Theoretical approaches to the ab-initio study of complex systems

Olivia Pulci

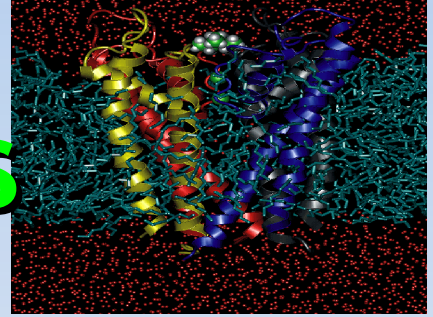
European Theoretical Spectroscopy Facilty (ETSF),
and CNR-INFM,
Dipartimento di Fisica Università di Roma Tor Vergata

http://www.fisica.uniroma2.it/~cmtheo-group
http://www.etsf.eu

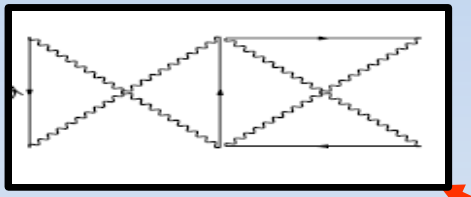
_Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

NAST-ISM

Group activities



Biological systems



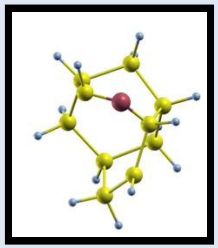
Theory

Code development

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

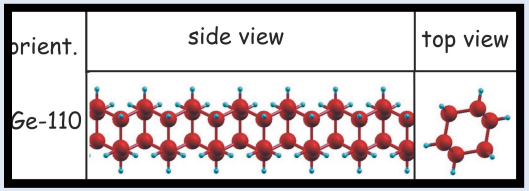
- **Generality, transferability 0D-3D**
- **detailed physical informations**

0-D



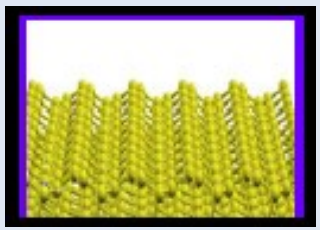
Nanoclusters

1-D



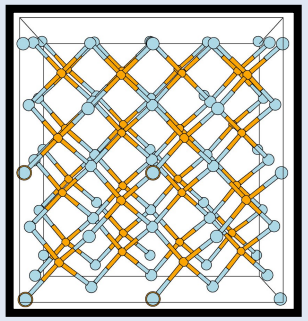
Nanowires

2-D



Surfaces

3-D



bulks

Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

European Theoretical Spectroscopy Facility

an initiative of the

Nanoquanta
Network of Excellence


X. Gonze
Université catholique de Louvain
C-O. Almbladh
Lunds Universitet
Lund
R. Godby
University of York
M. Scheffler
Fritz-Haber-Institut
Berlin
BEAMLINES:
Optics (O. Pulci)
EELS (F. Sottile)
X-ray (J. Rehr)
Transport (P. Bokes)
Time-resolved excitations (M. Marques)
Photoemission (C. Verdozzi)
Raman (G. Rignanese) new
E.K.U. Gross
Freie Universität
Berlin
L. Reining
Laboratoire des Solides Irradiés
Paris
F. Bechstedt
Friedrich-Schiller-Universität
Jena
Roma
A. Rubio
Universidad del País Vasco
San Sebastián
G. Onida
Universitá degli Studi
Milano
R. Del Sole
Istituto Nazionale per la Fisica della Materia
Roma

Development
of theory

training

Undergraduates
PhD Students
Post Docs
Other colleagues
exp + Industry!

Marie Curie Fellowships

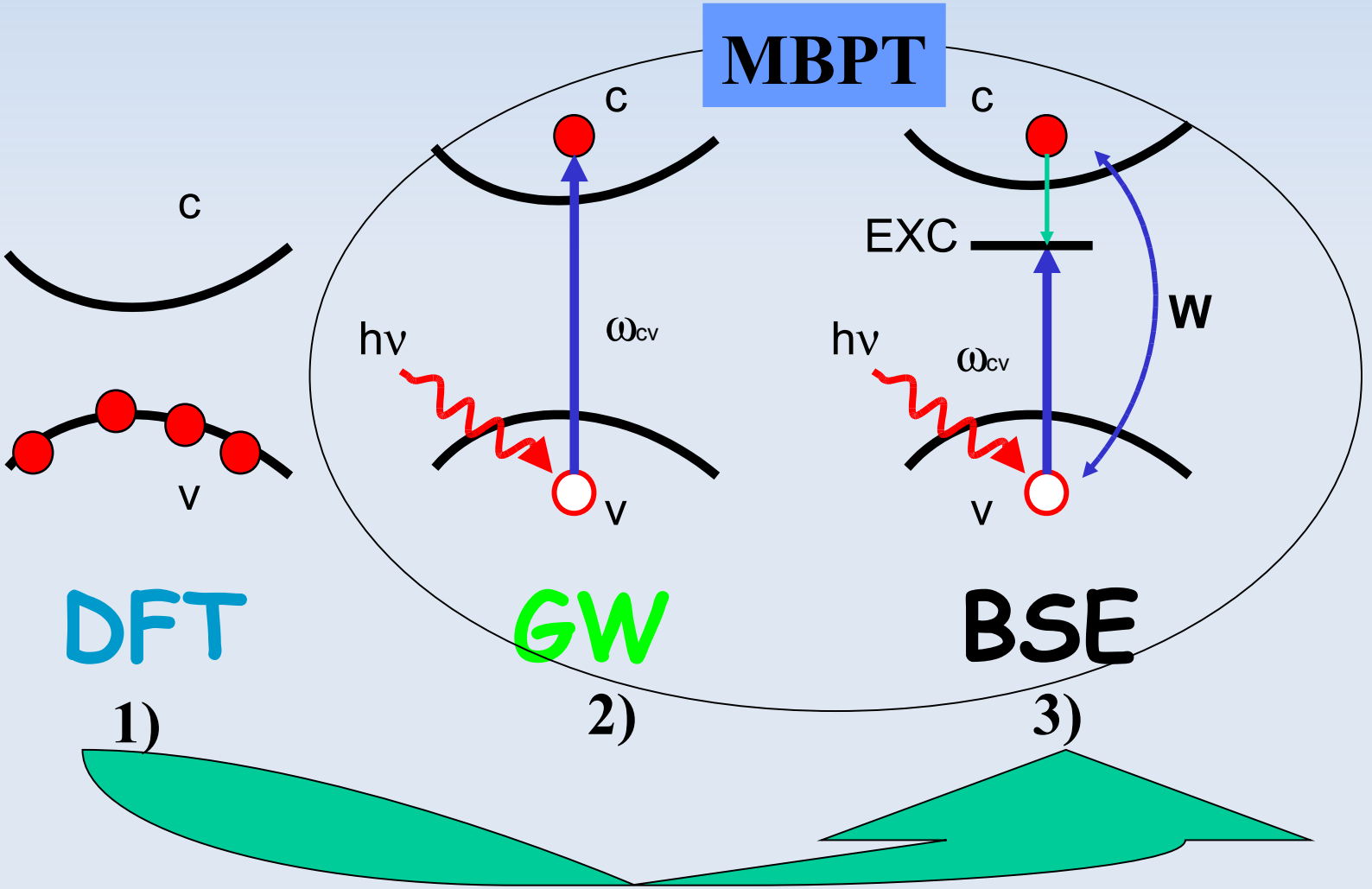
Development

Distribution:
ABINIT
FHI
OCTOPUS
Yambo
DP+EXC
TOSCA

Research

Carrying on
Projects for
users

METHODS



Theory development:

- **MB kernel for TDDFT**

(M. Marsili, A. Marini, R. Del Sole)

PRB2003, PRL2003, PRB2007

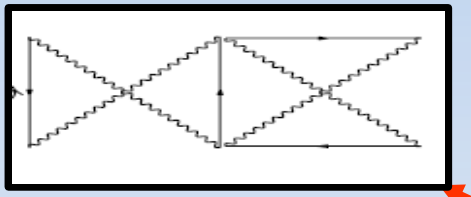
- **Electron-phonon coupling** (A. Marini)

A. Marini Phys. Rev. Lett. **101**, 106405 (2008)

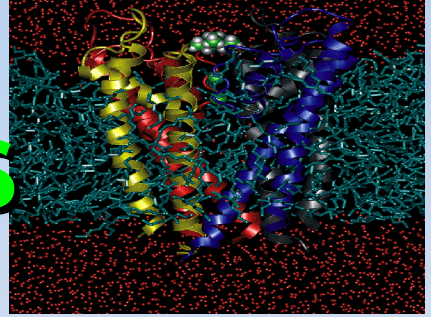
- **Vertex corrections** (M. Marsili, R. Del Sole)

M. Marsili, R. Del Sole, in preparation

Group activities



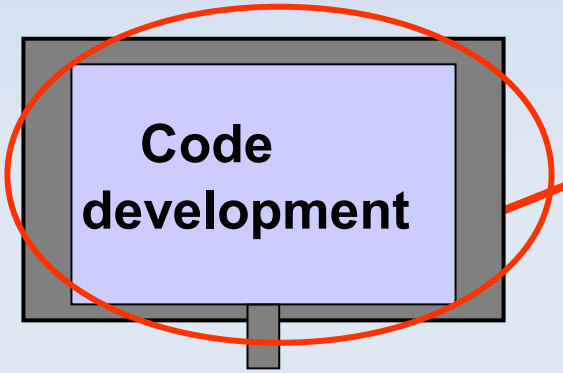
Theory



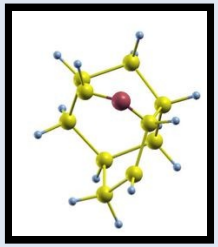
Biological systems

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

- **Generality, transferability 0D-3D**
- **detailed physical informations**

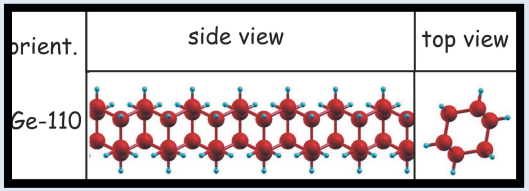


0-D



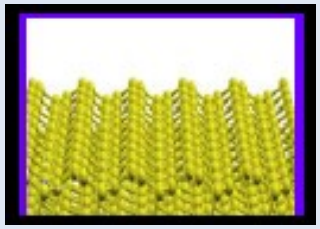
Nanoclusters

1-D



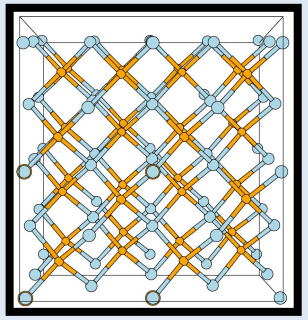
Nanowires

2-D



Surfaces

3-D



bulks

Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

Andrea Marini

YAMBO ©

Daniele Varsano

Conor Hogan

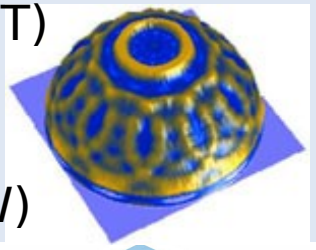
www.yambo-code.org

YAMBO is a multipurpose Ab-Initio Many-Body code for excited state calculations.

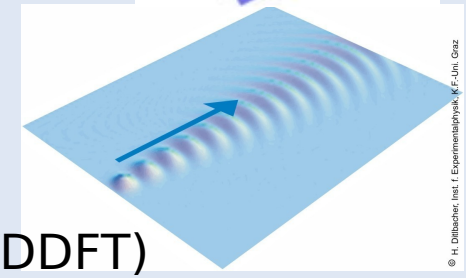
Myrta Gruning

released under the GPL license on Sept 1st 2008

Particles(DFT)



Quasiparticles(GW)



Plasmons (TDDFT)

In these first 6 months ...

more the **5000 contacts**...
more the **600 downloads** of the source...
documentation and tutorials **visited 1000 times**

Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

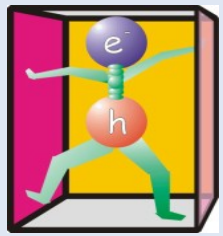
ELSEVIER

COMPUTER PHYSICS COMMUNICATIONS

doi:10.1016/j.cpc.2009.02.003

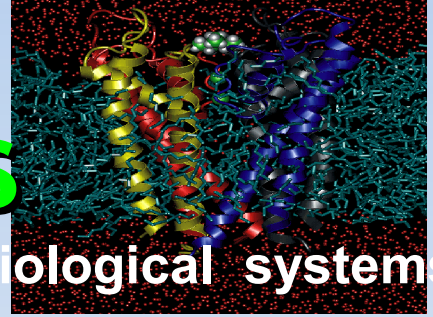
yambo: An *ab initio* tool for excited state calculations ☆

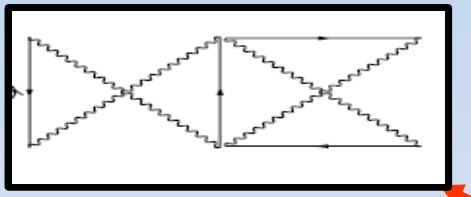
Andrea Marini [a,e,*], Conor Hogan [b,e], Myrta Grüning [c,e], Daniele Varsano [d,e]



Excitons (Bethe-Salpeter equation)

Group activities





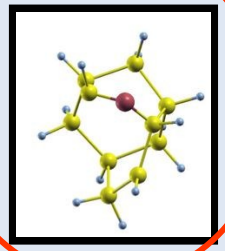
Theory

Code development

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

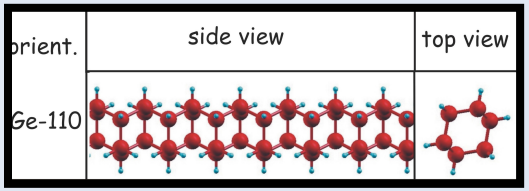
- **Generality, transferability 0D-3D**
- **detailed physical informations**

0-D



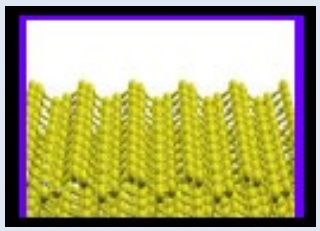
Nanoclusters

1-D



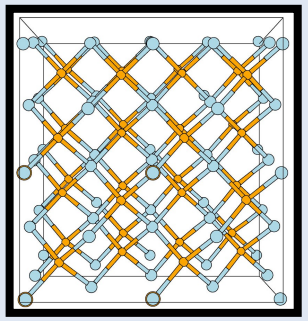
Nanowires

2-D



Surfaces

3-D

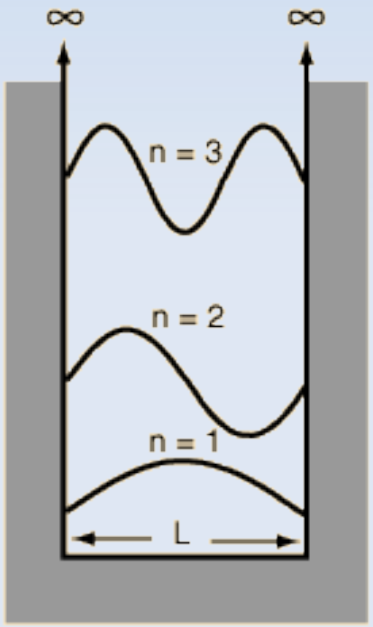


bulks

Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

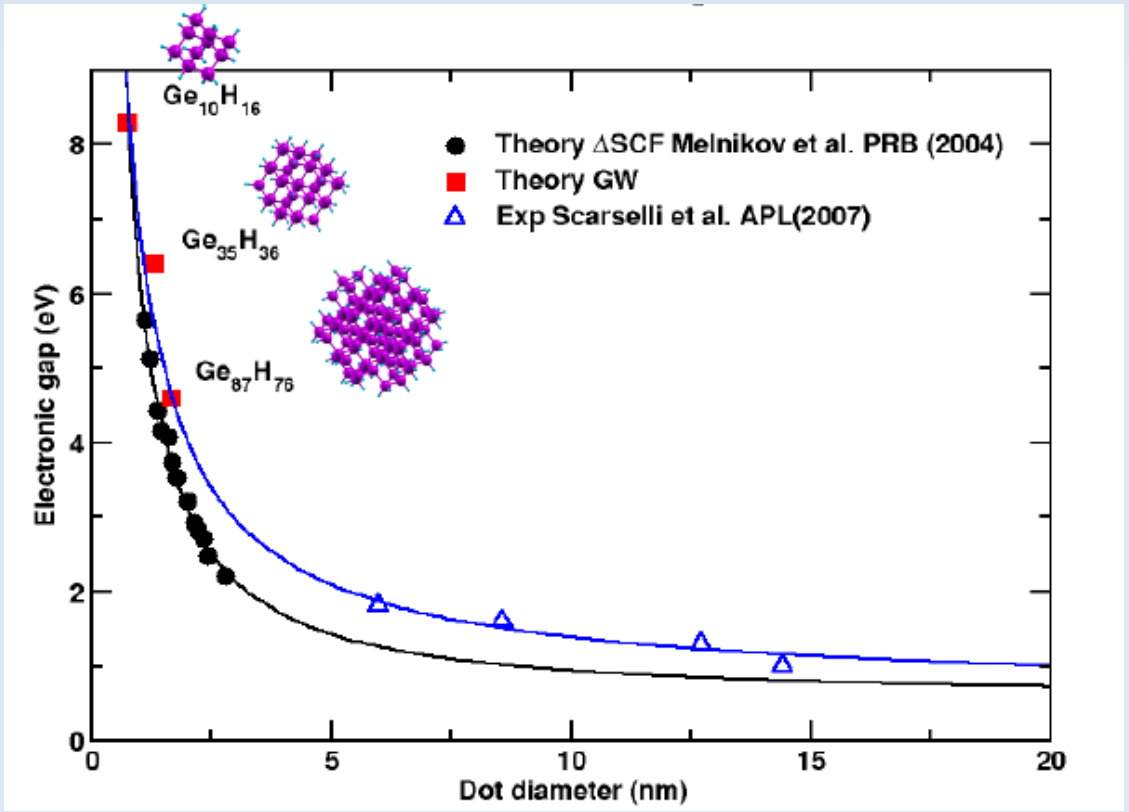
0D nanodots

nanoclusters: electronic gap vs. size



$$E_n = \frac{\pi^2 \hbar^2}{2m_e}\frac{n^2}{L^2}$$

Quantum confinement



M. Marsili, M. Palummo, O. Pulci

(c)

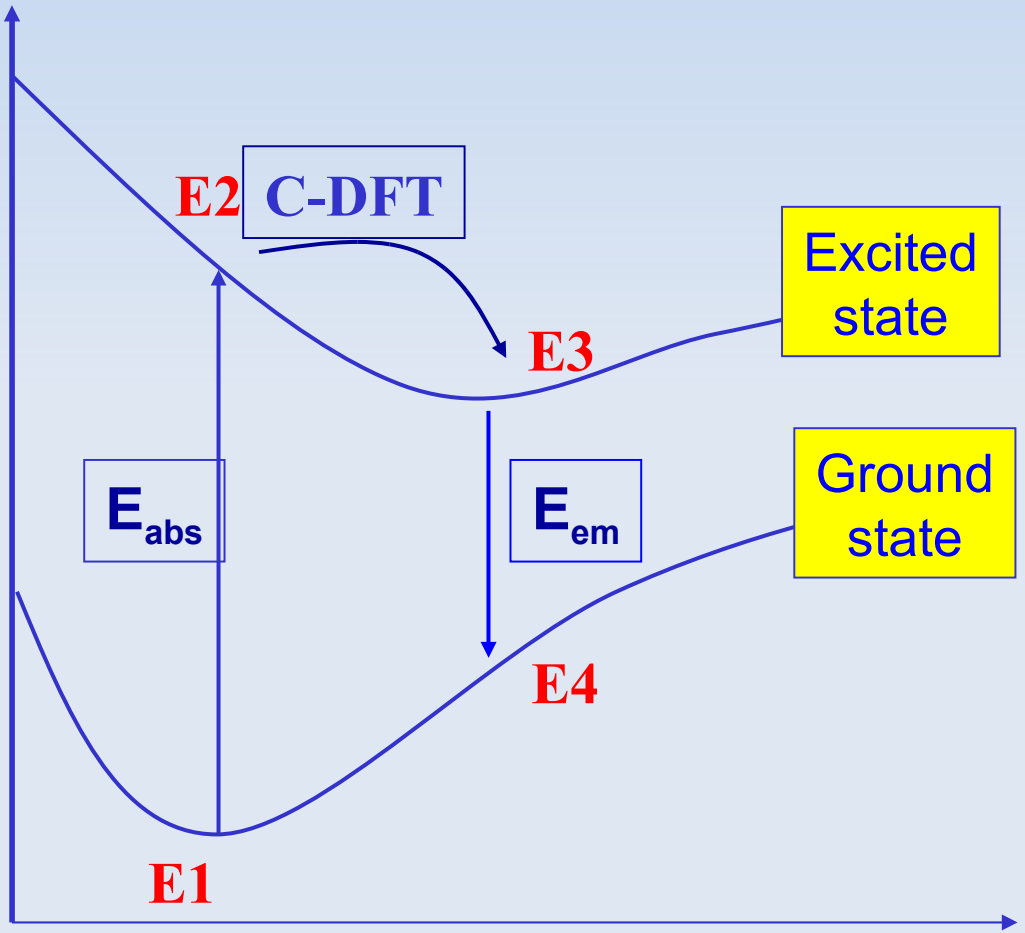
$$E_g(\mathrm{QD}) \approx E_{g0} + \frac{\hbar^2\pi^2}{2m_{eh}R^2}$$

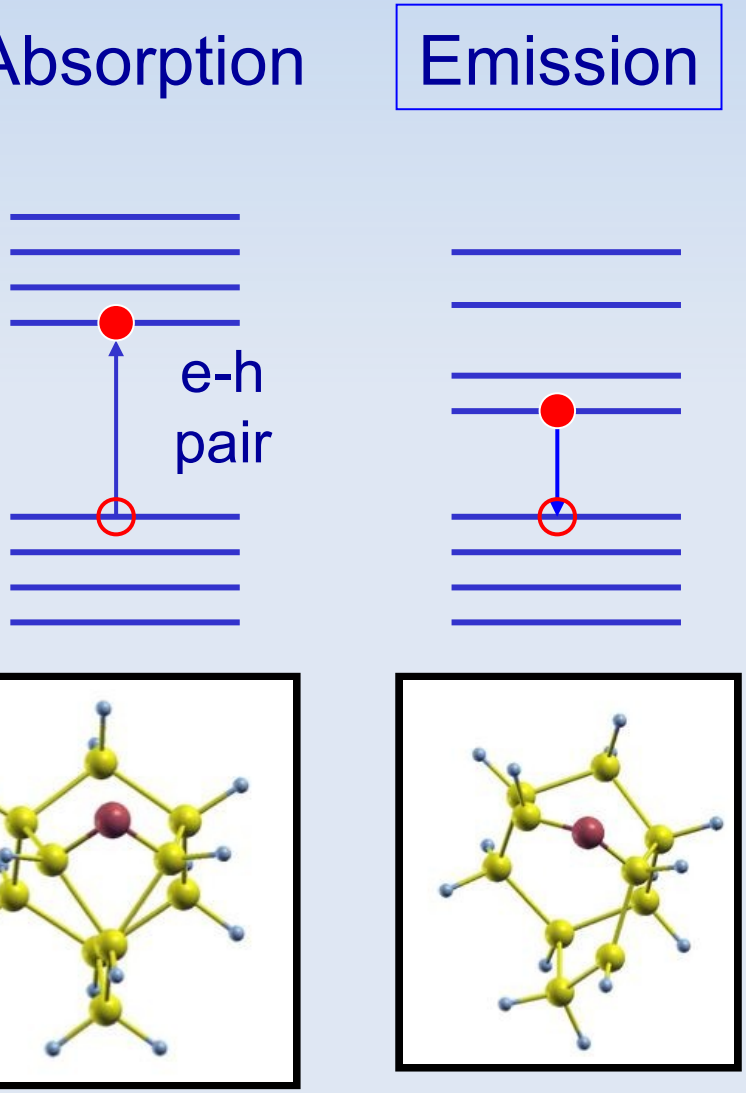
$$m_{eh} = \frac{m_e m_h}{m_e + m_h}$$

m_e = effective electron mass

m_h = effective hole mass

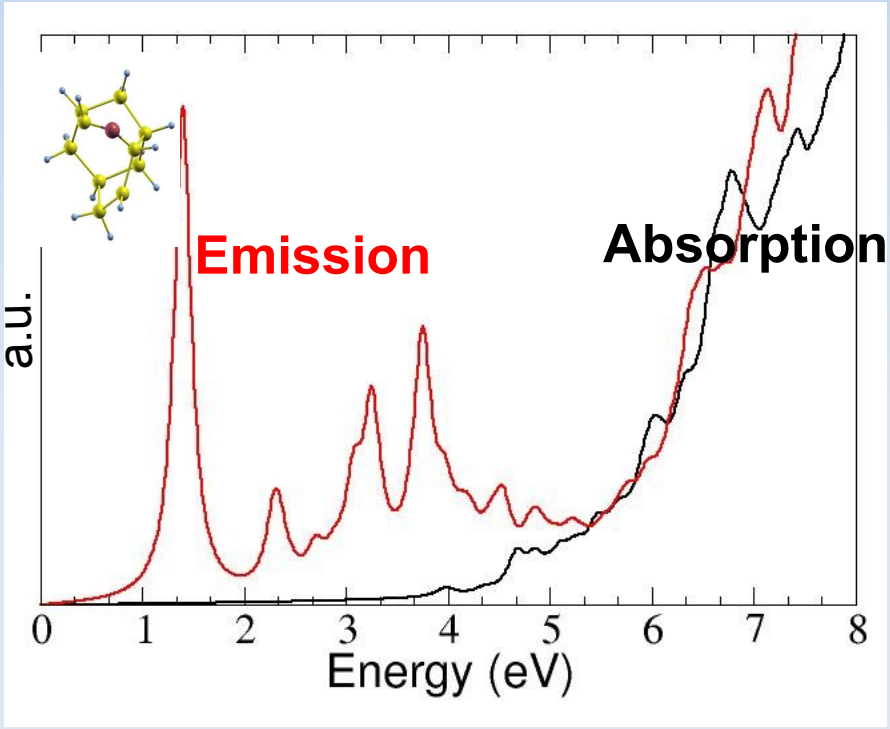
0D nanodots: absorption and emission



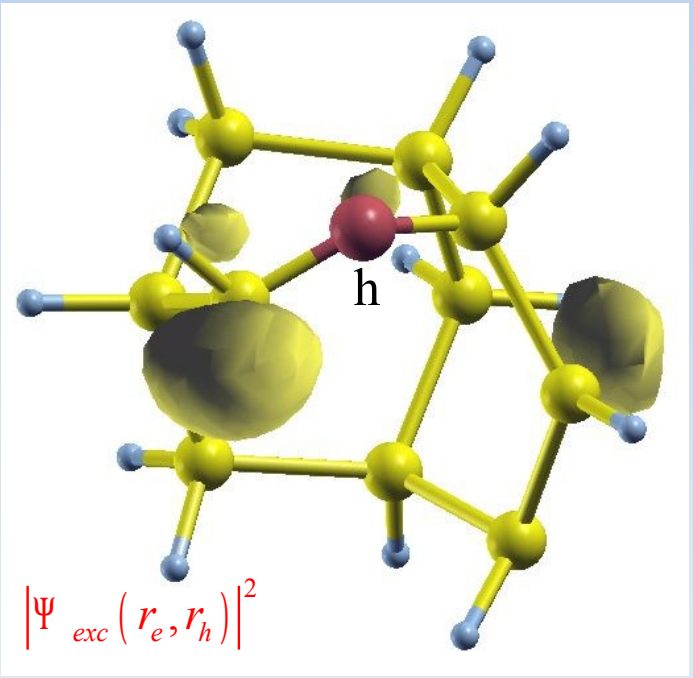


Structural minimization performed both in the ground state and in presence of the e-h pair

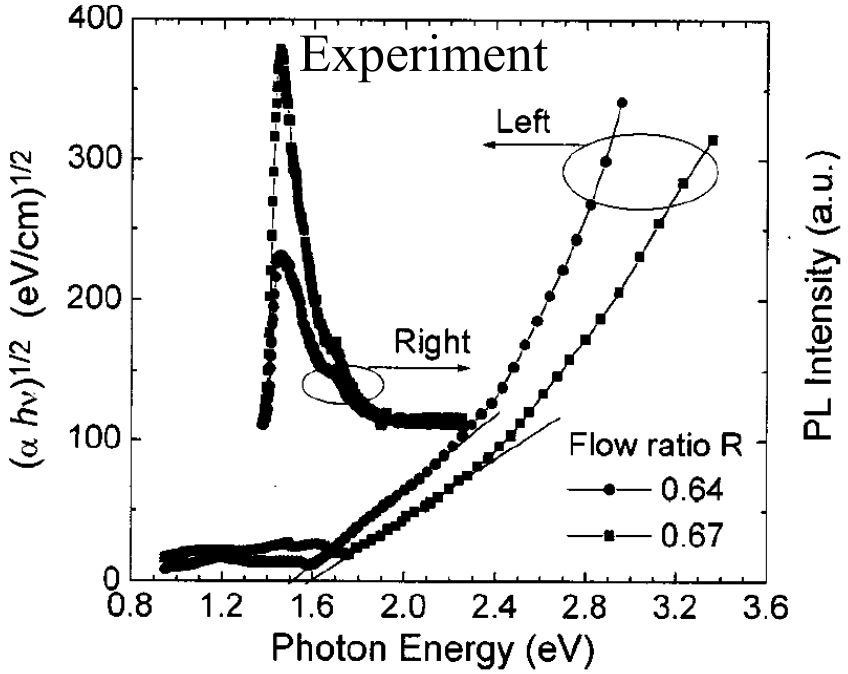
0D nanodots (O. Pulci)



PRB 2007



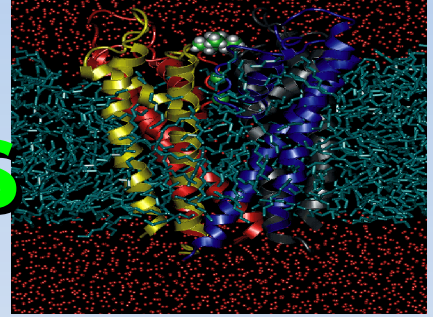
PL peak related to O ***bridge***



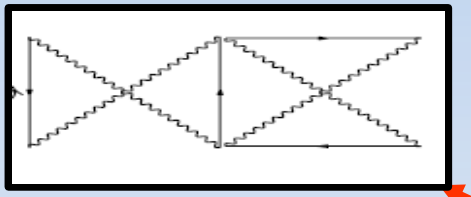
Ma et al. APL, **75** 1857 (1999))

O. Pulci in collaboration with S. Ossicini group (Modena

Group activities



Biological systems



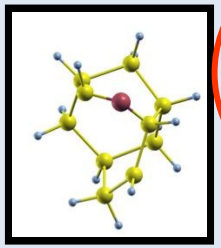
Theory

Code development

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

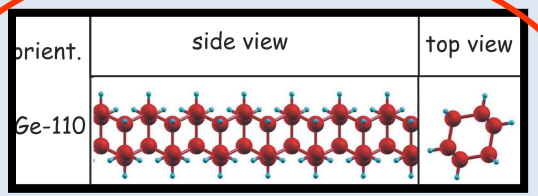
- **Generality, transferability 0D-3D**
- **detailed physical informations**

0-D



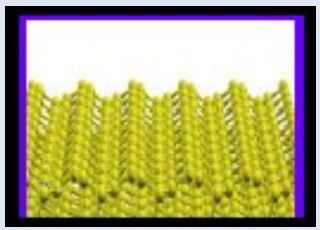
Nanoclusters

1-D



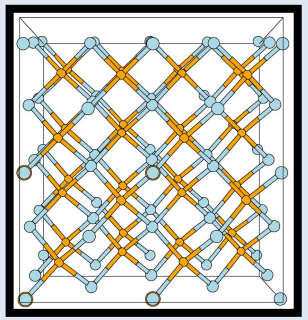
Nanowires

2-D



Surfaces

3-D

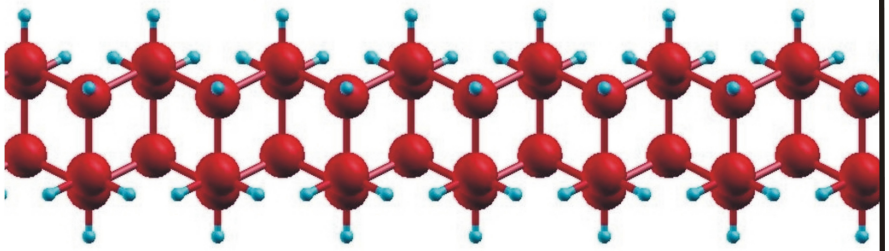
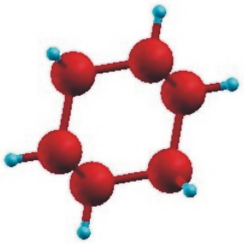
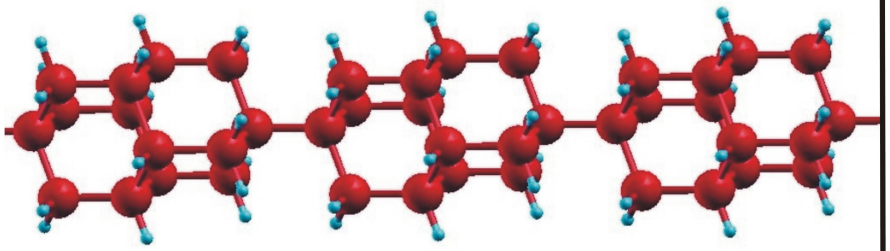
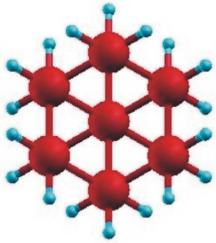
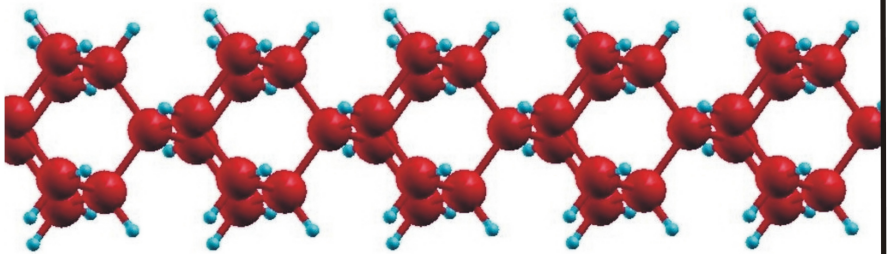
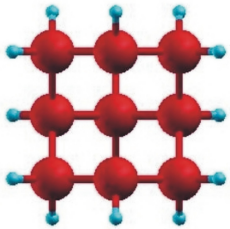


bulks

Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

1D nanowires (Palummo)

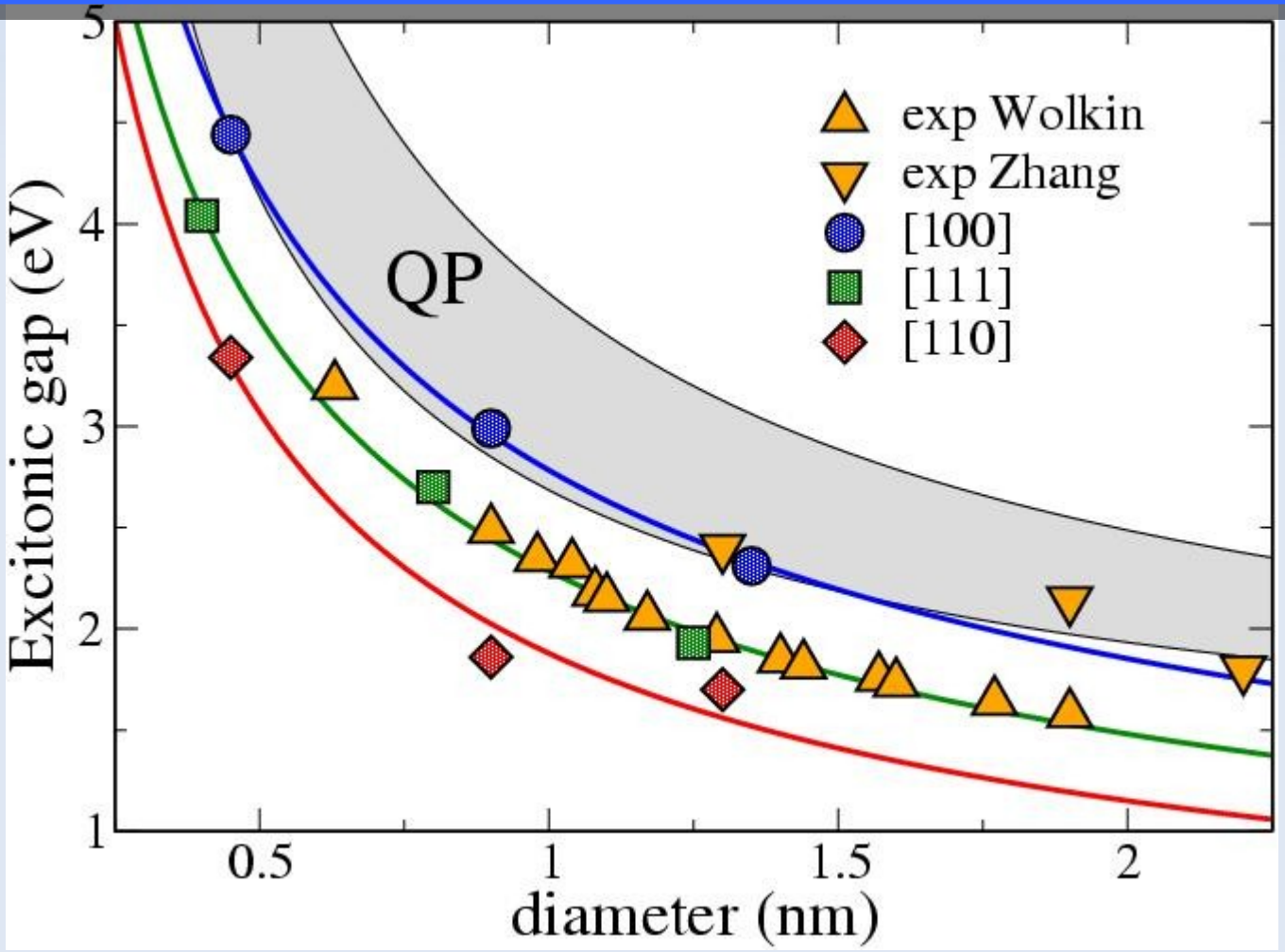
Si Wires' atomic structure

orient.	side view	top view
110		
111		
100		

d=4Å

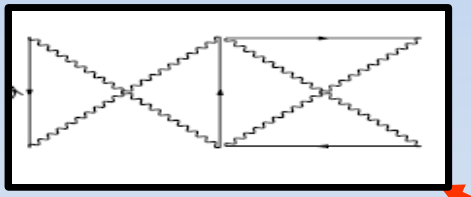
1D nanowires

Si NWs Excitonic Gap: theory vs exp.

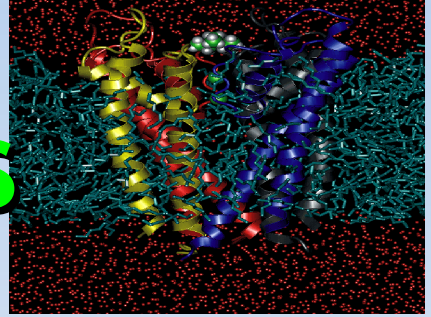


M.Bruno et al. PRL 2007

Group activities



Theory



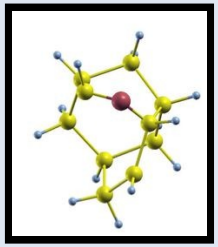
Biological systems

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

- **Generality, transferability 0D-3D**
- **detailed physical informations**

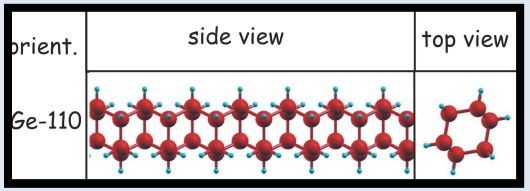
Code development

0-D



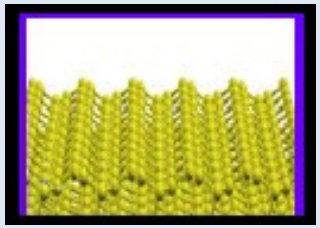
Nanoclusters

1-D



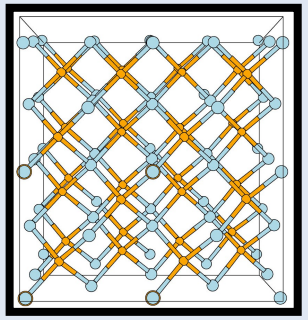
Nanowires

2-D



Surfaces

3-D



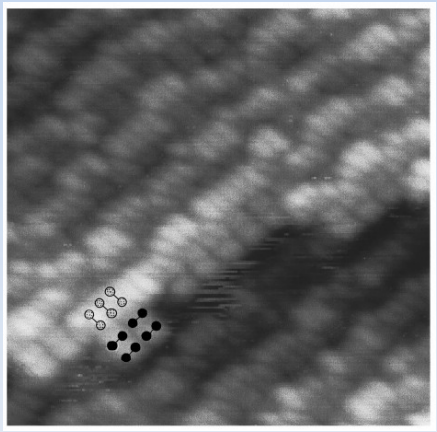
bulks

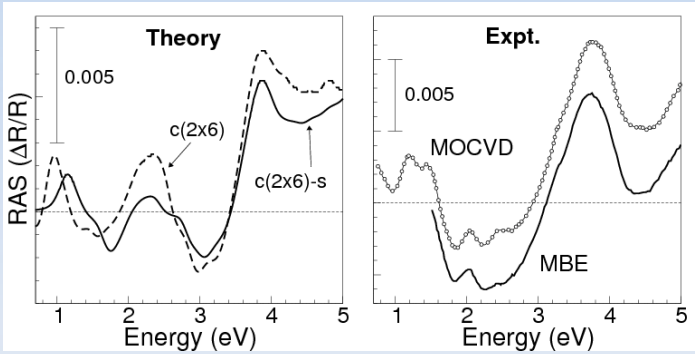
Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

2D: surfaces (ongoing projects)

- GaSb(001) c2x6

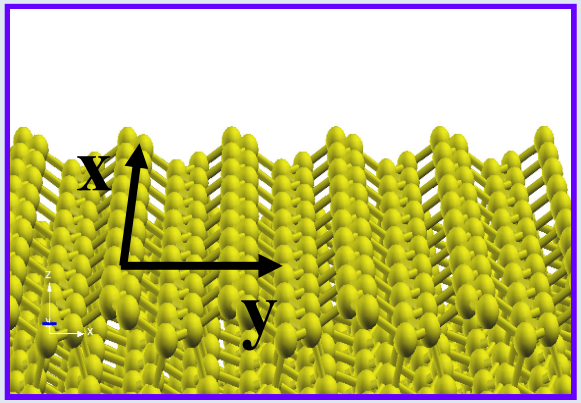
Conor Hogan





- C(111)2x1

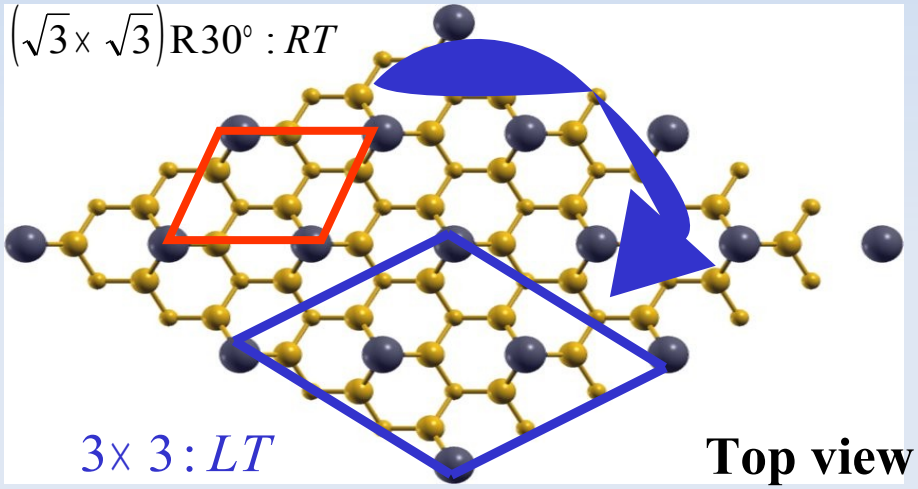
Margherita Marsili

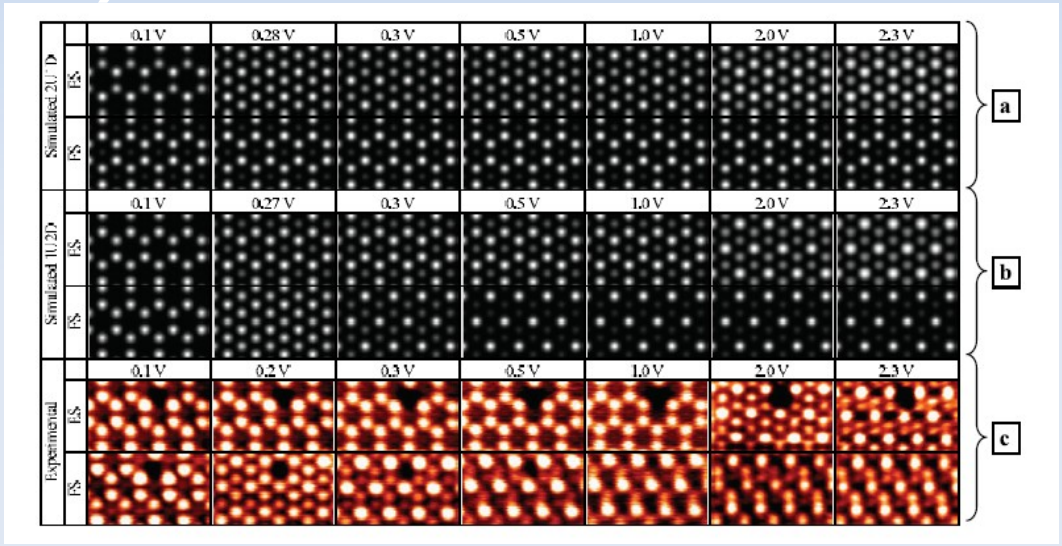


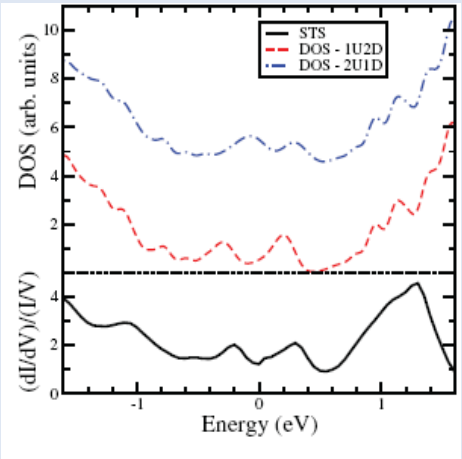
- Ice (0001)

Viviana Garbuio

ISM-NAST collaboration (1):
Ge(111):Sn







Metal semiconductor interfaces: electronic properties at the GW level and comparison experimental/calculated STM images

Eur. Phys. Lett. 2009

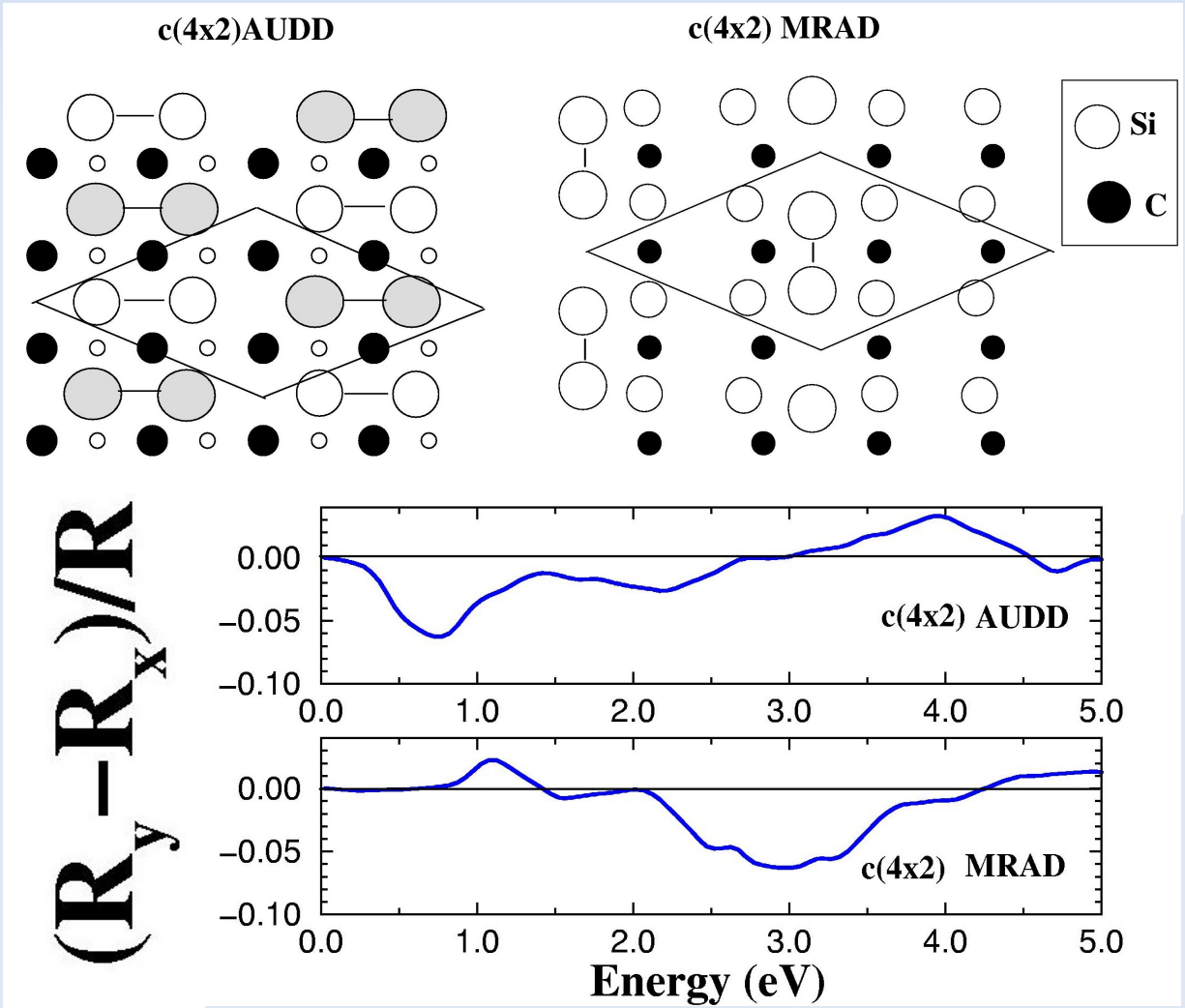
With Paola Gori, Fabio Ronci, Stefano Colonna, and Antonio Cricenti (ISM)

ISM-NAST collaboration (2):

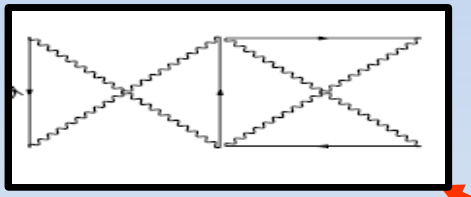
3C-SiC(001) c(4x2)

Group IV surfaces: determination of actual ground state via comparison with RAS results

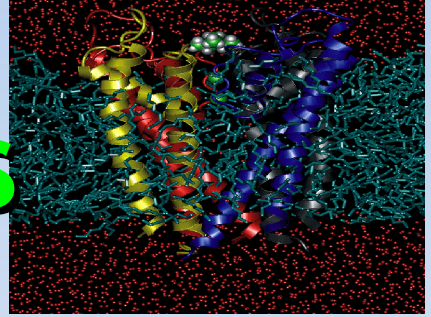
O. Pulci, Paola Gori and Antonio Cricenti (ISM)



Group activities



Theory



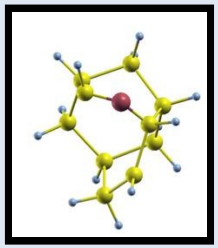
Biological systems

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

- **Generality, transferability 0D-3D**
- **detailed physical informations**

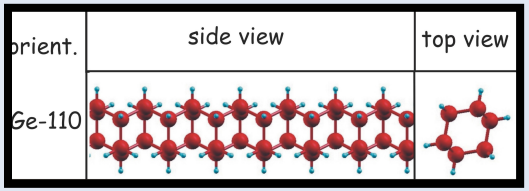
Code development

0-D



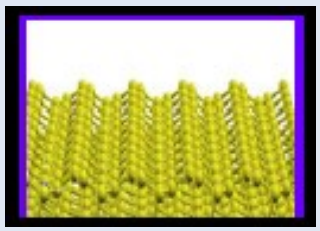
Nanoclusters

1-D



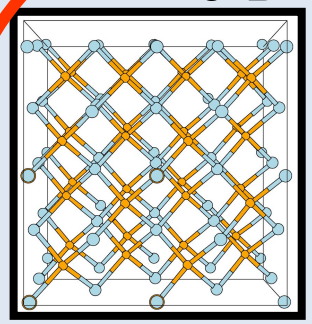
Nanowires

2-D



Surfaces

3-D

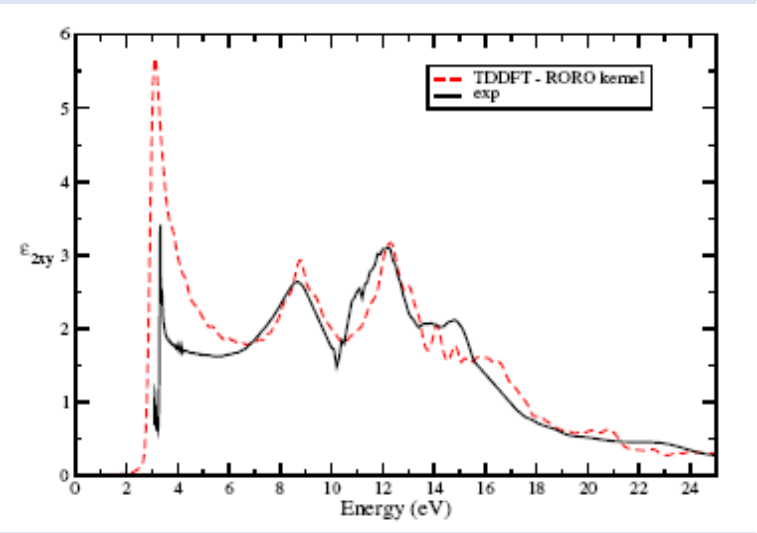


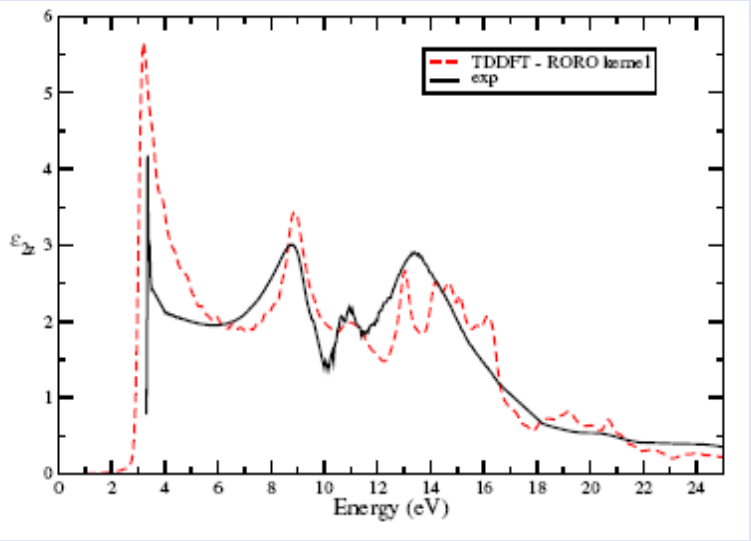
bulks

Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

ISM-NAST collaboration (3): oxides

excitonic effects in ZnO

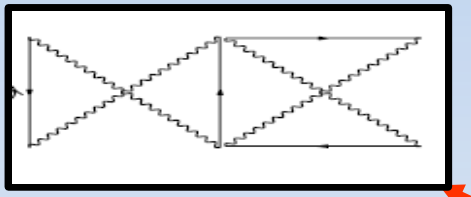




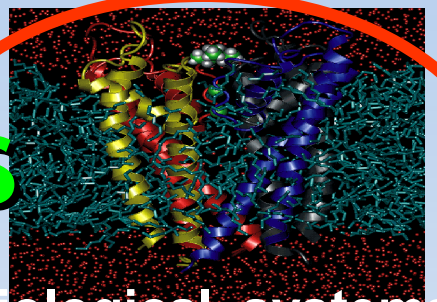
Optical properties of oxides: inclusion of excitonic effects at the BSE or TDDFT level

with Paola Gori and Antonio Cricenti (ISM)

Group activities



Theory



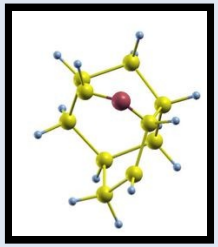
Biological systems

Code development

Ab-initio: *(NOT "one puts nothing in, one gets nothing out"!!)*

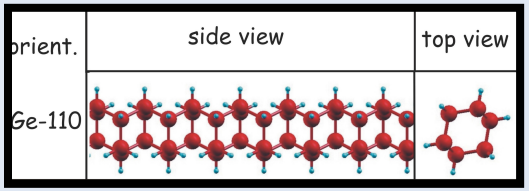
- **Generality, transferability 0D-3D**
- **detailed physical informations**

0-D



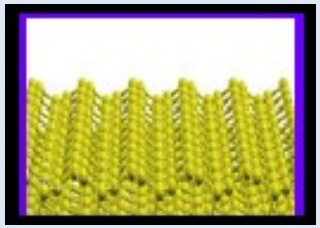
Nanoclusters

1-D



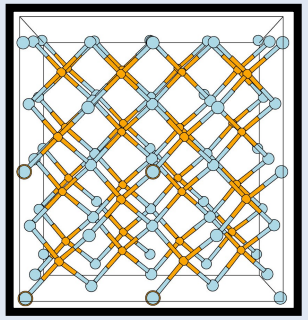
Nanowires

2-D



Surfaces

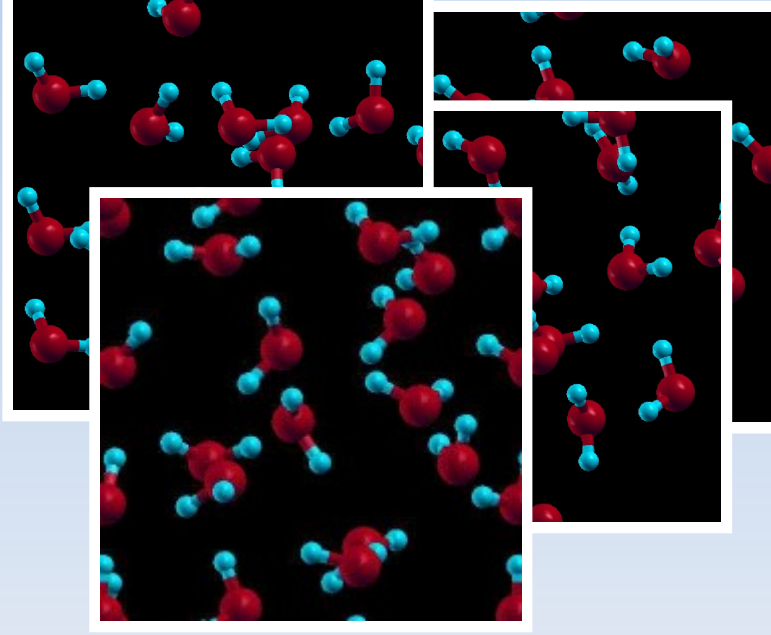
3-D



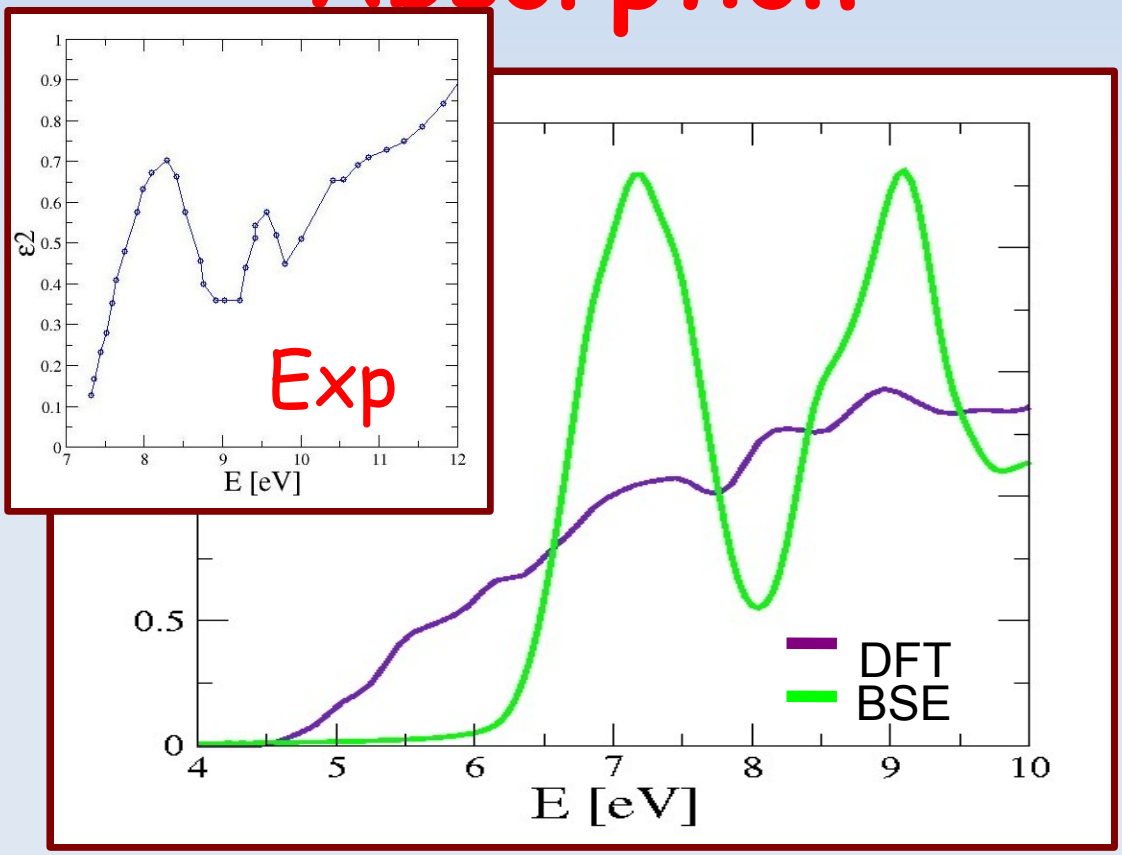
bulks

Olivia Pulci, Maurizia Palummo, Conor Hogan, Andrea Marini, Margherita Marsili, Viviana Garbuio, Adriano Mosca Conte, Elena Cannuccia, Rodolfo Del Sole

H_2O (Garbuio-Pulci)

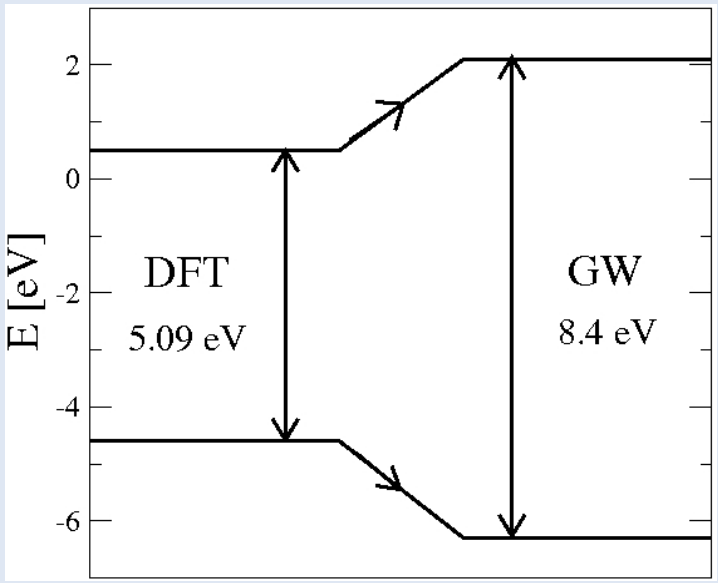


Absorption



Exciton binding energy **2.4 eV**

Electronic Gap

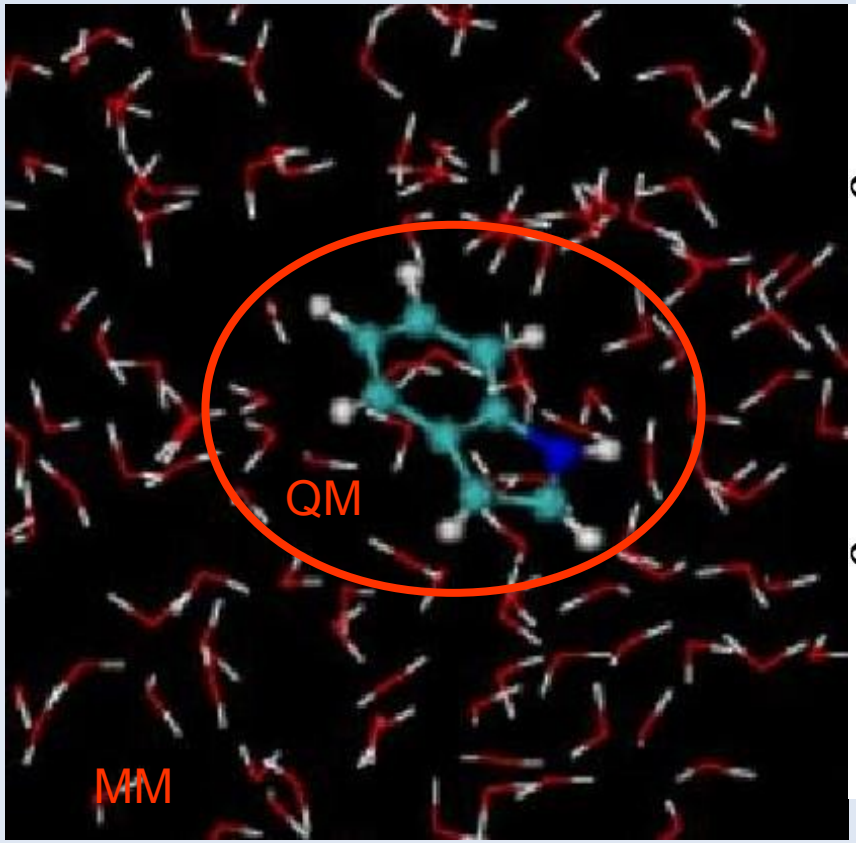


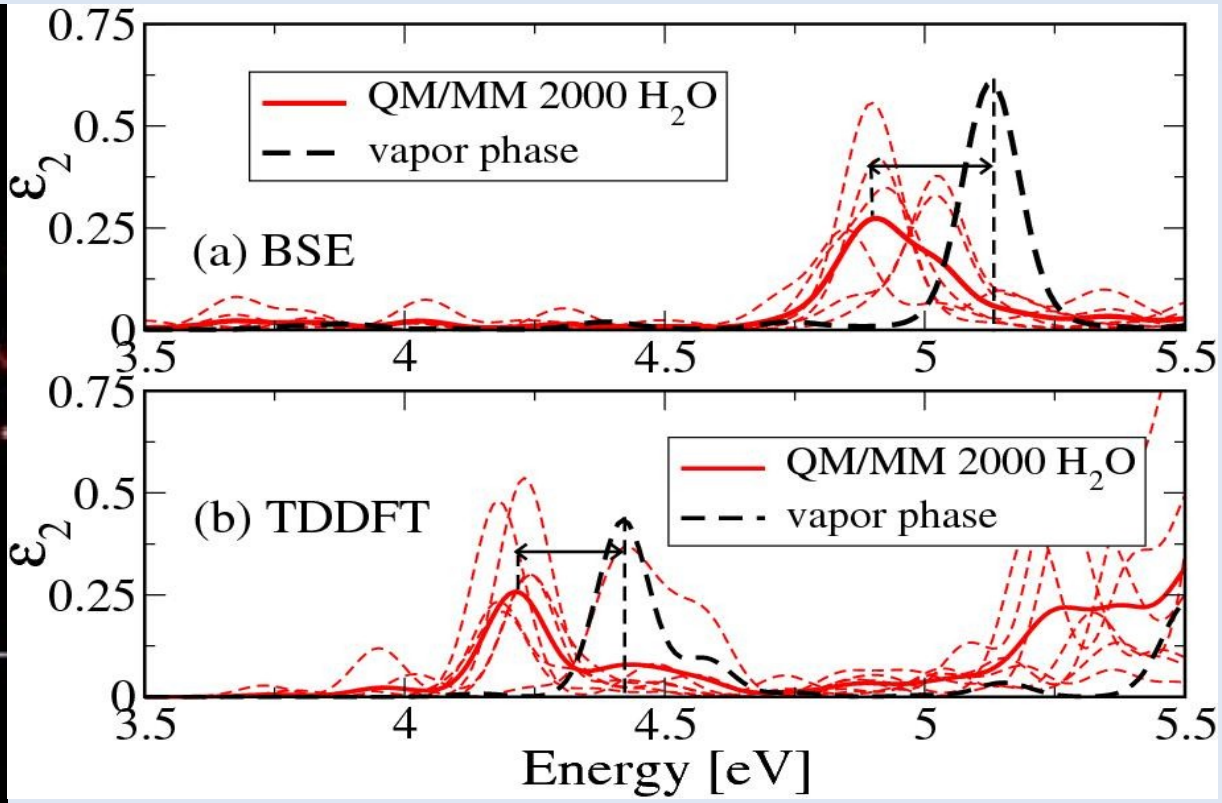
EXP-L.R. Painter *et al*., Phys. Rev. Lett. **21**, 282 (1968) – G.D. Kerr *et al.,* Phys. Rev. A **5**, 2523 (1972)

Bio: conquering the environment (Mosca Conte-Pulci)

OPTICAL PROPERTIES OF INDOLE IN WATER SOLUTION BY MBPT/MM

A COMBINATION OF MANY BODY METHODS (GW+BSE) WITH QM/MM TO STUDY BIOLOGICAL MOLECULES IN SOLUTION

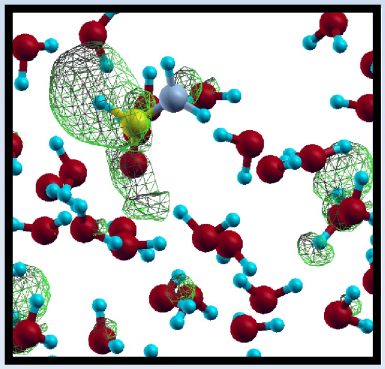




A. Mosca Conte, E. Ippoliti,R. Del Sole, P. Carloni, O. Pulci, JCTC (in press)

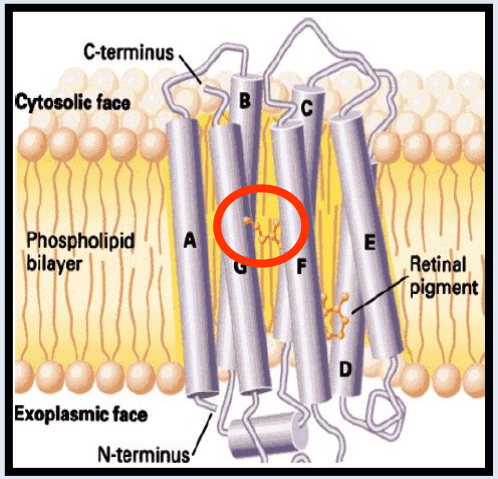
Towards Biological Systems

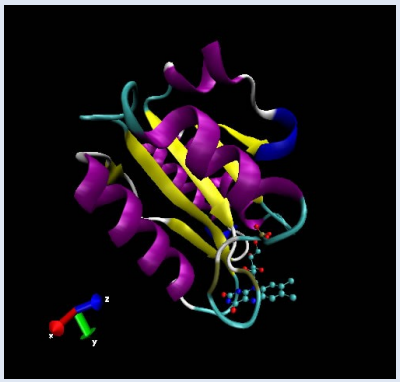
Ongoing projects:



Study of solutions:
formamide in water
V. Garbuio

Rhodopsin:
retinal photoisomerization
osca Conte, NAST project with L. Guidoni





Flavin
Cannuccia

Conclusions and Perspectives

- WHAT WE DO

ab-initio electronic and optical properties of 0-3D systems

- WHAT WE CAN DO WITH SOME EFFORT..

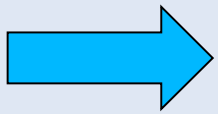
200 atoms all ab-initio (hybrid methods needed)

- WHAT (RIGHT NOW) WE CANNOT DO

(but we are working on it)

excited state molecular dynamics


ETSF
European
Theoretical
Spectroscopy
Facility
an initiative of the
nanoquanta
Network of Excellence
Call for projects always opened
Thank you for your attention
http://www.etsf.eu



Theory (Marsili-Del Sole)

GWΓ approch
to band energies calculations

Theory (Sangalli)

Casida's approach to TDDFT

$$\chi(\omega) = \chi_{KS}(\omega) + \chi_{KS}(\omega) f_{Hxc}(\omega) \chi(\omega) \tag{1}$$

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_I \\ Y_I \end{pmatrix} = \omega_I \begin{pmatrix} X_I \\ Y_I \end{pmatrix} \tag{2}$$

$$A_{ij\sigma,hk\tau} = \delta_{i,h}\delta_{j,k}\delta_{\sigma,\tau}(\epsilon_{i\sigma} - \epsilon_{j\sigma}) + f^{Hxc}_{ij\sigma,hk\tau}(\omega)$$

$$B_{ij\sigma,hk\tau} = f^{Hxc}_{ij\sigma,kh\tau}(\omega)$$

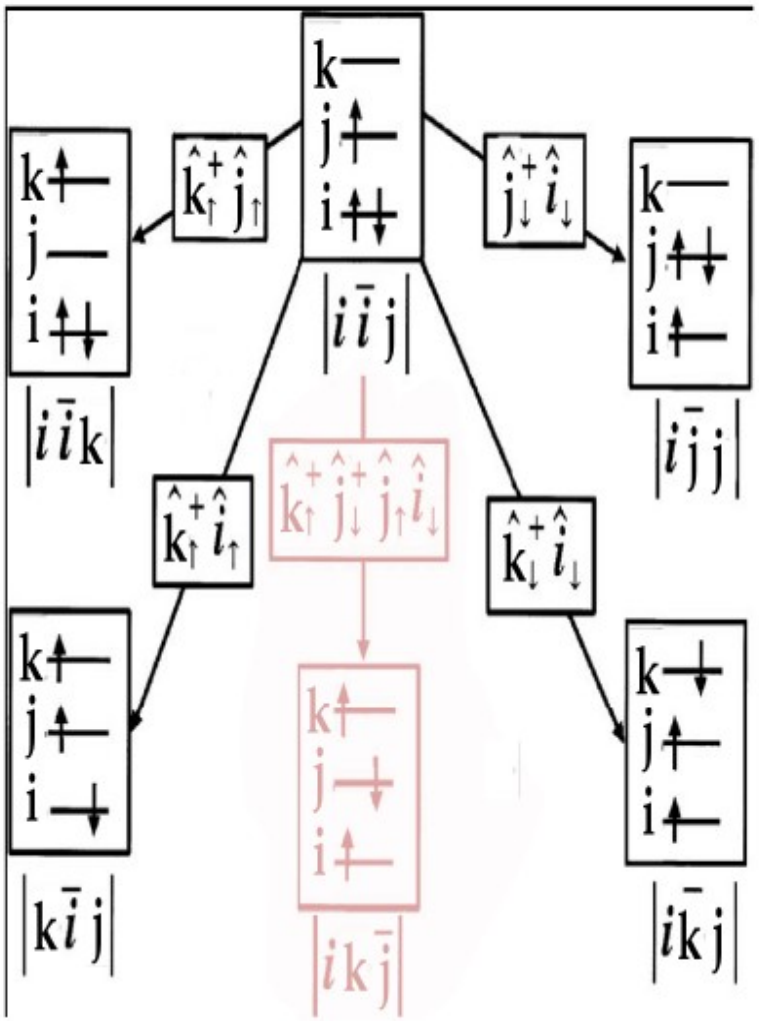
$$f^{Hxc}_{ij\sigma,hk\tau} = \int d^3\mathbf{r} d^3\mathbf{r}' \psi_{i\sigma}(\mathbf{r})\psi^*_{j\sigma}(\mathbf{r}) \left[\frac{1}{|\mathbf{r} - \mathbf{r}'|} + f^{xc}_{\sigma\tau}(\mathbf{r}, \mathbf{r}'; \omega) \right] \psi^*_{h\tau}(\mathbf{r}')\psi_{k\tau}(\mathbf{r}') \tag{3}$$

- Matrix elements dimension = number of Khon-Sham single excitations (N)
- If $f_{xc}(\omega) \simeq f_{xc}(0) \rightarrow$ N solutions!
- $\Psi \simeq \sum_{ij\sigma} X_{ij\sigma} \hat{a}^\dagger_{j\sigma} \hat{a}_{i\sigma} \Psi_0$

Theory (Sangalli)

Why double excitations are important: spin symmetry

An open shell system



Complete basis

$$\Phi^2_{1/2} = |i\bar{i}k\rangle$$
$$\Phi^2_{1/2} = |i\bar{j}j\rangle$$
$$\Phi^2_{1/2} = \frac{1}{\sqrt{2}}(|\bar{i}jk\rangle - |ij\bar{k}\rangle)$$
$$\Phi^2_{1/2} = \frac{1}{\sqrt{6}}(|\bar{i}jk + |ij\bar{k}\rangle - 2|i\bar{j}k\rangle)$$
$$\Phi^4_{1/2} = \frac{1}{\sqrt{3}}(|\bar{i}jk\rangle + |ij\bar{k}\rangle + |i\bar{j}k\rangle)$$

TDDFT (ALDA!)

$$\Phi^2_{1/2} = |i\bar{i}k\rangle$$
$$\Phi^2_{1/2} = |i\bar{j}j\rangle$$
$$\Phi^2_{1/2} = \frac{1}{\sqrt{2}}(|\bar{i}jk\rangle - |ij\bar{k}\rangle)$$

"Triplet":

$$\Phi^3_{1/2} = \frac{1}{\sqrt{2}}(|\bar{i}jk\rangle + |ij\bar{k}\rangle)$$

Theory (Sangalli)

Mathematical point of view

$$\begin{pmatrix} S & C \\ C^\dagger & D \end{pmatrix} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \end{pmatrix} = \omega_I \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \end{pmatrix} \tag{4}$$

$$\left(S + C(\omega_I - D)^{-1} C^\dagger\right) \mathbf{e}_1 = \omega_I \mathbf{e}_1 \ . \tag{5}$$

Contraction from n-dimensional space to m-dimensional subspace

Structure of the matrix

- If $n = 3$ and $m = 2$:

$$C(\omega_I - D)^{-1} C^\dagger = \frac{1}{\omega - d} \begin{pmatrix} a^2 & ab \\ ba & b^2 \end{pmatrix}$$

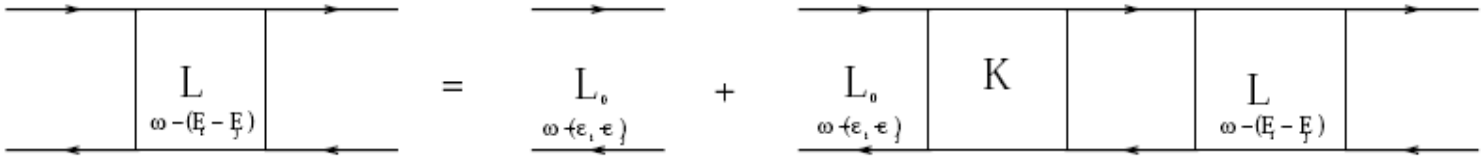
This comes from the product

$$C \ C^\dagger = \begin{pmatrix} a \\ b \end{pmatrix} (a \ b)$$

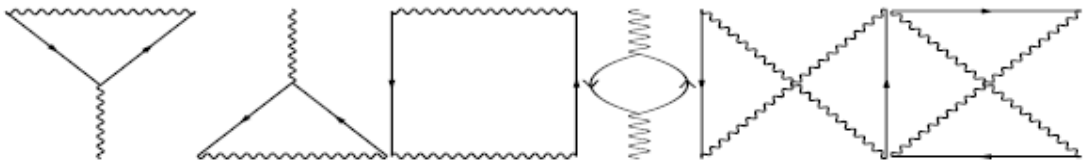
Theory (Sangalli)

The physics behind the kernel

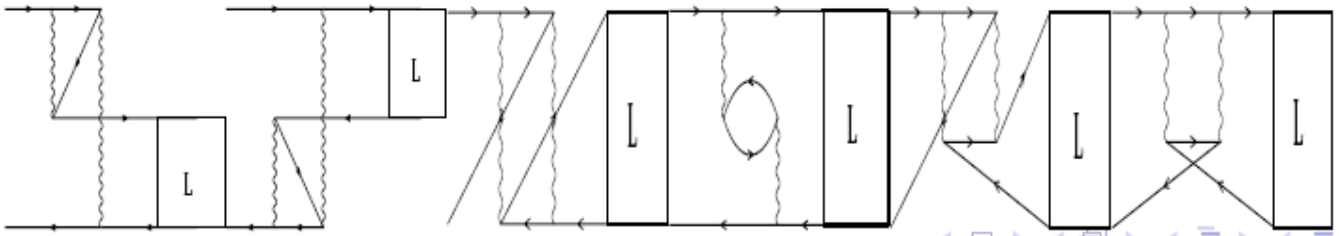
- The dynamic kernel moves the poles from L_0 to L



- Second order kernel respect coulom potential U_0.



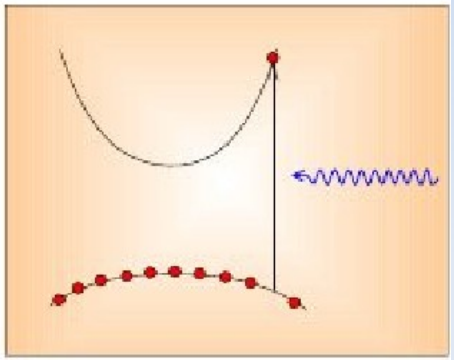
- Diagrams (deformed)...we see double excitations.



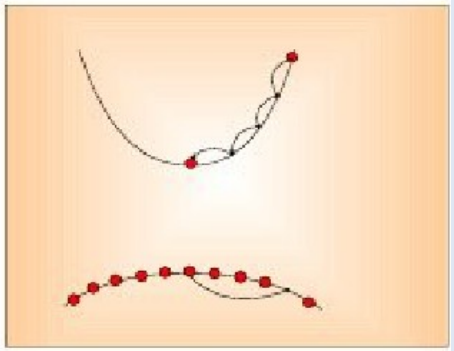
Theory (Attacalite-Marini)

Luminescence by using non-equilibrium Green Function

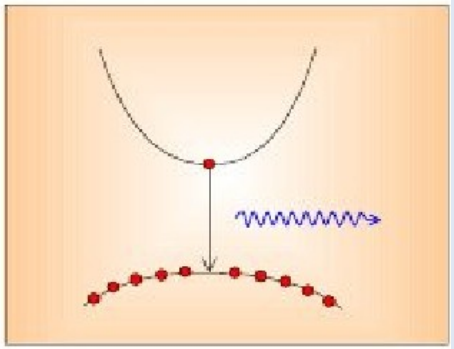
(1) Excitation with laser pulse (25 fs … 400 fs)



(2) Relaxation via phonons (100 fs … 3 ps)



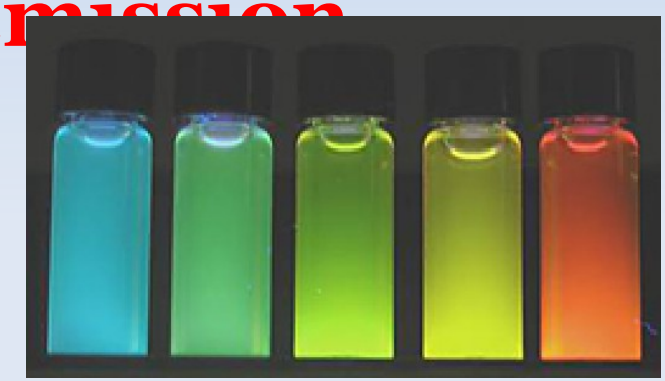
(3) Recombination/ Photoluminescence (PL) (> 100 ps)



Theory (Attacalite-Marini)

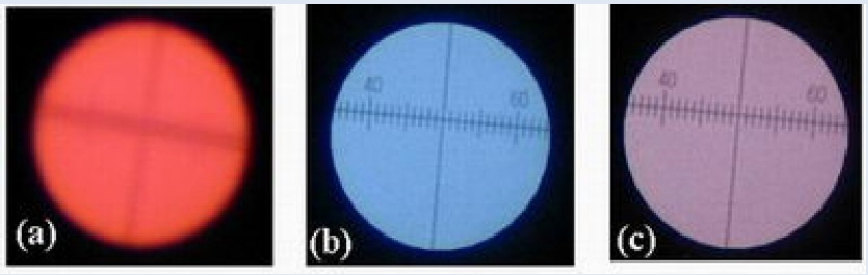
Prospective:

Create a theoretical and computational tool to study and predict light emission



1) Luminescence:

Catho and photo luminescence

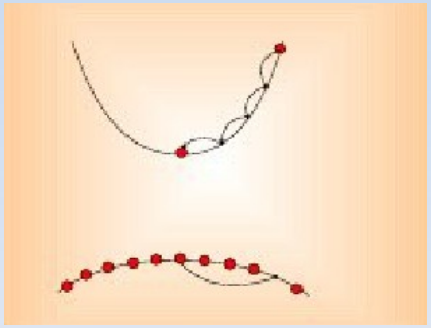


2) Role of **temperature**, **defects** and **confinement**

3) Non-linear Optics,
optical gain, Optical Switching

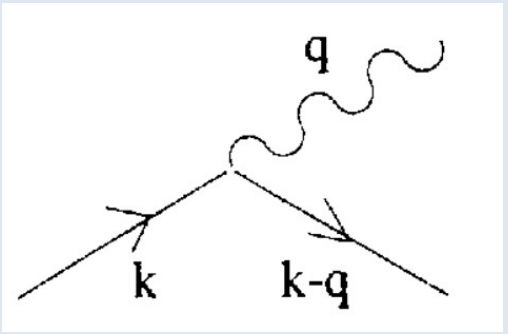
Theory (Attacalite-Marini)

Working Plan



I. **Real-time dynamics of electrons**
by using Non-Equilibrium Green Functions.
Luminescence of bulk materials

$$(i\frac{\partial}{\partial t_1} - H_0)G^<(t_1, t_2) = [U(t_1) + \Sigma^{HF}(t_1)]G^<(t_1, t_2) + I^<(t_1, t_2)$$



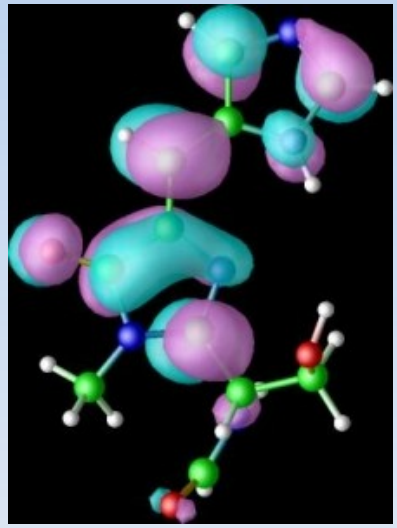
II. **Electron-phonon coupling**.
Relaxation through emission of phonons.
Luminescence from indirect-gap systems

$$\Sigma_k^<(t_1, t_2) = i\sum_q g_q^2 D_q^<(t_1, t_2) G_{k-q}^<(t_1, t_2)$$

III. **Forces in the excited state**.
Luminescence from cluster, wires,
polymers and defects (exciton trapping)

Theory (Attacalite-Marini)

Ab-initio Approach



The single particle electronic states are first evaluated using density functional theory (DFT)

Why Non-equilibrium Green Functions?

$$G^{<}(t_1,t_2) = i\langle a^{+}(t_2)\,a(t_1)\rangle$$

$$G^{>}(t_1,t_2) = -i\langle a(t_1)\,a^{+}(t_2)\rangle$$

Systematic approach to progressively include electronic correlation effects and electron-phonon interaction

Can be used as starting point to derive approximate theory (Kinetic equations, Bloch equations, Boltzmann equations)

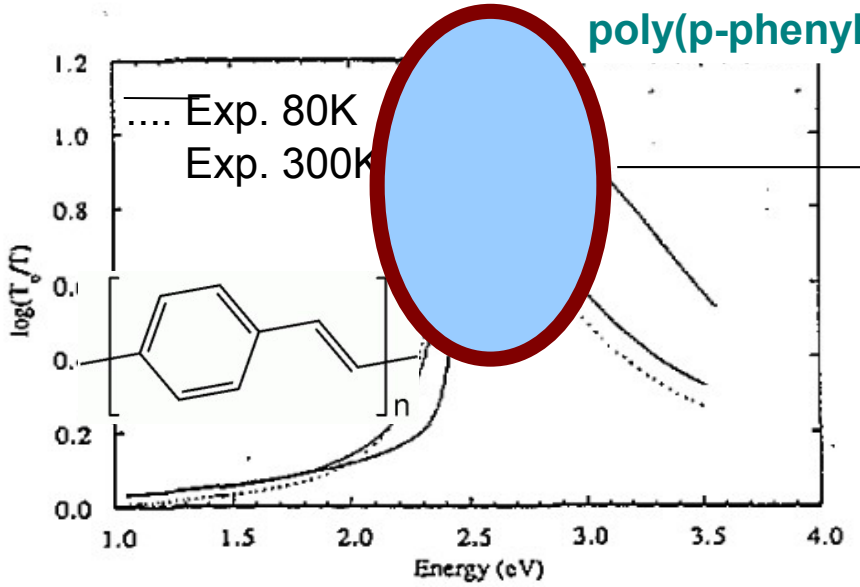
All this theory will be implemented in ->

Yambo ©

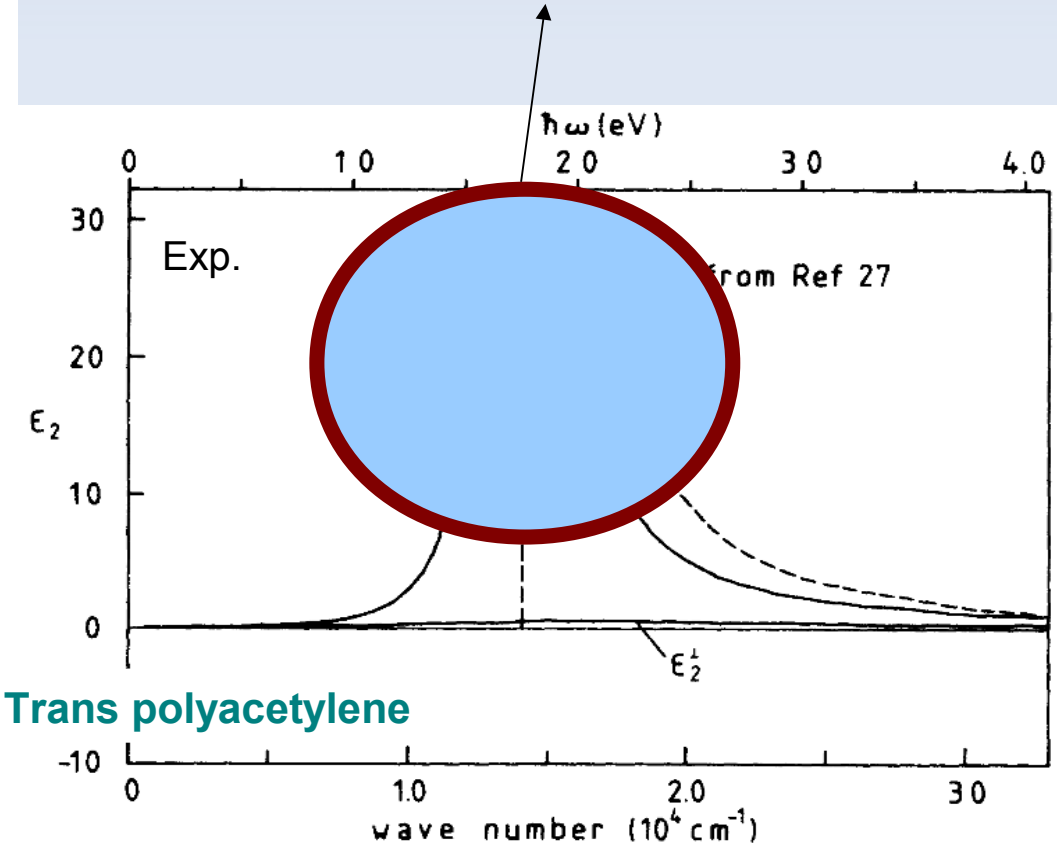
1D CONJUGATED POLYMERS (Cannuccia-Marini)

EXCITON-VIBRON INTERACTION IN ONE DIMENSIONAL CONJUGATED POLYMERS

poly(p-phenylene vinylene)



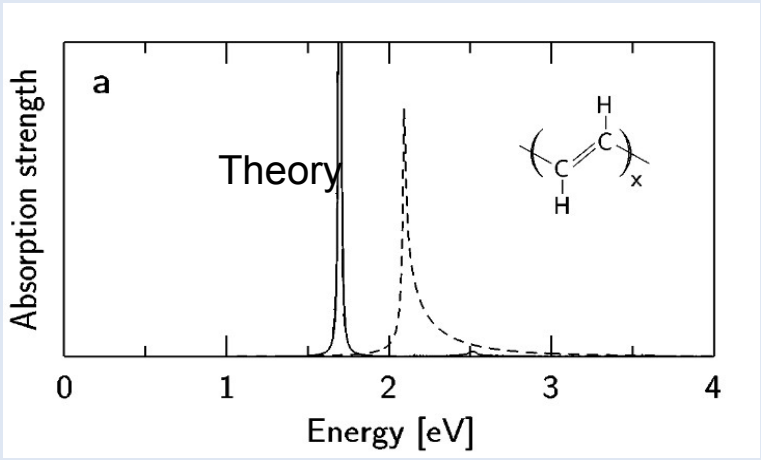
Bound exciton characterized by an **asymmetric line-shape,** together with strong **vibronic-induced side bands**



Trans polyacetylene

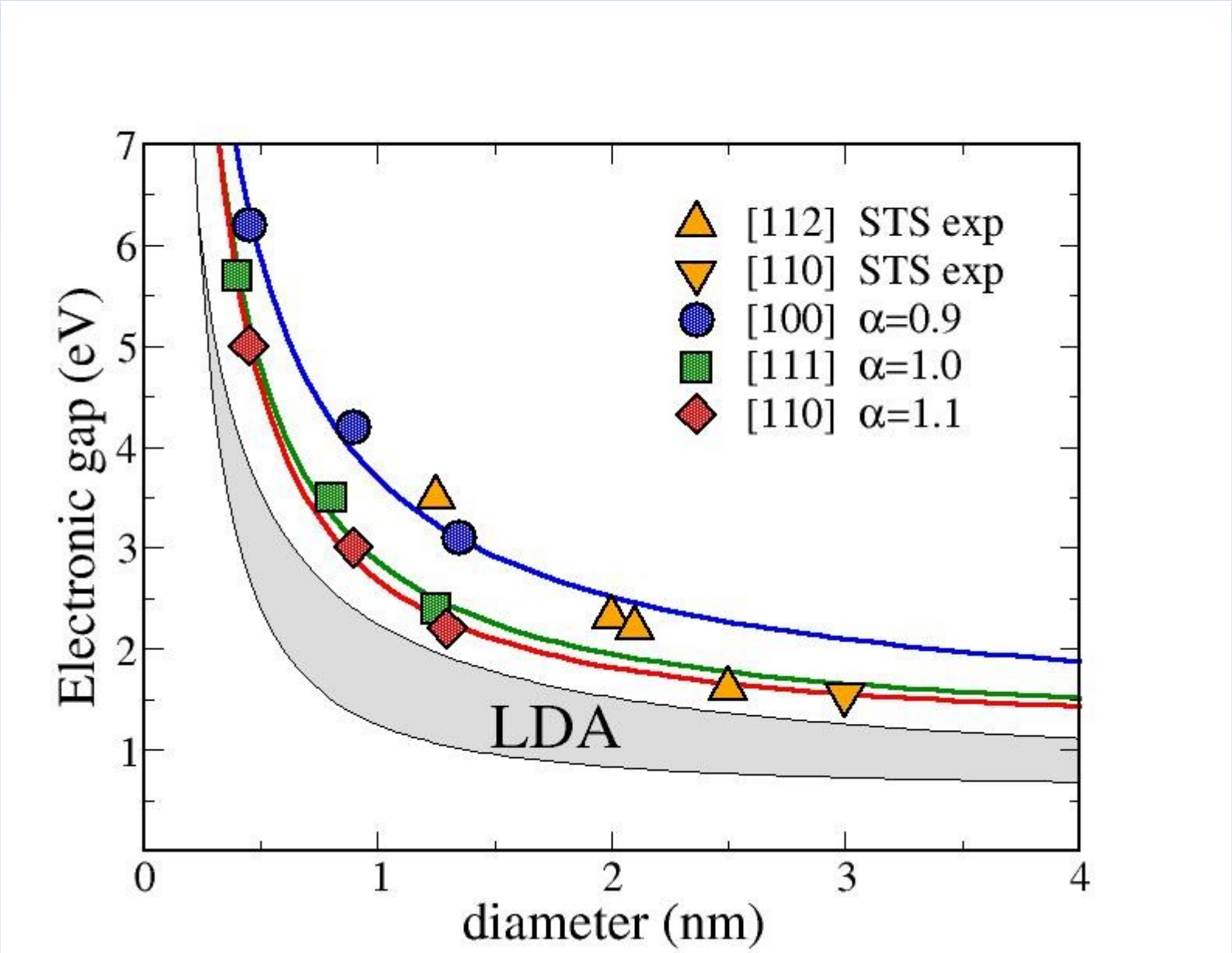
Phys. Rev. B 38, 10313 - 10322 (1988)

K Pichler et al 1993 J. Phys.: Condens. Matter 5 7155



Phys. Rev. Lett. 82, 1959 - 1962 (1999)

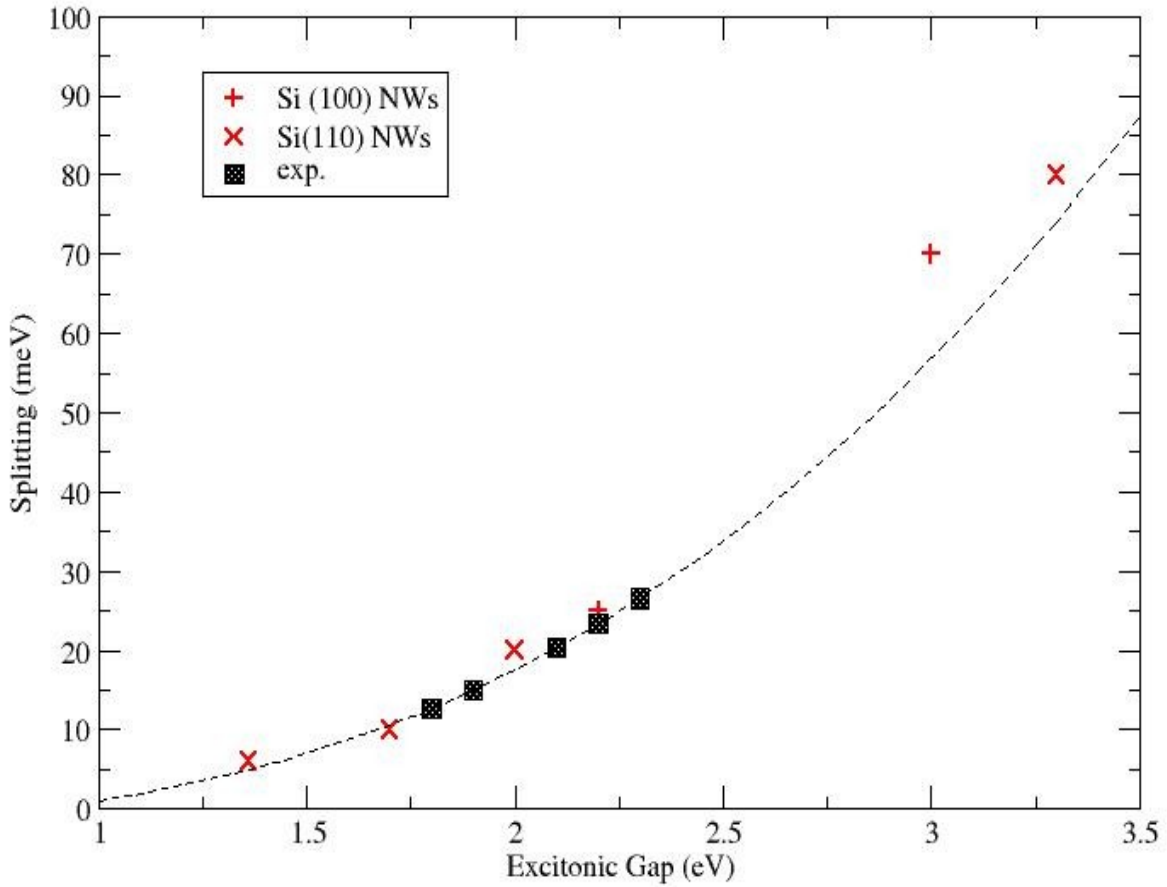
1D nanowires (Palummo)



Experiment: Ma et al., Science 2003

1D nanowires (Palummo)

Si NWs Exchange splitting : BSE theory vs Exp.



YAMBO (Hogan-Marini)

Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

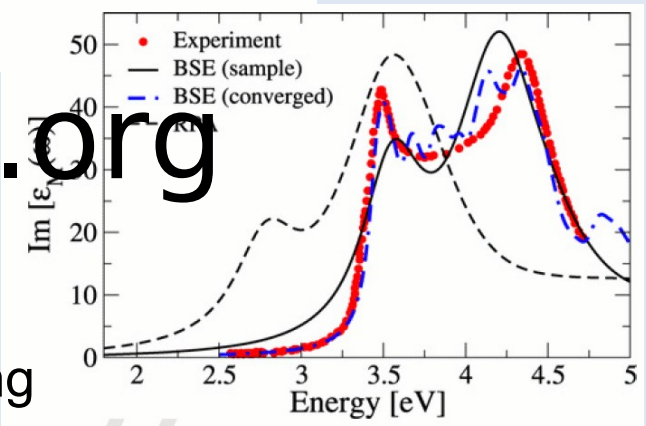
doi:10.1016/j.cpc.2009.02.003

yambo: An *ab initio* tool for excited state calculations ☆

Andrea Marini [a,e,*], Conor Hogan [b,e], Myrta Grüning [c,e], Daniele Varsano [d,e]

[a] Dipartimento di Fisica, CNISM, and SMC Institute for Statistical Mechanics and Complexity, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, I-00133 Roma, Italy
[b] Dipartimento di Fisica and INFM-CNR, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, I-00133 Roma, Italy
[c] Unité PCPM, Université Catholique de Louvain, 1348 Louvain-la-Neuve, Belgium
[d] National Center on nanoStructures and Biosystems at Surfaces (S3) of INFM-CNR, I-41100 Modena, Italy
[e] European Theoretical Spectroscopy Facility (ETSF)

Yambo ©



www.yambo-code.org

Many-body perturbation theory:

- Quasiparticle corrections (GW)
- Optical and energy loss spectra including excitons and local field effects

....and much more!

Finite temperature. Electron-phonon and polarons

Real-axis GW

Self-consistent COHSEX, HF, EXX ... (_SC)

Surface Spectroscopy

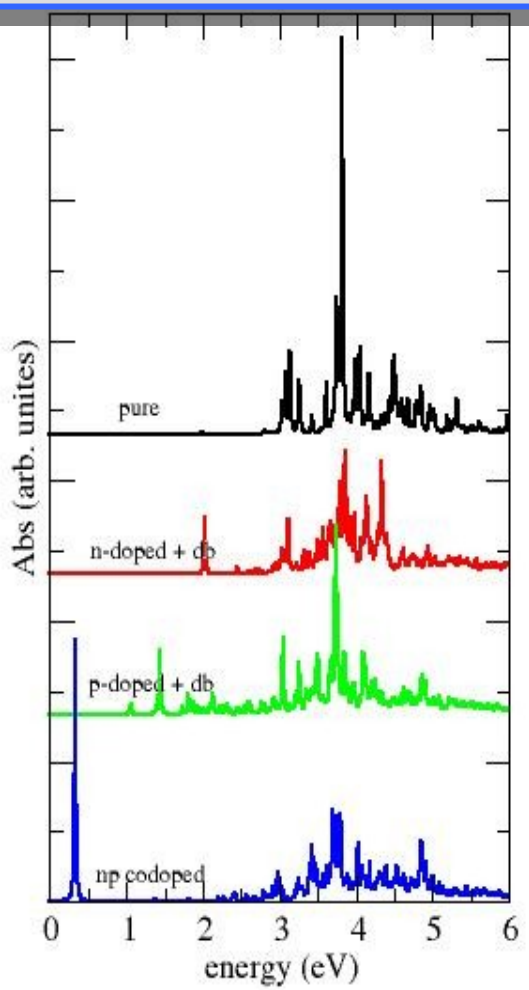
Collinear and non-collinear spin

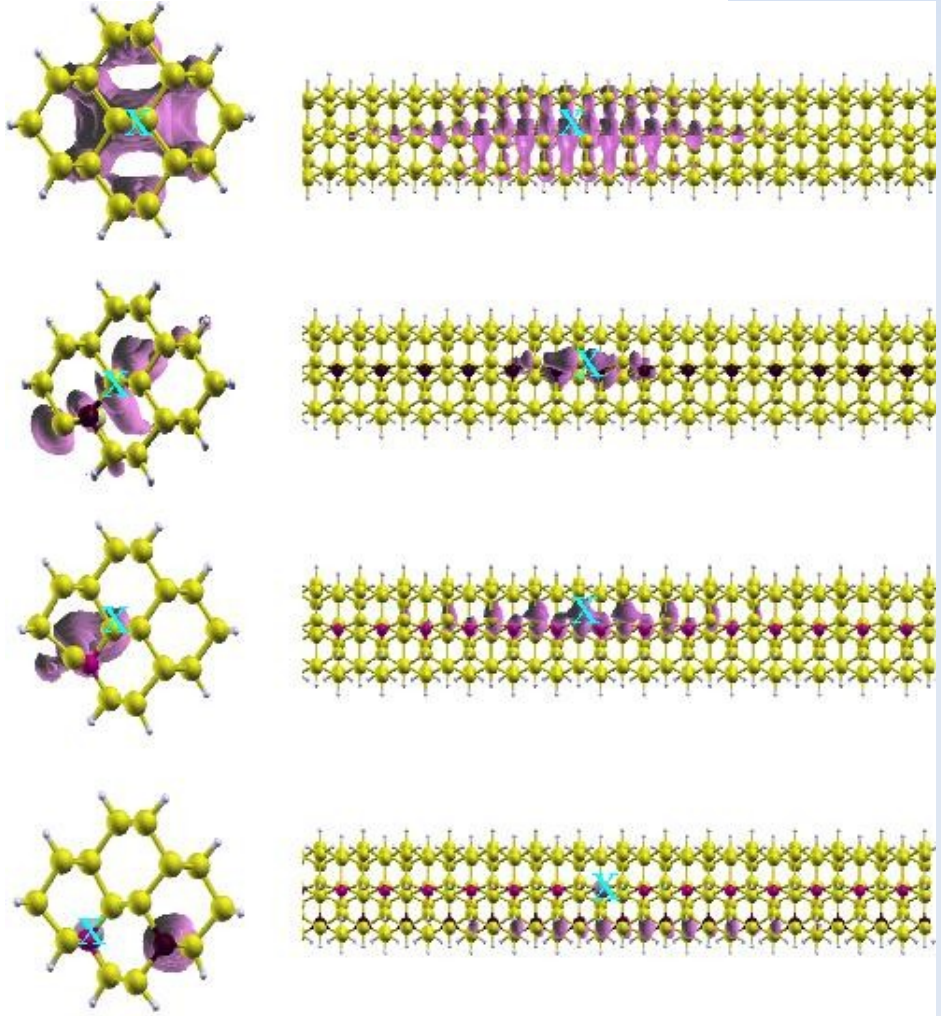
Many-Body TDDFT kernel

Total Energy (ACFDT)

1D nanowires (Palummo)

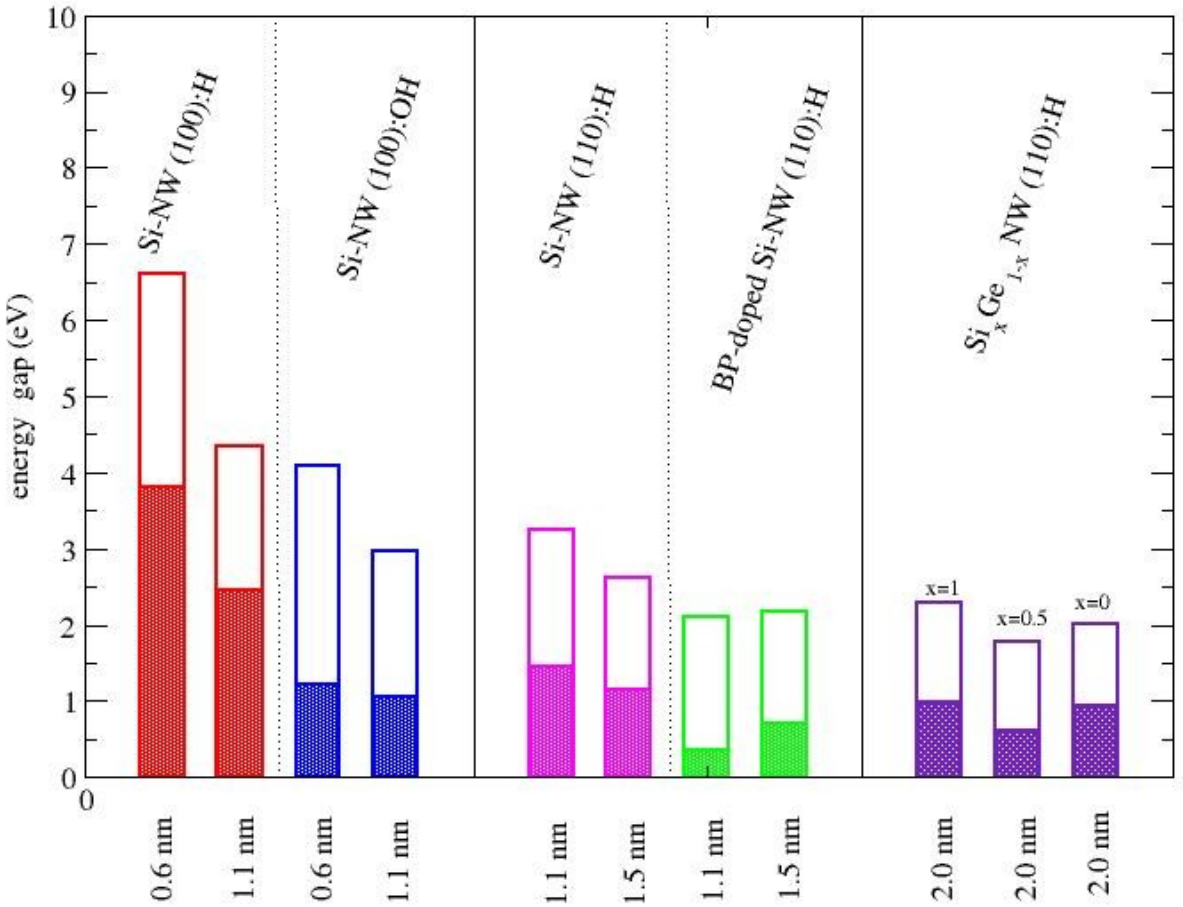
Doping Si NWs: influence on the optical properties





1D nanowires (Palummo)

GW corrections: doping and surface termination

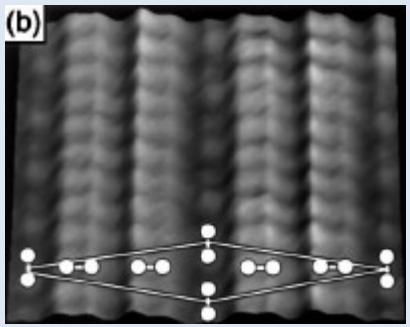


2D GaSb(001) (Hogan)

Structure and Optical Properties of Sb-stabilized GaSb(001)

Conor Hogan, Rodolfo Del Sole (Rome)

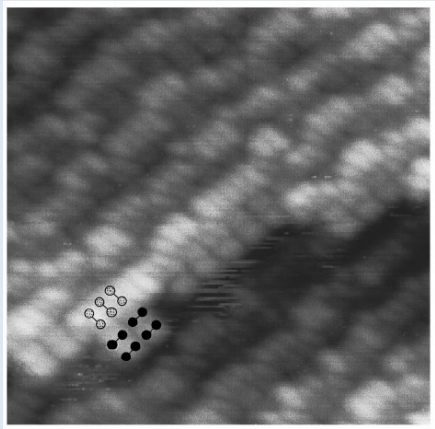
Rita Magri (Modena)



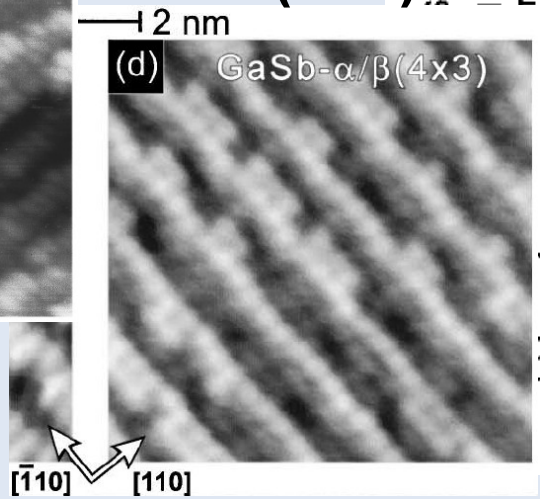
c(2x10)

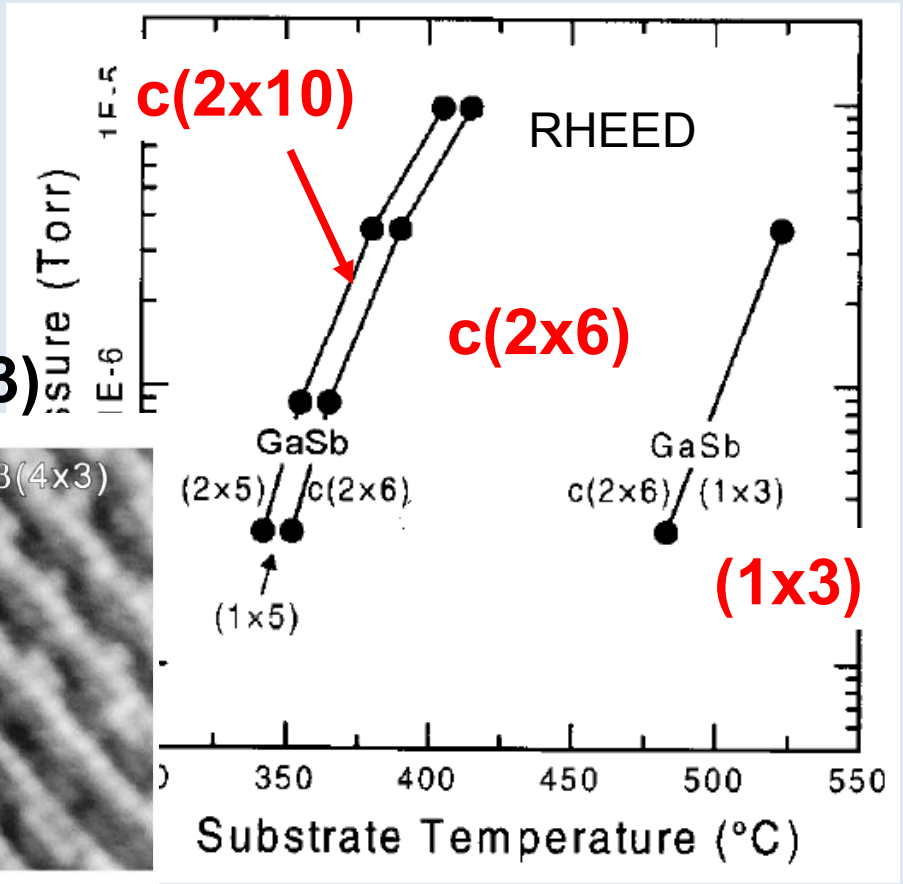
Houze (2007)
Resch-Esser (1997)
Barvosa-Carter (2000)

c(2x6)



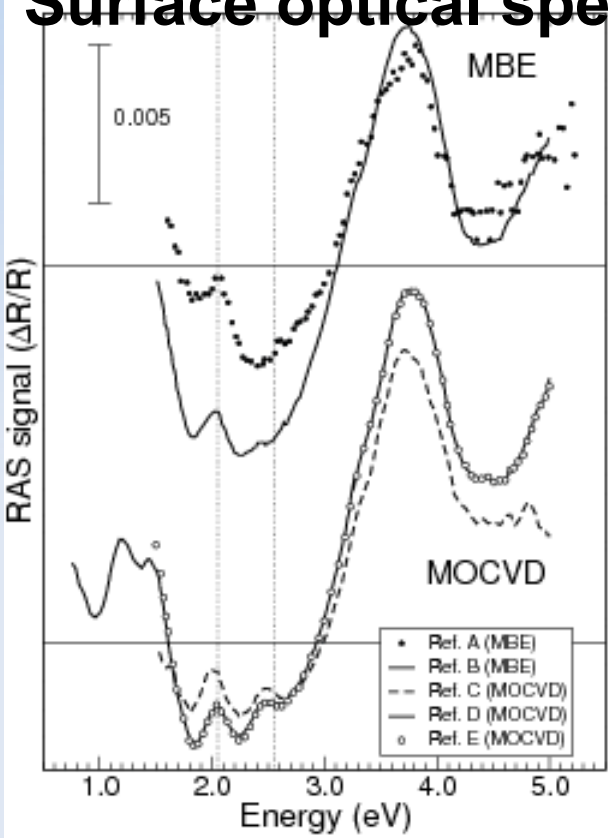
(1x3)

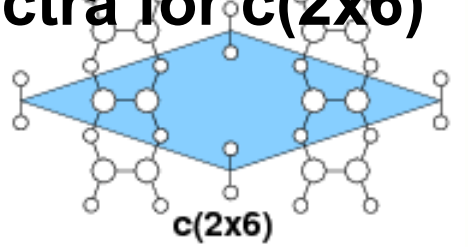


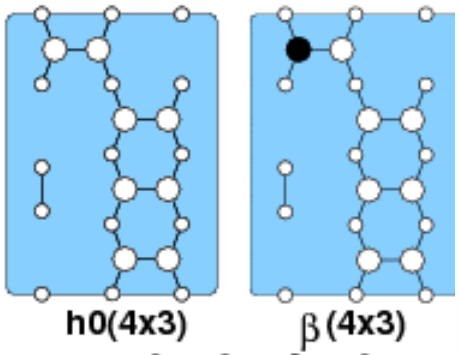


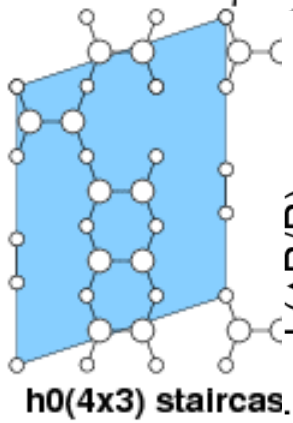
2D GaSb(001) (Hogan)

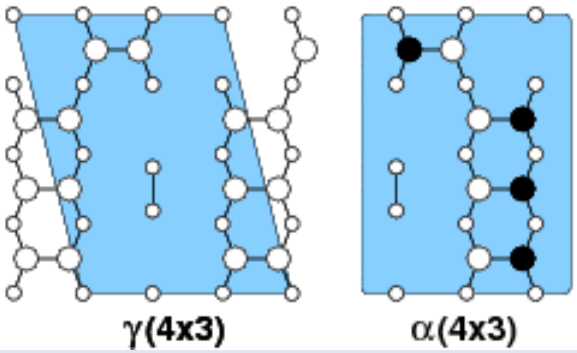
Surface optical spectra for c(2x6)

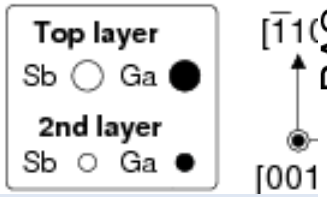


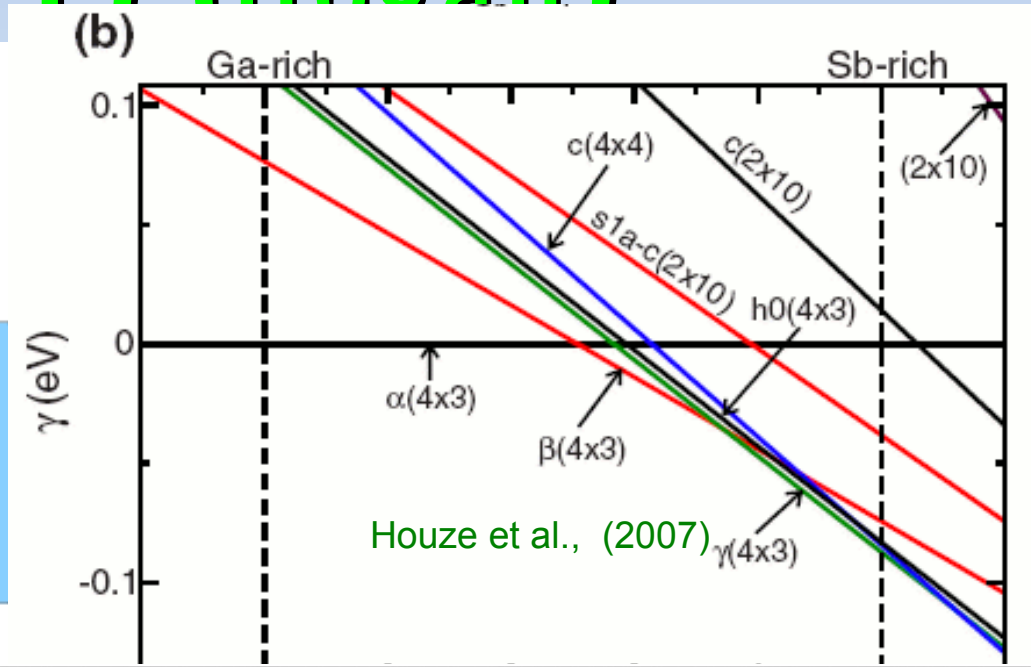


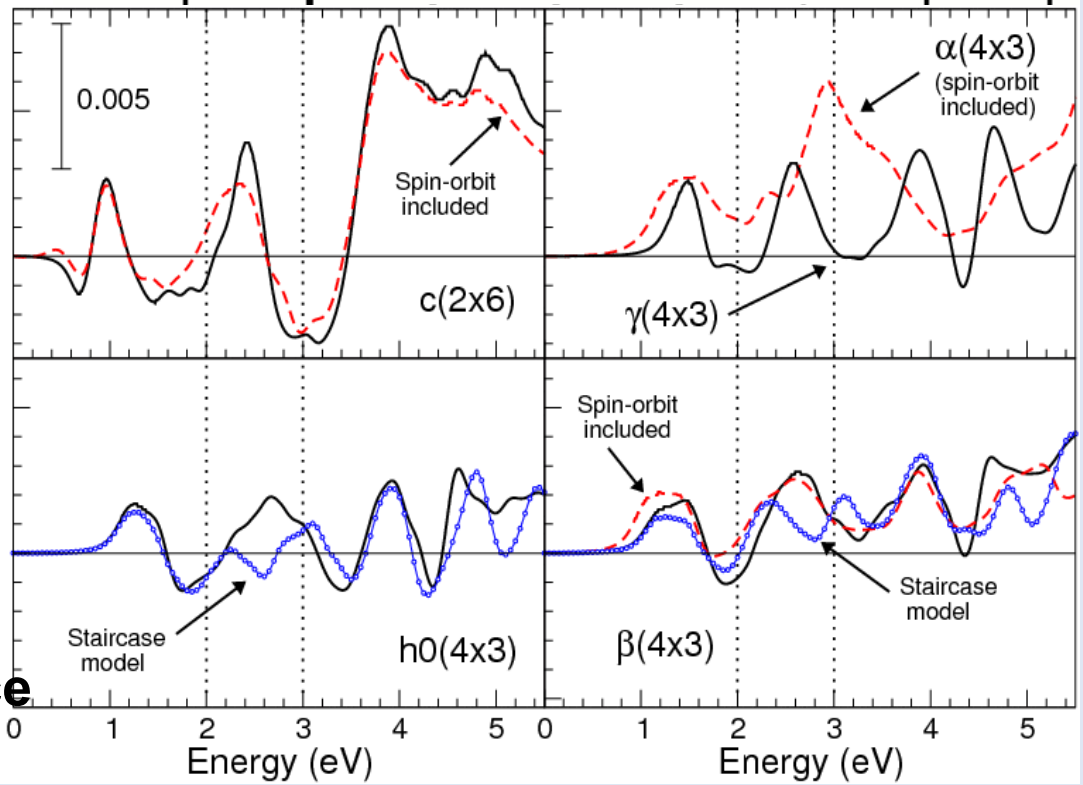












All previous structures fail to reproduce correctly the experimental RA spectra

2D GaSb(001) (Hogan)

New structure

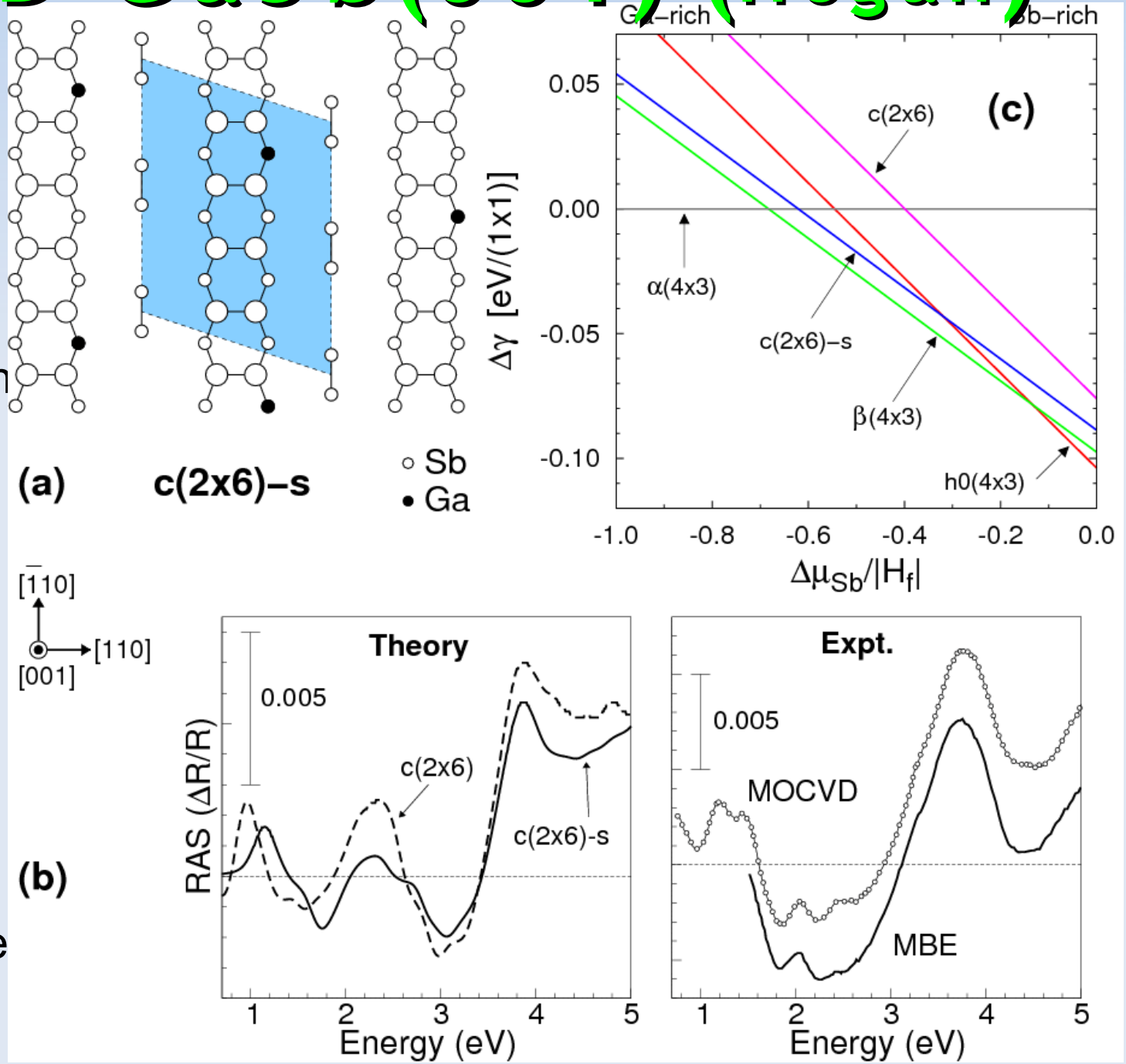
Second layer
Ga 'doping'

Electron counting
rule fulfilled
(1 Ga per (2x6) un

Low energy,
semiconducting
surface
(stable at 500C?)

Better agreement
with RA spectra

True surface base
on long chains
with interruptions

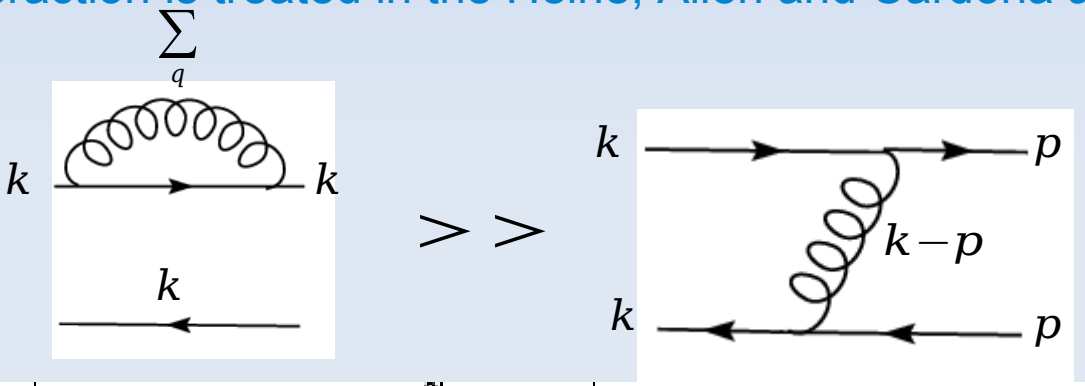


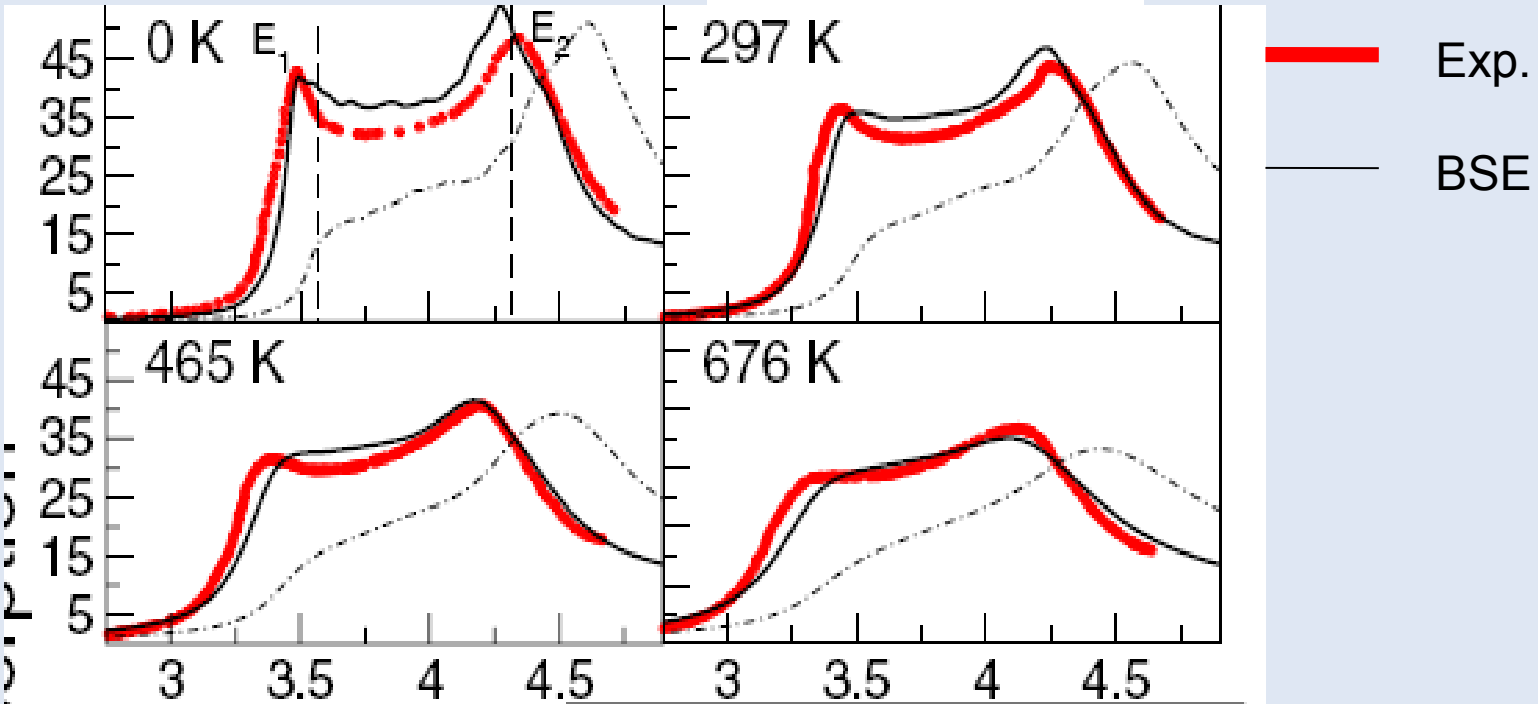
Ab-initio Finite-Temperatures Excitons

A. Marini Phys. Rev. Lett. **101**, 106405 (2008)

BSE is solved, in ab-initio manner, including the coupling with the lattice vibrations.

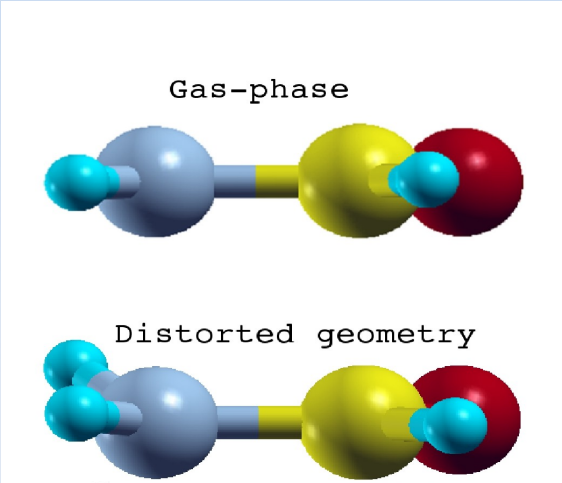
E-ph interaction is treated in the Heine, Allen and Cardona approach.

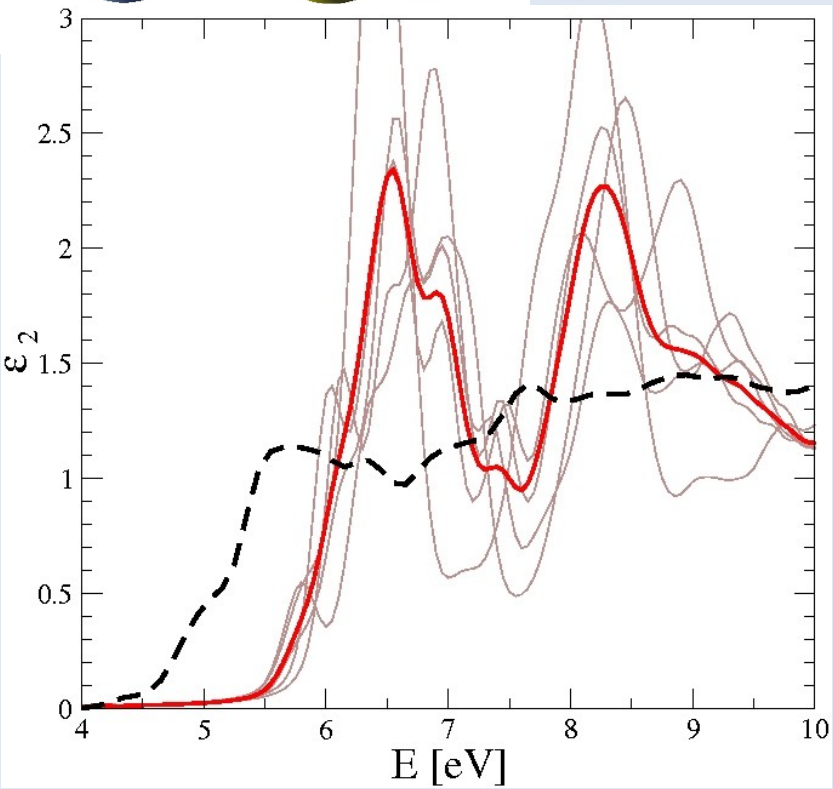


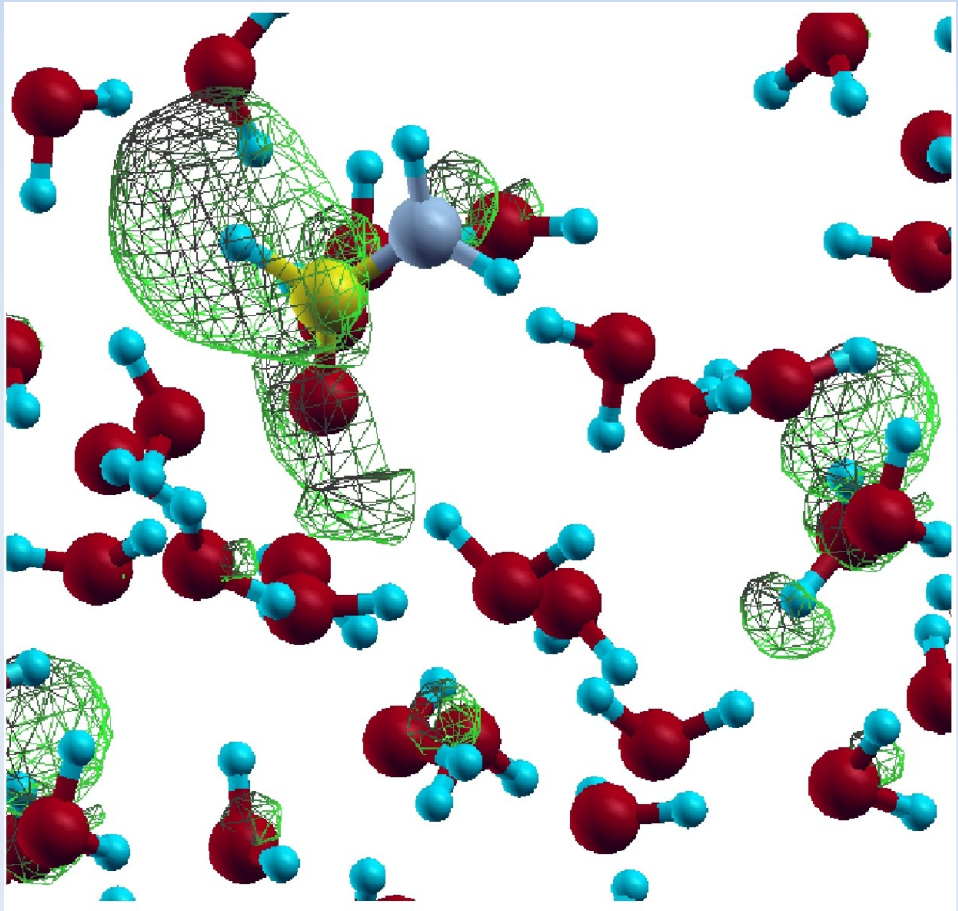


3D Bio (Garbuio-Pulci)

FORMAMIDE in water

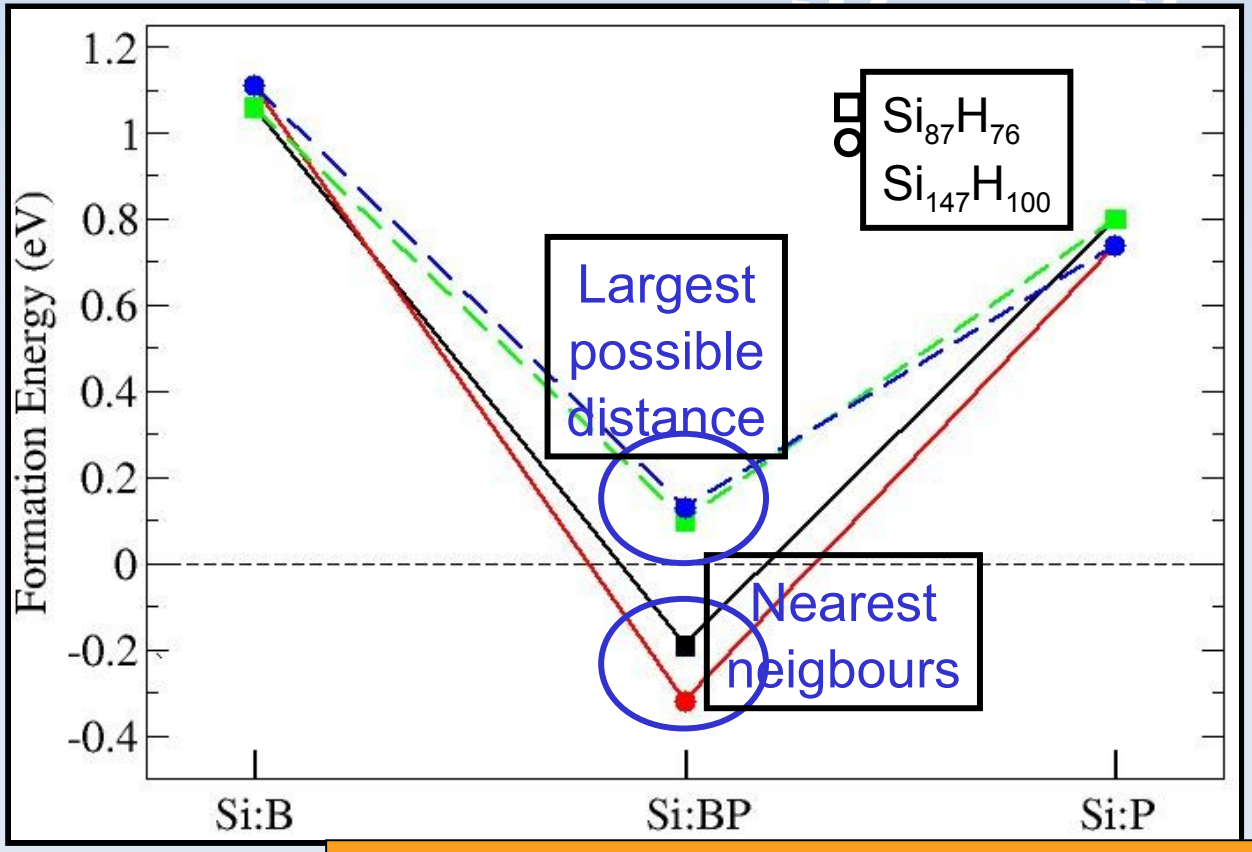






0D: nanodots

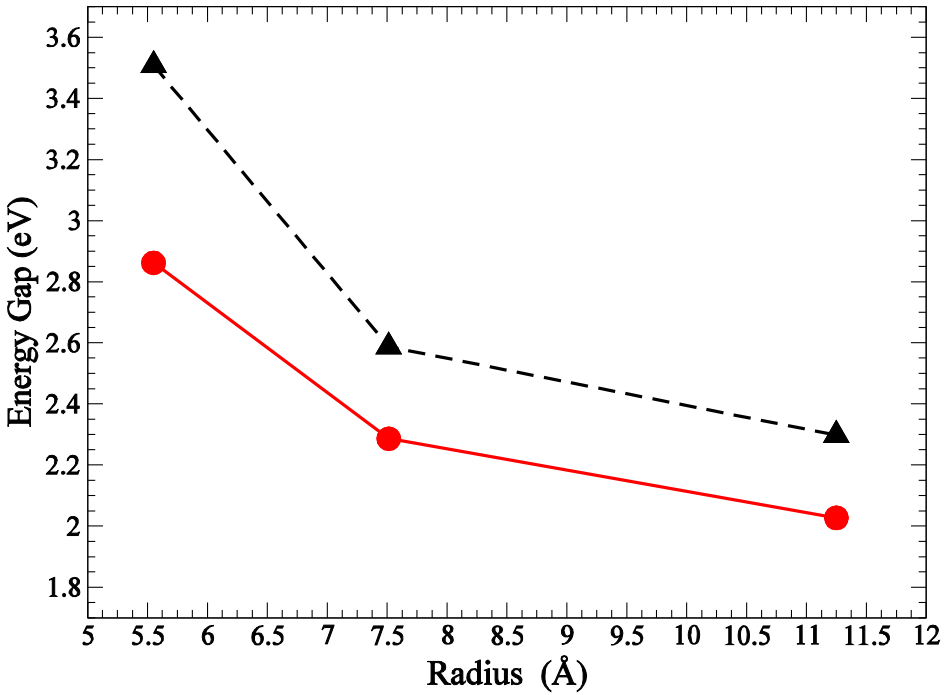
Formation energy: Single- *vs* co-doping



- Co-doping easier due to charge compensation
- No size dependence
  - **Cantele et al, *Phys. Rev. B* 72, 113303 (2005)**
  - **S. Ossicini, F. Iori et al, *Appl. Phys. Lett.* 87 173120 (2005)**
  - **F. Iori, E. Degoli, S. Ossicini et al., *J. Lum.* (2006)**

0D nanodots

Gap Homo-Lumo



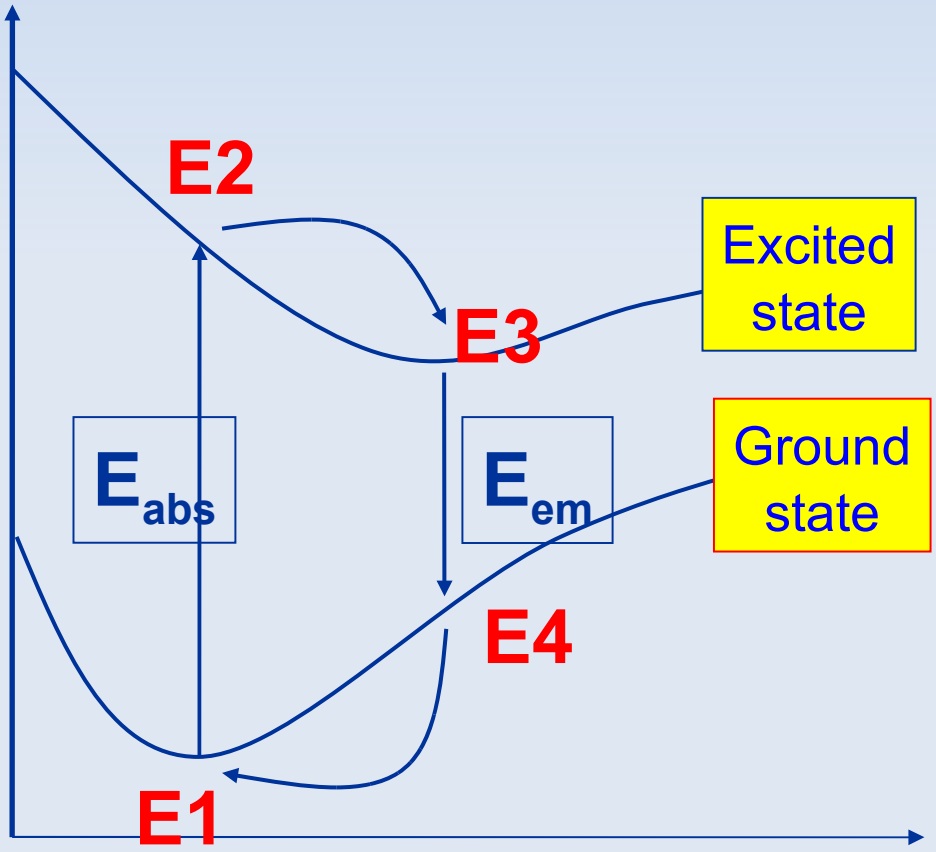
▲ undoped

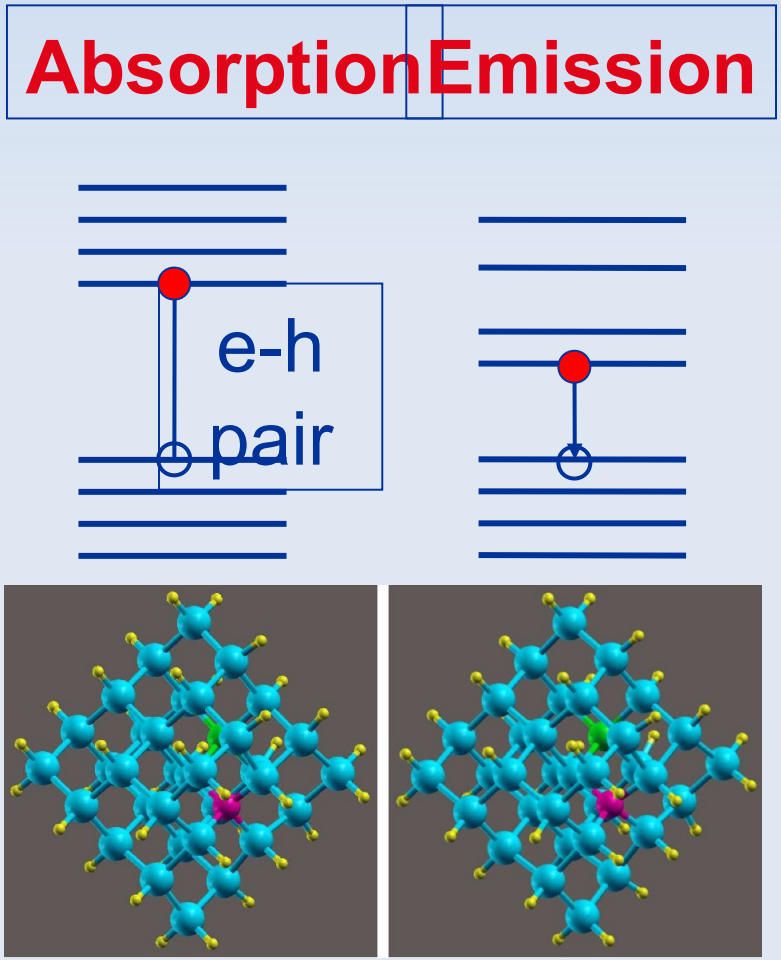
● codoped

- **Eg decrease as nc's size increase**
- **Eg of codoped is shifted towards lower energies**

0D nanodots

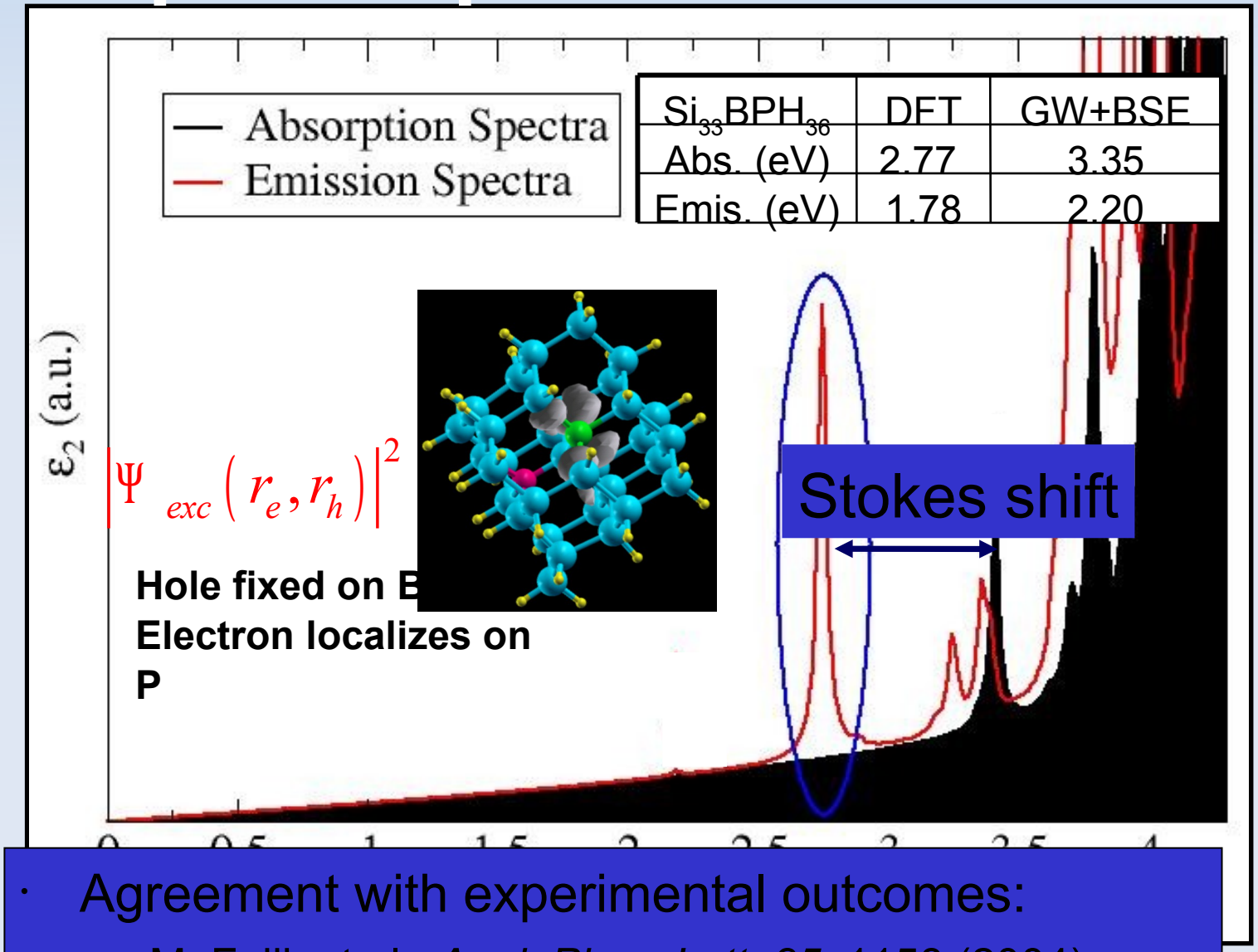
Absorption and Emission processes





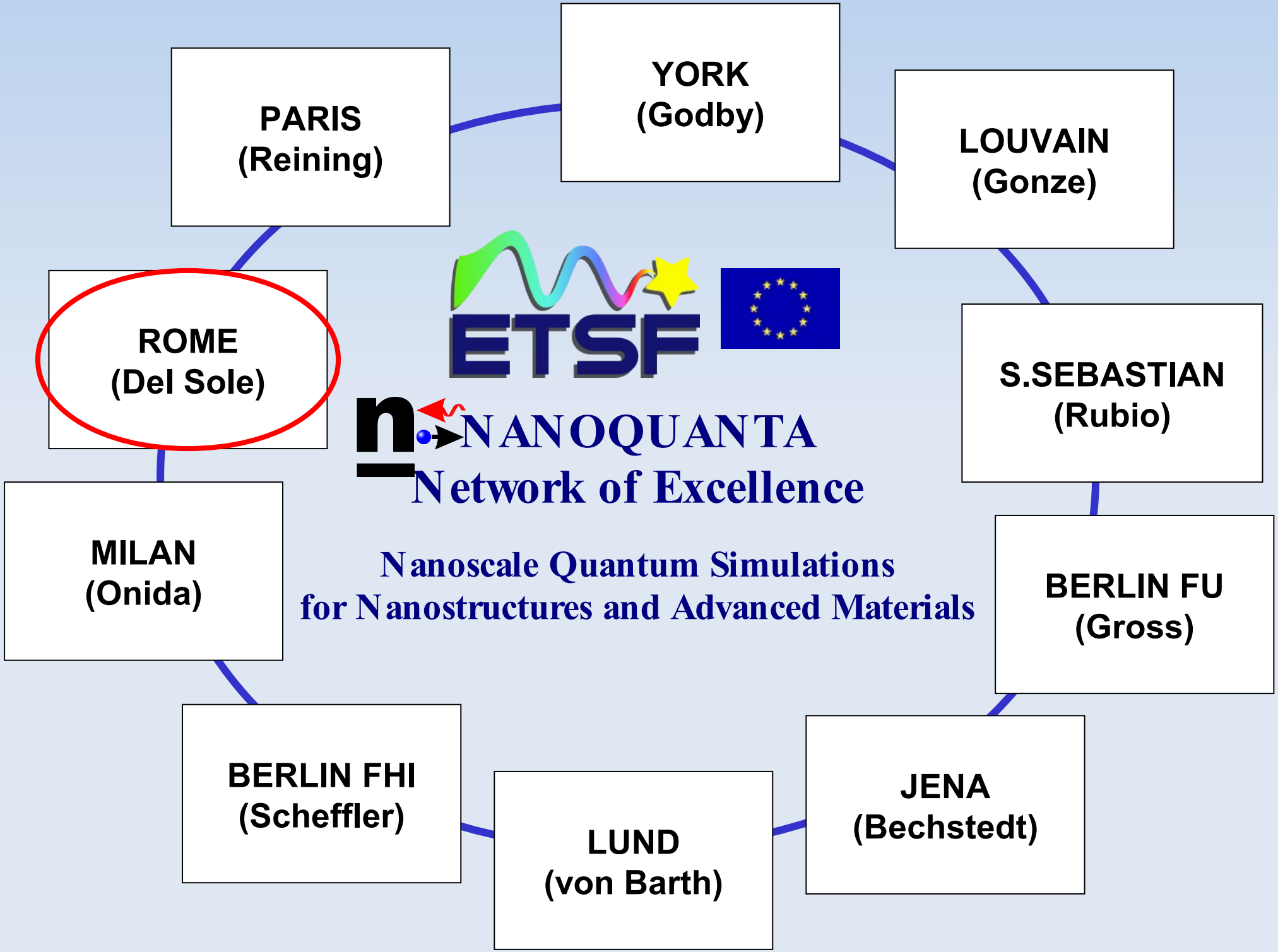
0D nanodots (Pulci-Marsili-Palummo)

Optical spectra within GW+BSE

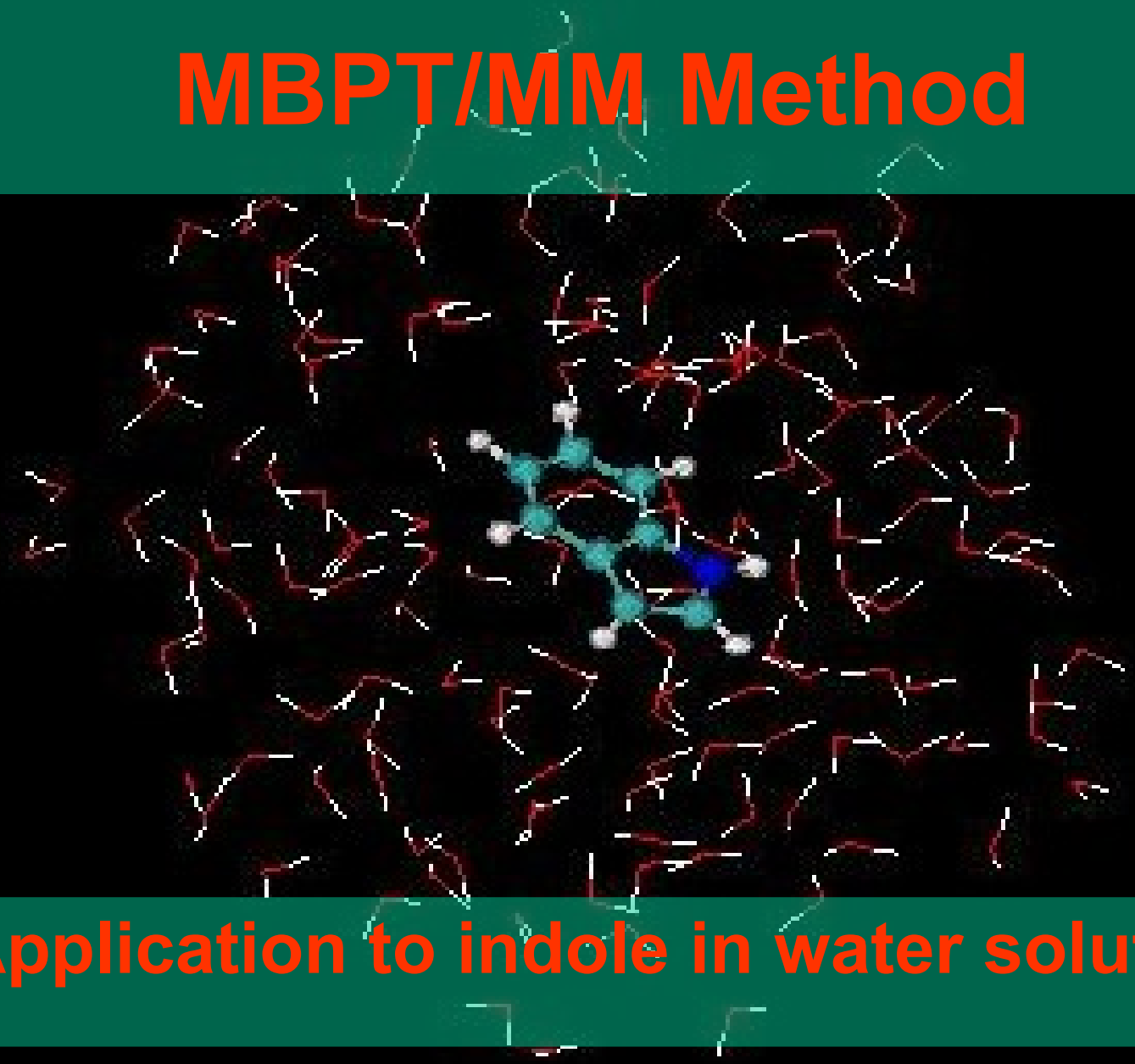


$Si_{33}BPH_{36}$	DFT	GW+BSE
Abs. (eV)	2.77	3.35
Emis. (eV)	1.78	2.20

- Agreement with experimental outcomes:
  - M. Fujii, et al., *Appl. Phys. Lett. 85*, 1158 (2004)


PARIS
(Reining)
YORK
(Godby)
LOUVAIN
(Gonze)
ROME
(Del Sole)
ETSF
S.SEBASTIAN
(Rubio)
NANOQUANTA
Network of Excellence
Nanoscale Quantum Simulations
for Nanostructures and Advanced Materials
MILAN
(Onida)
BERLIN FU
(Gross)
BERLIN FHI
(Scheffler)
JENA
(Bechstedt)
LUND
(von Barth)

MBPT/MM Method

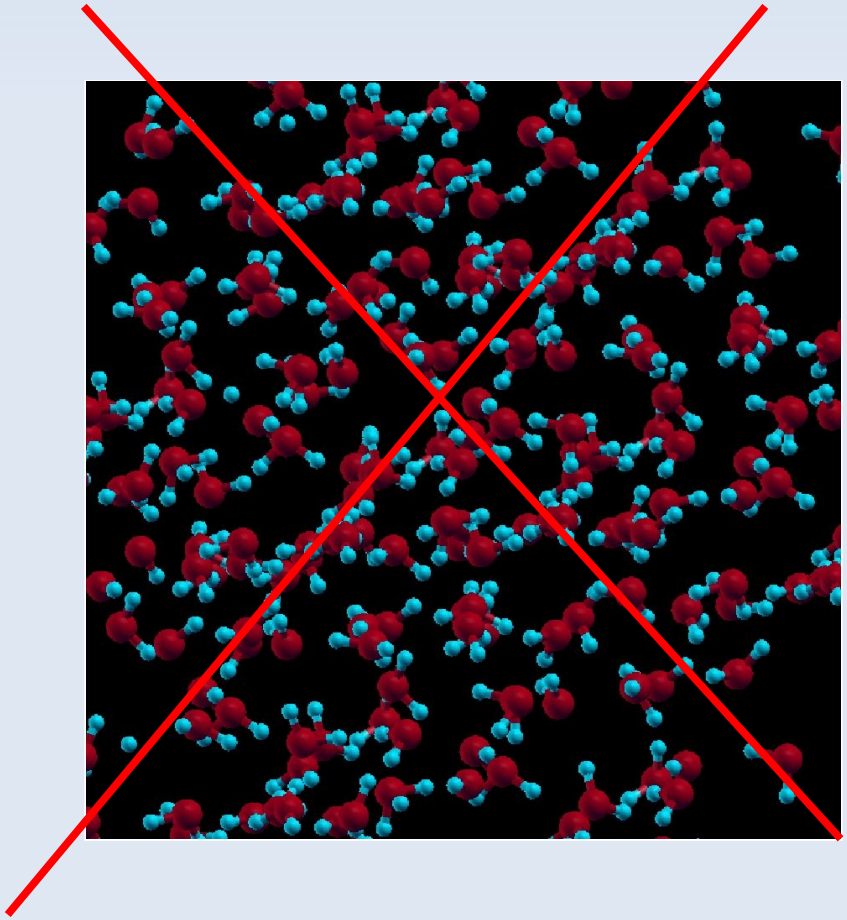


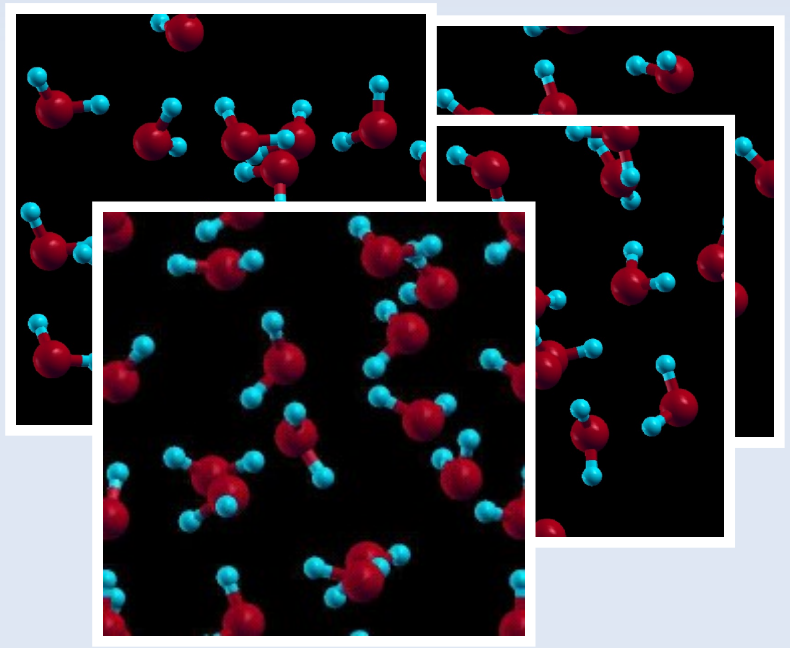
Application to indole in water solution

3D Bio (Garbuio-Pulci)

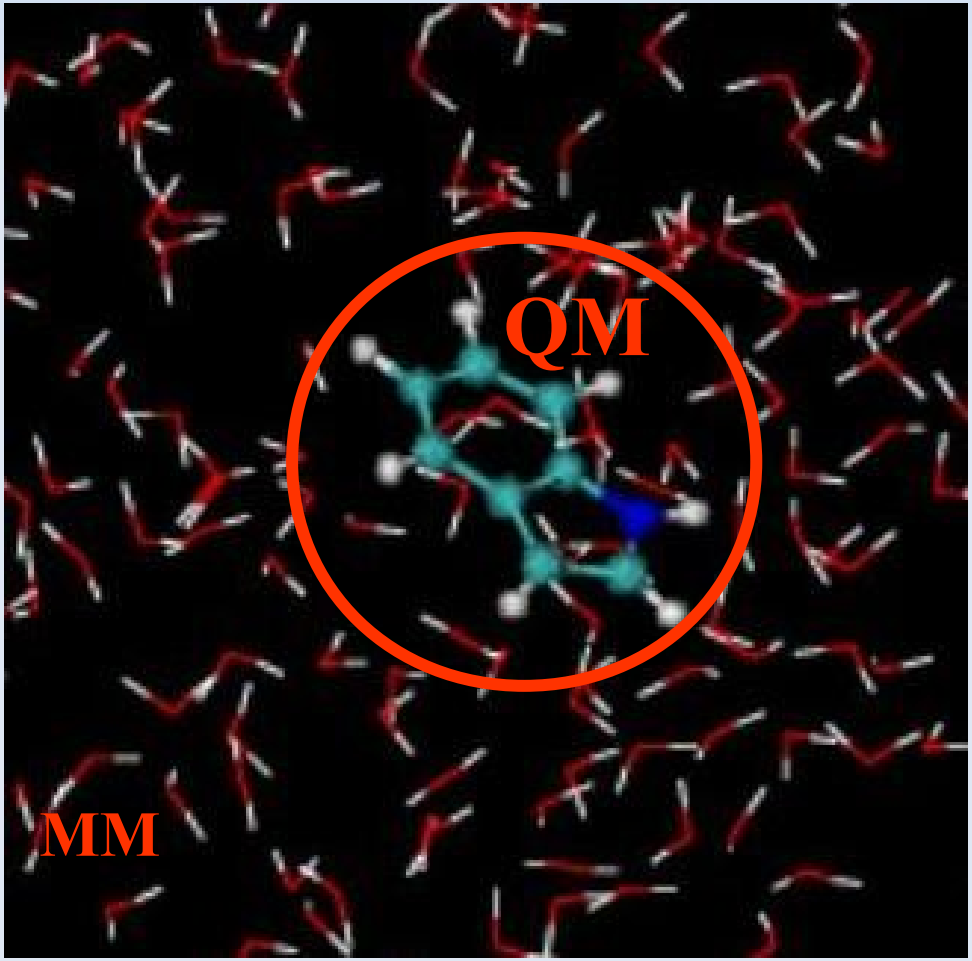
LIQUID WATER

Liquid water = disordered system= huge unit cell





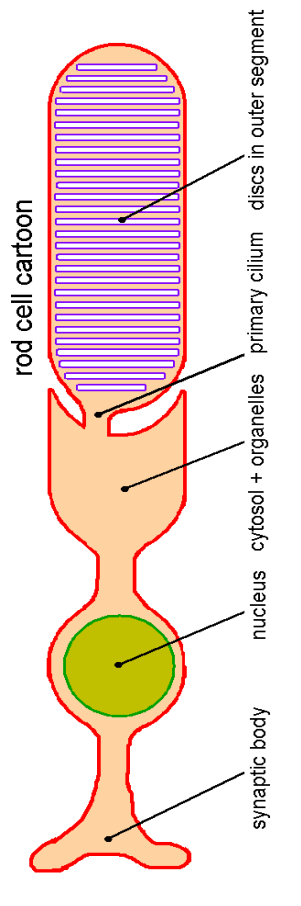
20 MD snapshots and average of results.

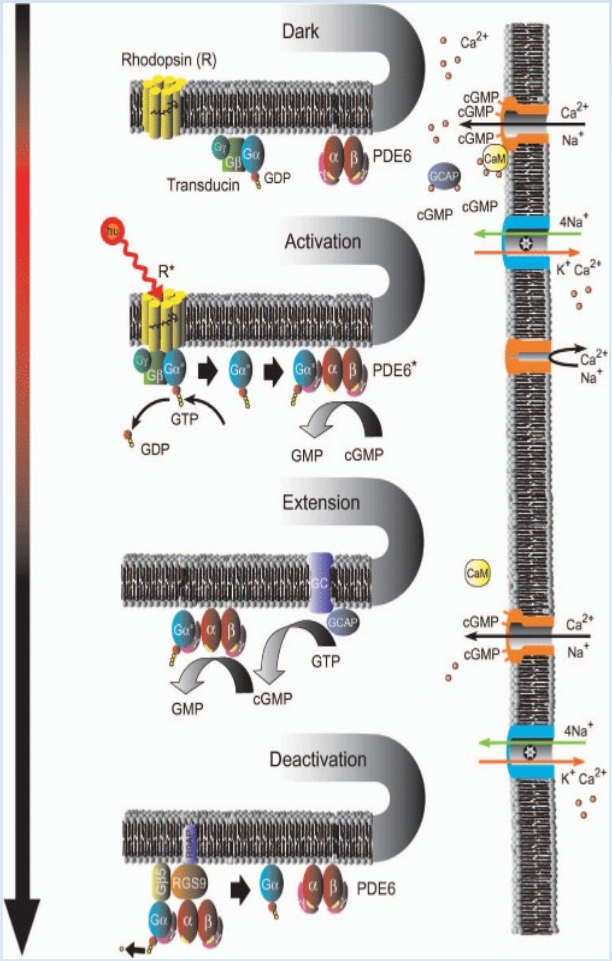

QM
MM

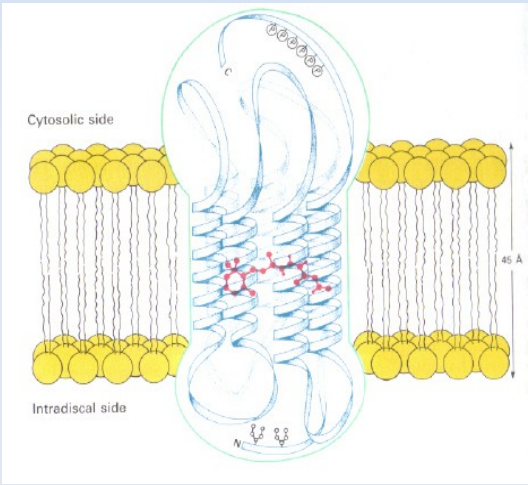
3D Bio (Mosca Conte-Pulci)

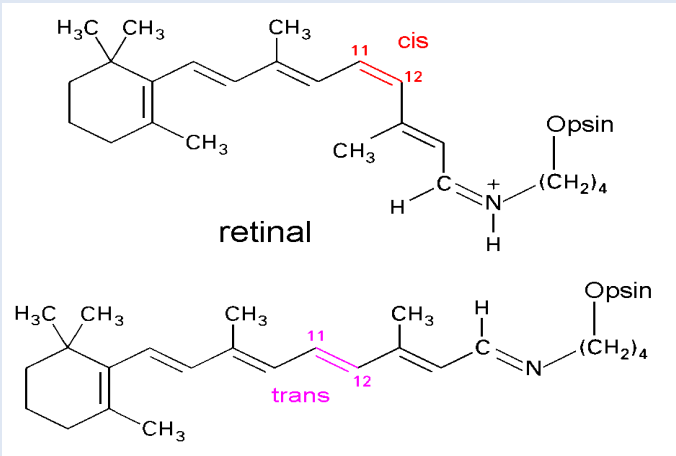
PHOTO-ISOMERIZATION OF RETINAL IN RHODOPSIN

FIRSTS STEPS OF THE MECHANISMS OF VISION IN LIVING BEINGS







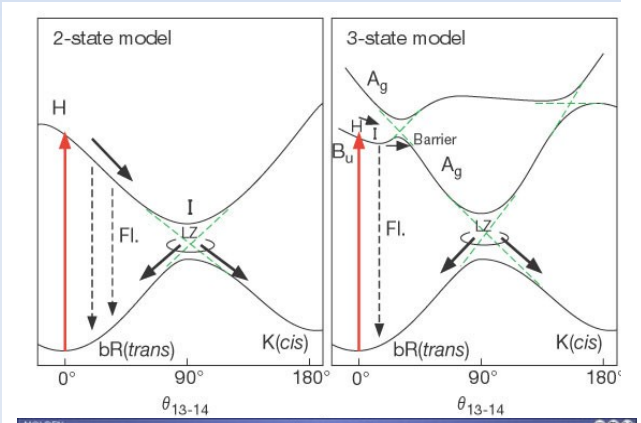


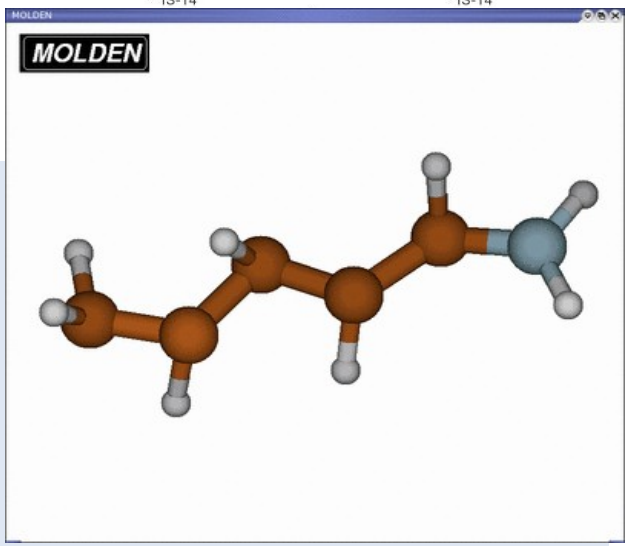
Adriano Mosca Conte, Olivia Pulci, Rodolfo Del Sole, Leonardo Guidoni

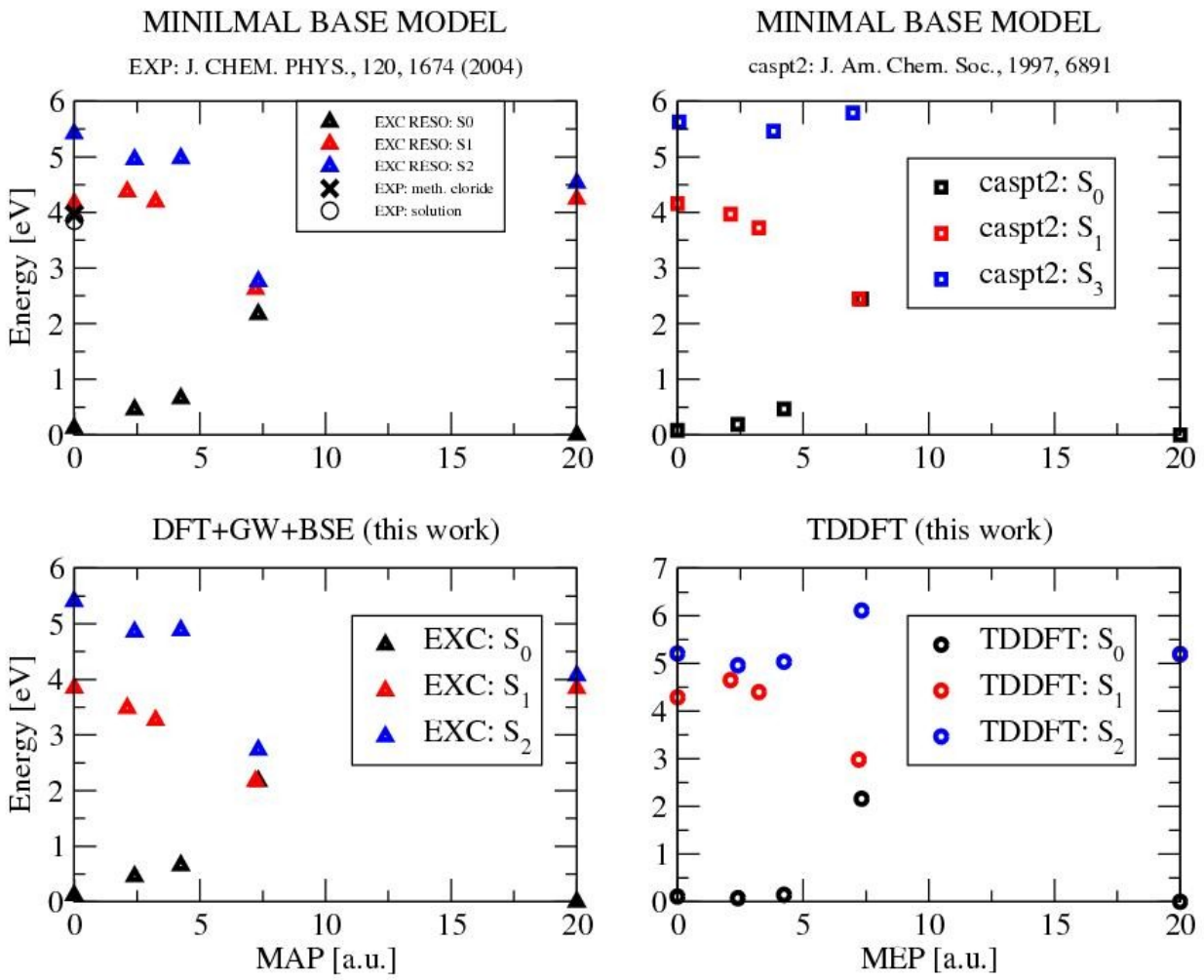
3D Bio (Mosca Conte-Pulci)

PHOTO-ISOMERIZATION OF RETINAL IN RHODOPSIN

MINIMAL BASE MODEL







Adriano Mosca Conte, Olivia Pulci, Rodolfo Del Sole, Leonardo Guidoni