

Not yet GPL

Non-equilibium physics

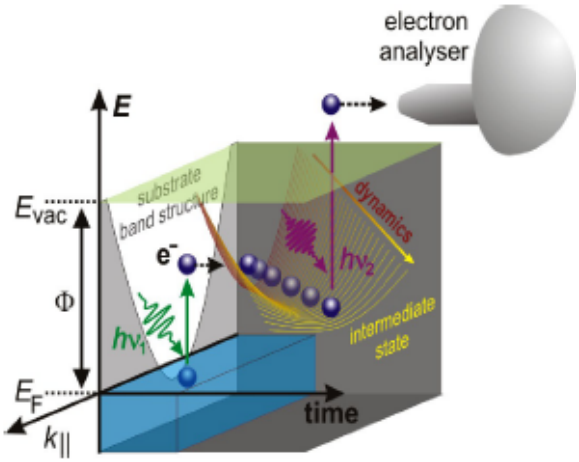


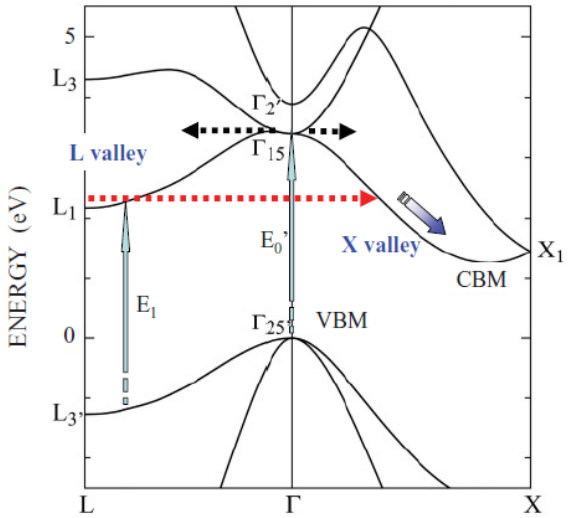


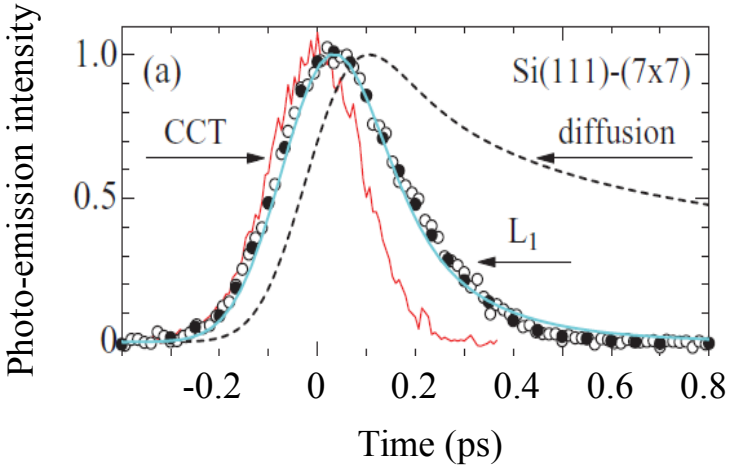


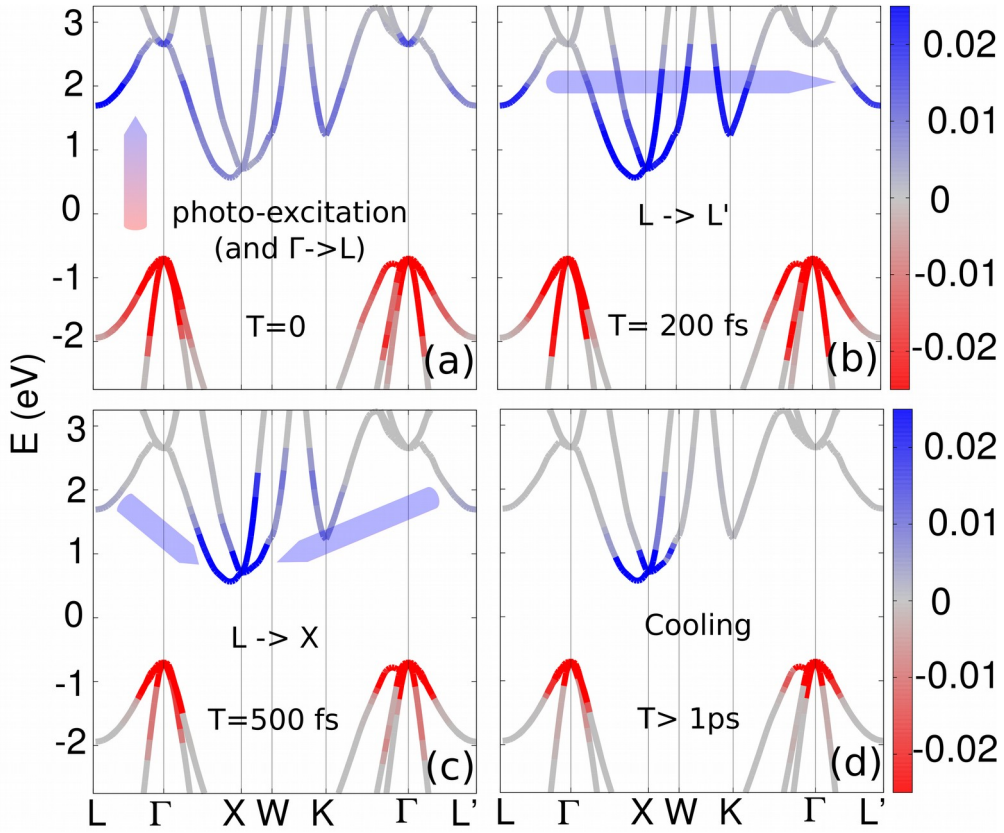
Not yet GPL

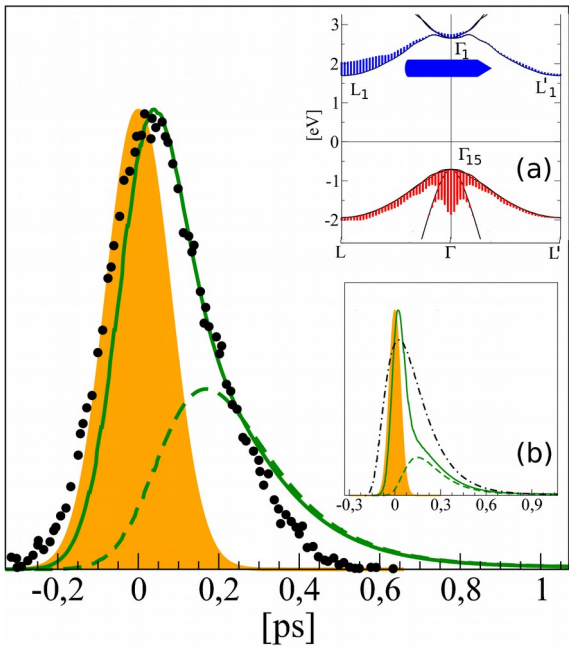
Non-equilibium physics











D. Sangalli, and A. Marini,
Europhysics Letters 110, 47004 (2015)

CNR
Istituto di Struttura
della Materia

Thank you for your attention

www.yambo-code.org

en.wikipedia.org/wiki/YAMBO_code

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github.com/yambo-code
github.com/henriquemiranda/yambopy