Non Equilibrium Many-Body Perturbation Theory from first principles

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CNR
Istituto di Struttura
della Materia

MaX conference 2018
29th – 31st January 2018, Trieste, Italy

Yambo ©

MaX DRIVING THE EXASCALE TRANSITION

Yambo and HPC

New computational resources make possible
to tackle more **challenging computational problems**
from first-principles

QP vs KS energies
BSE vs IP absorption

Higher accuracy

High throughput

AiiDA
Automated Interactive Infrastructure and Database for Computational Science

yambo plugin

yambopy

Ultra-fast and
non equilibrium physics

New physics

Larger systems

Surfaces, interfaces,
nanostructures ab-initio

Extend the limits of system size
DFT (10^3 – 10^4 atoms) - MBPT (10^2 10^3 atoms)

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Why so fast ?

Spatial resolution of ~0.06 mm = 60 μm

Time resolution of ~0.04 s = 40 ms

We can use technology to explore
shorter space and time scales

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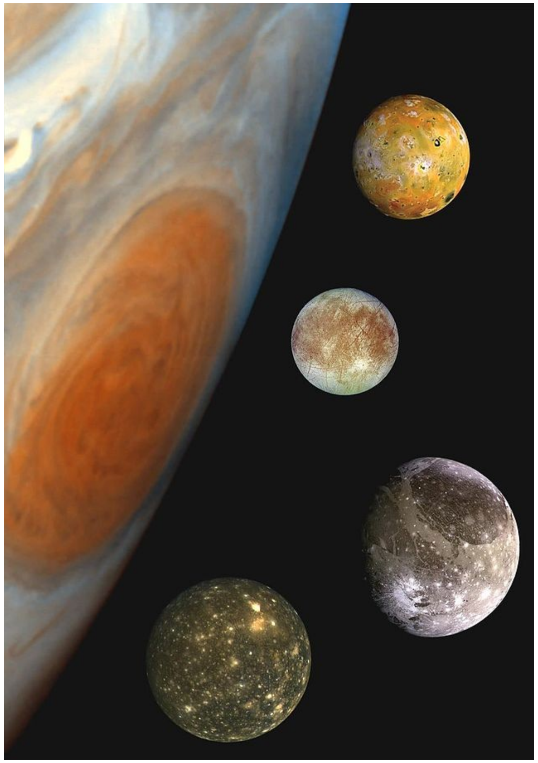
Enlarge space:
Telescope, Galileo (1609)

Magnification ~ x20



1610
Moons of Jupiter

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Enlarge space:
Telescope, Microscope, … ,
Scanning electron microscopy,
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Resolution ~ 1 Angstrom = 10^{-10} mt
Magnification ~ 10^6 - 10^7

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Slow down time ?
1791 George Stubbs (english painter)

1878 “Sallie Gardner at a Gallop” is a series of photographs consisting of a galloping horse

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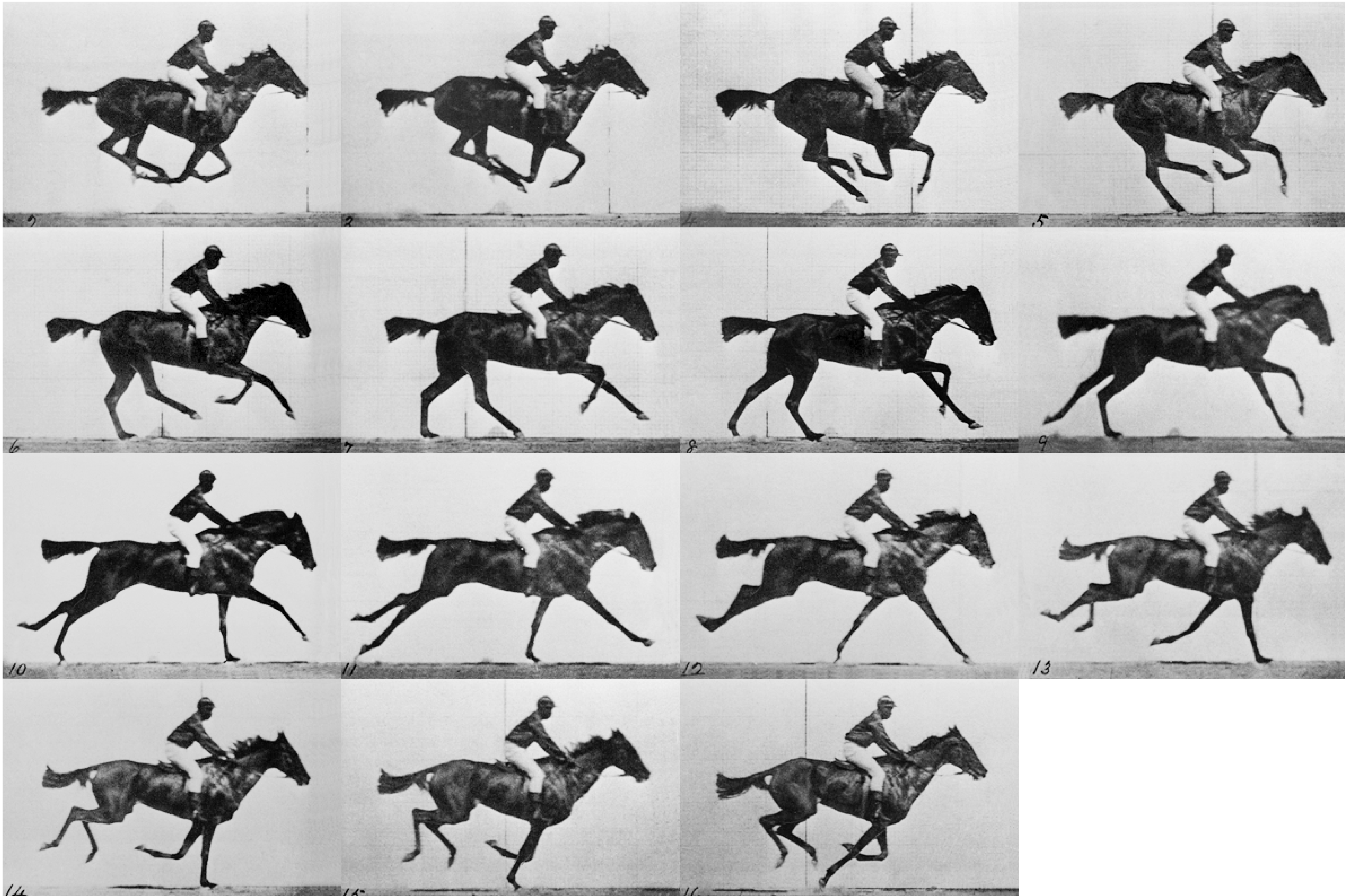

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Slow down time
1878 “Sallie Gardner at a Gallop” is a series of photographs consisting of a galloping horse
~ 0.5 ms = 500 μm resolution (x80)

How fast can we go ?

The Nobel Prize in Chemistry 1967
Manfred Eigen, Ronald G.W. Norrish, George Porter

Flash photolysis method 1949

Why so fast ?

The Nobel Prize in Chemistry 1967

Manfred Eigen
Prize share: 1/2

Ronald George Wreyford Norrish
Prize share: 1/4

George Porter
Prize share: 1/4

The Nobel Prize in Chemistry 1967 was divided, one half awarded to Manfred Eigen, the other half jointly to Ronald George Wreyford Norrish and George Porter *"for their studies of extremely fast chemical reactions, effected by disturbing the equlibrium by means*

10^{-6} μs Chemical reactions

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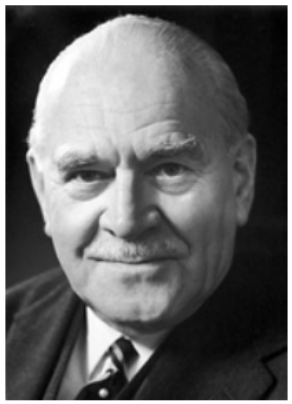

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George Porter

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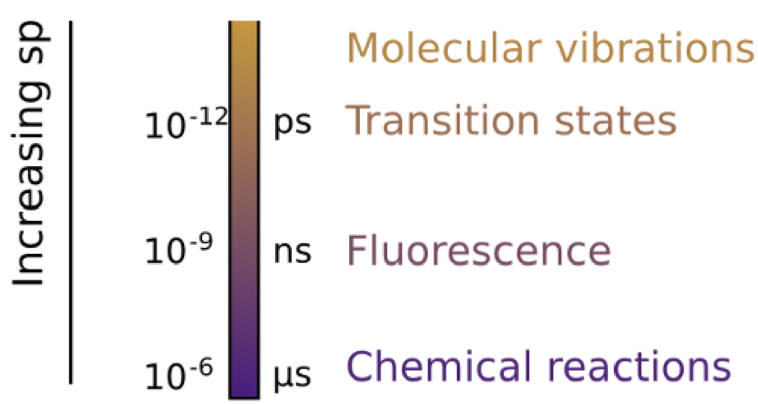

Why so fast ?

$$a = \frac{F_{coulomb}(d)}{m} \qquad d = 0.5\, a\, t^2$$

Atoms ~ 10^{-13} s = 100 fs

The Nobel Prize in Chemistry 1999

Ahmed Zewail

Femto-chemestry

The Nobel Prize in Chemistry 1999

Breaking of an ICN molecule on the fs time-scale

Ahmed H. Zewail

Prize share: 1/1

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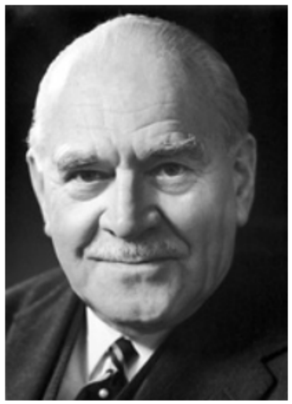

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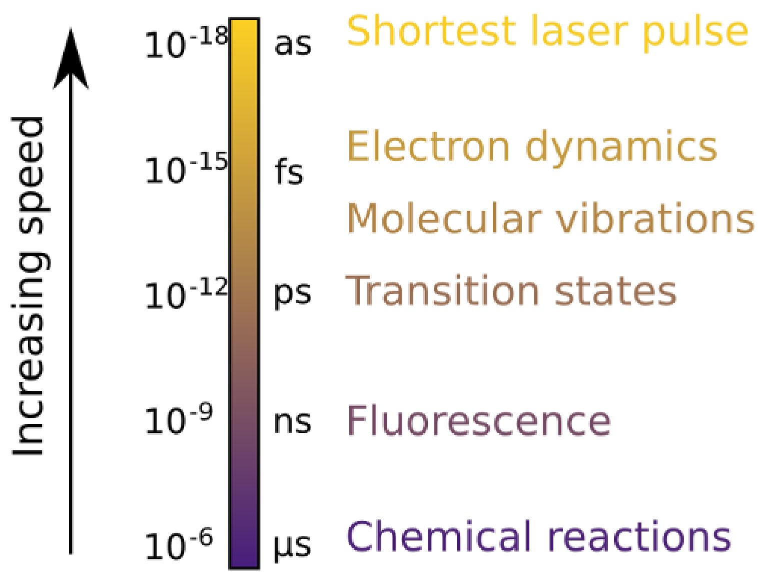

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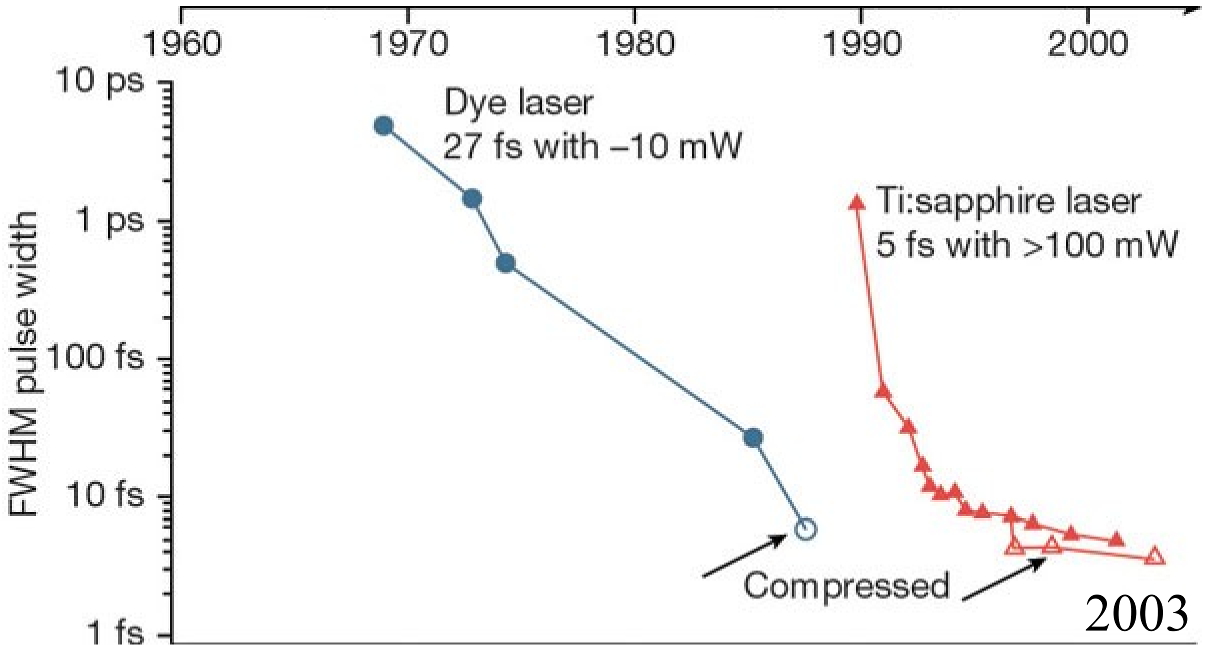
Electrons $\sim 10^{-16}$ s = 0.1 fs (Bohr model)



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5 fs ~ 10^{13} slow down of time

(1 Ang ~ 10^6–10^7 space magnification)

Shortest laser pulses <1 fs (X-Ray)

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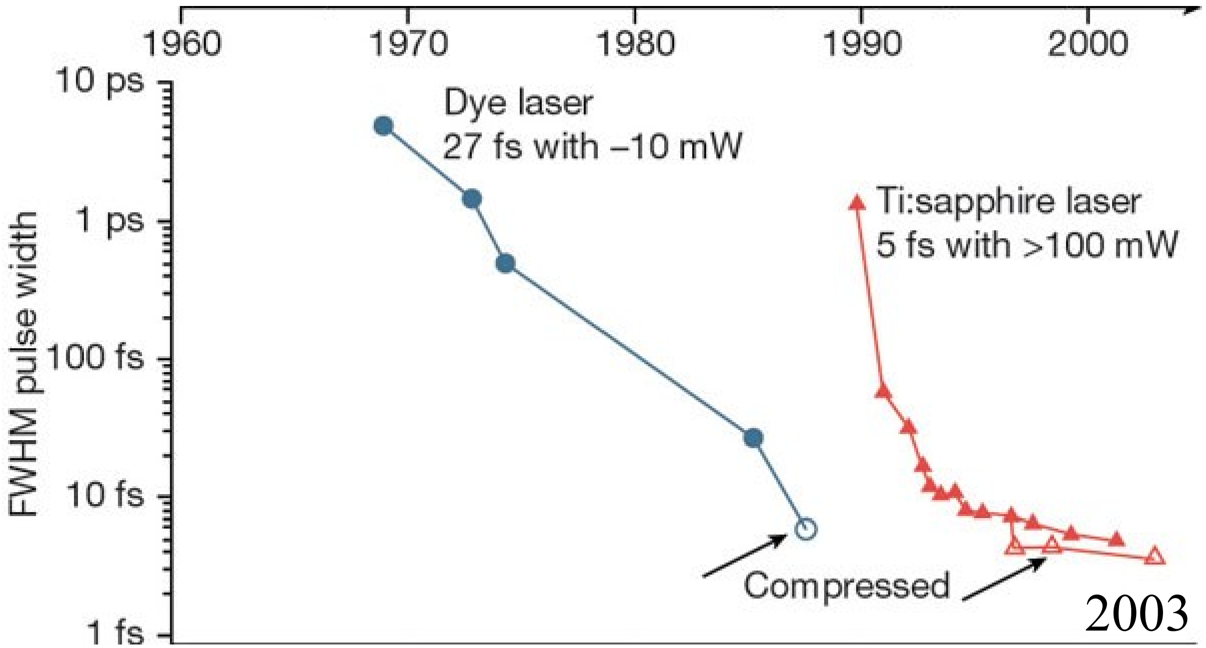

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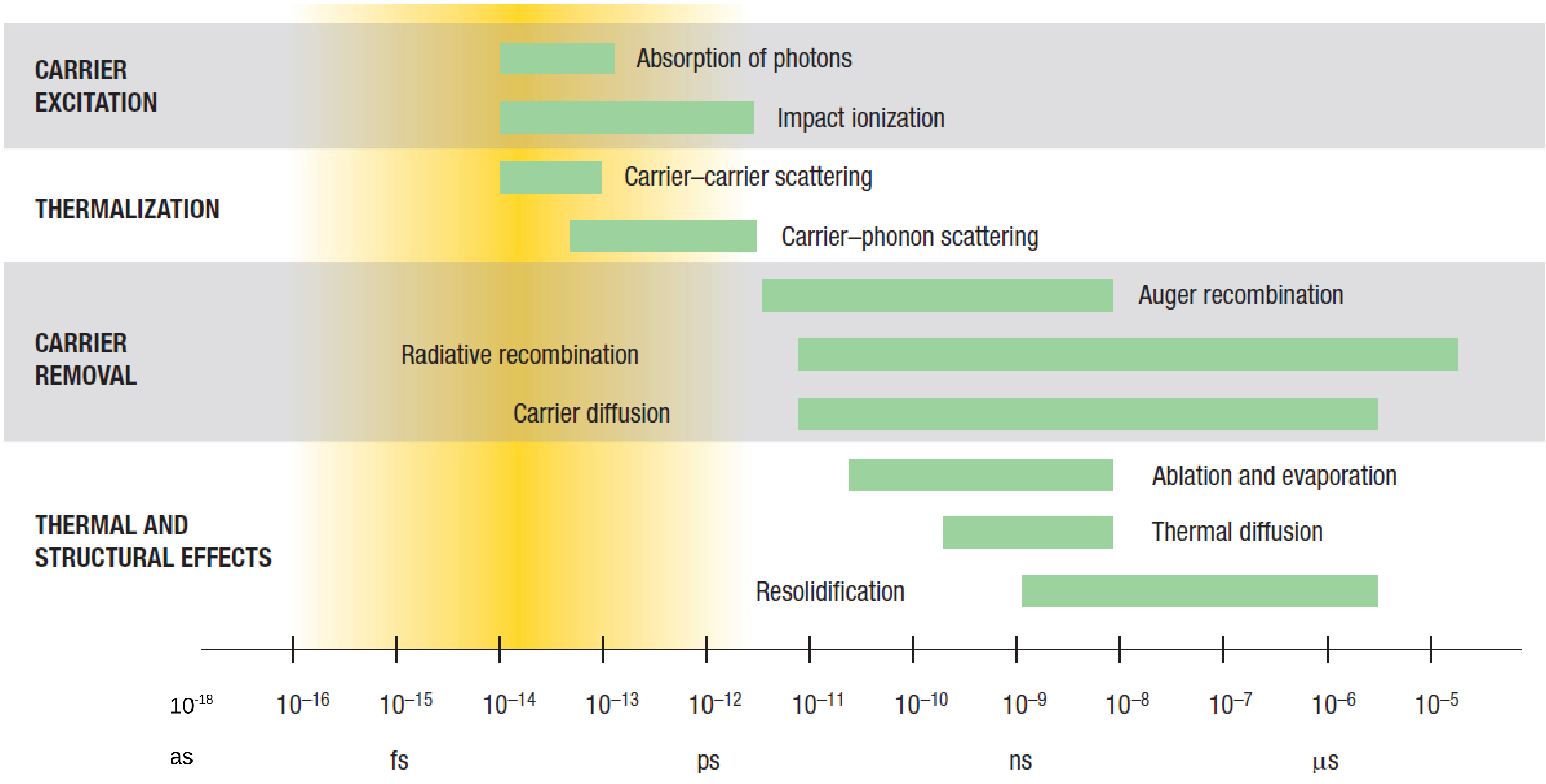
nature materials | VOL 1 | DECEMBER 2002



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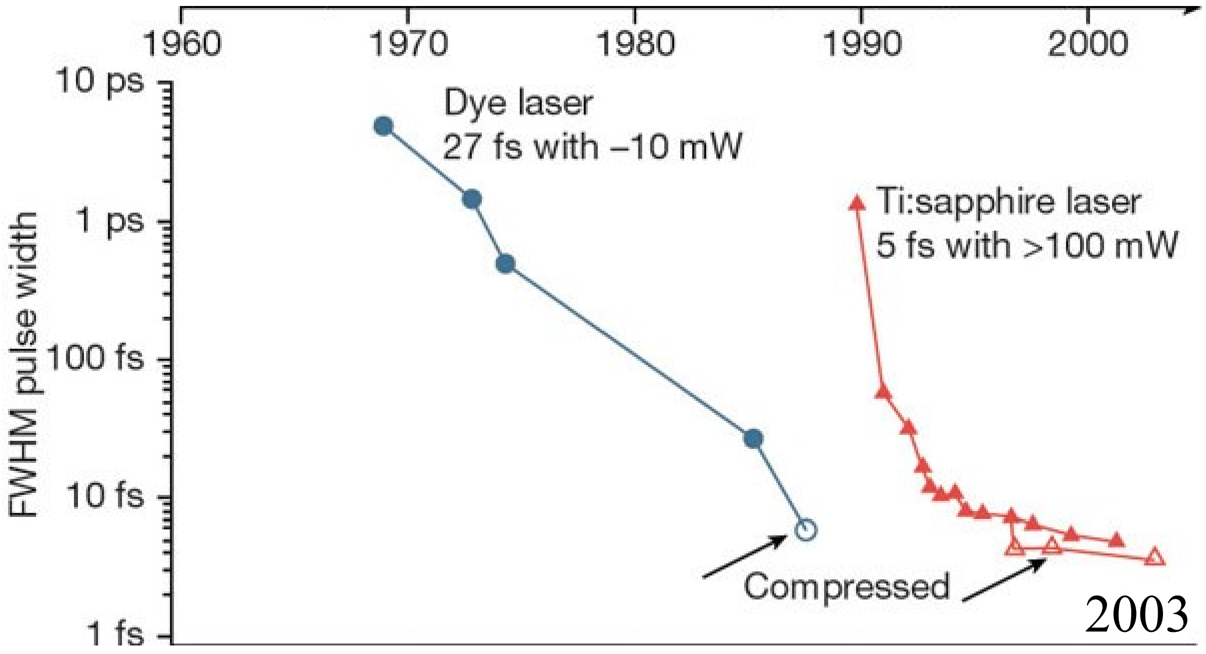

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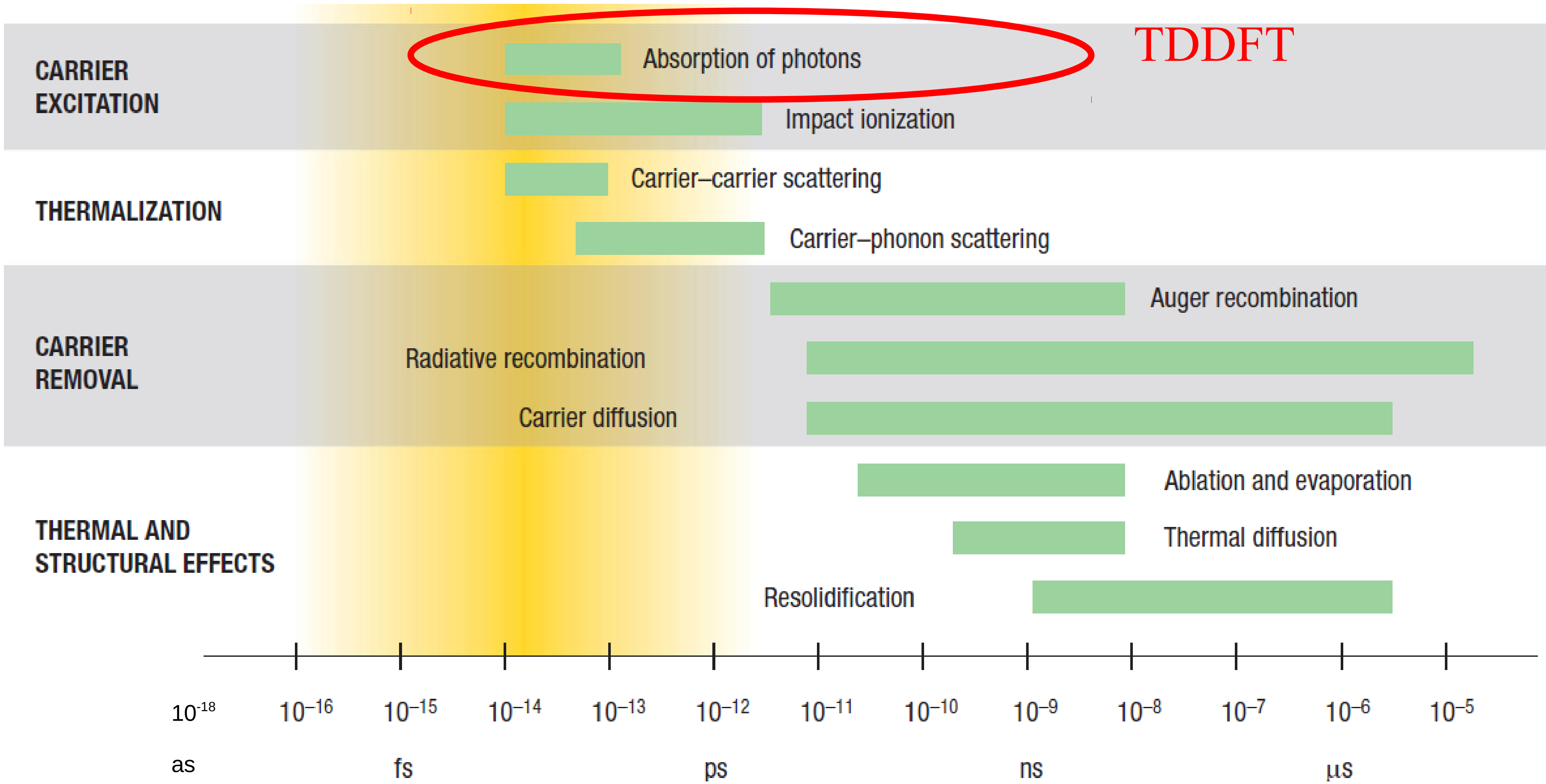

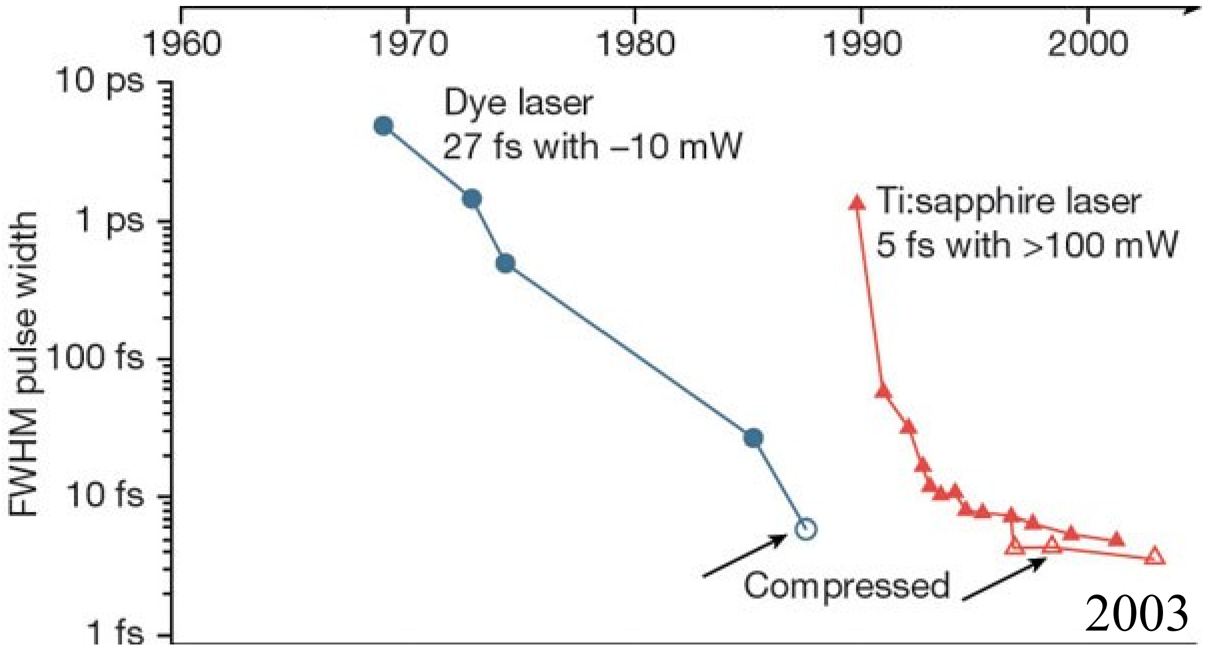

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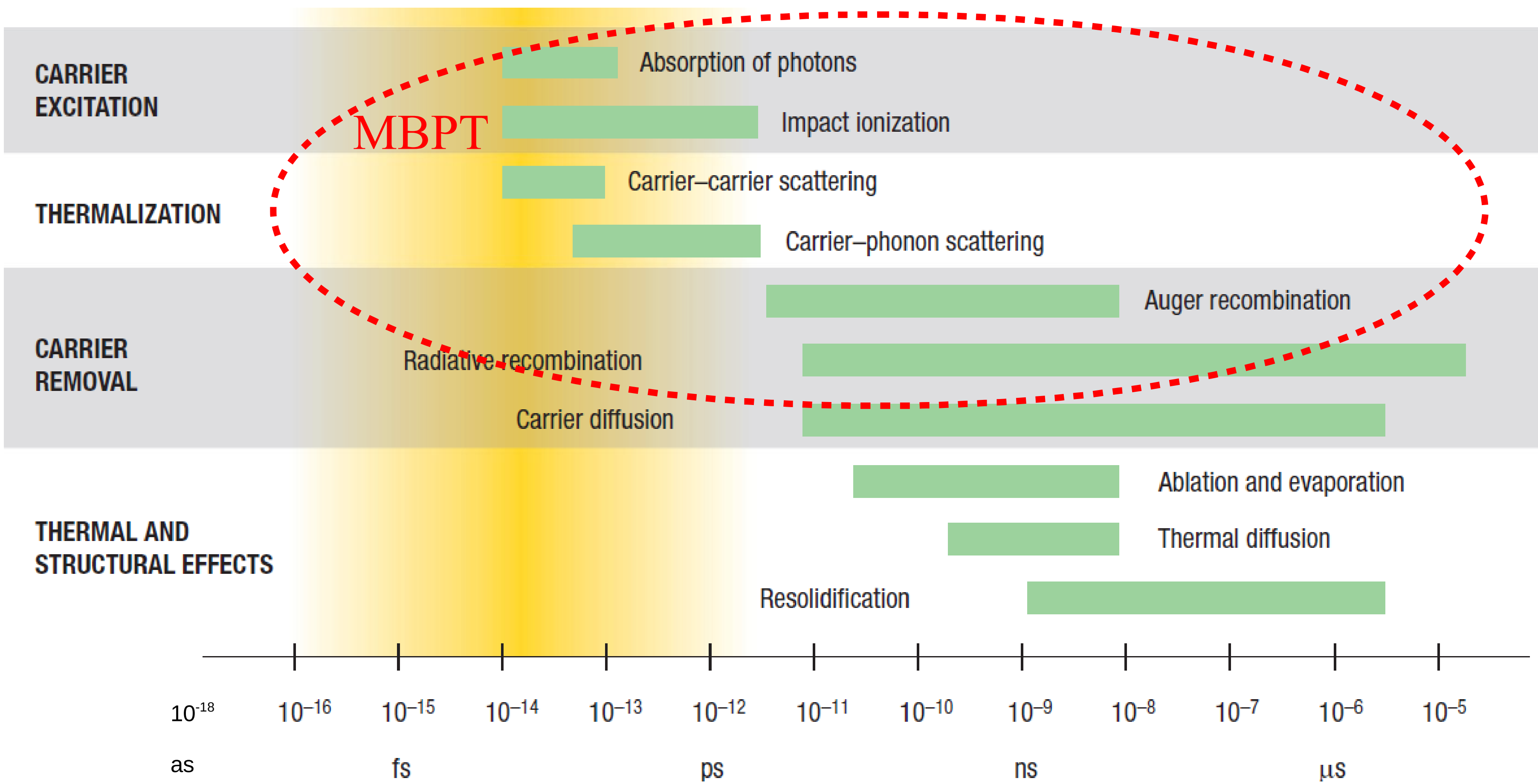
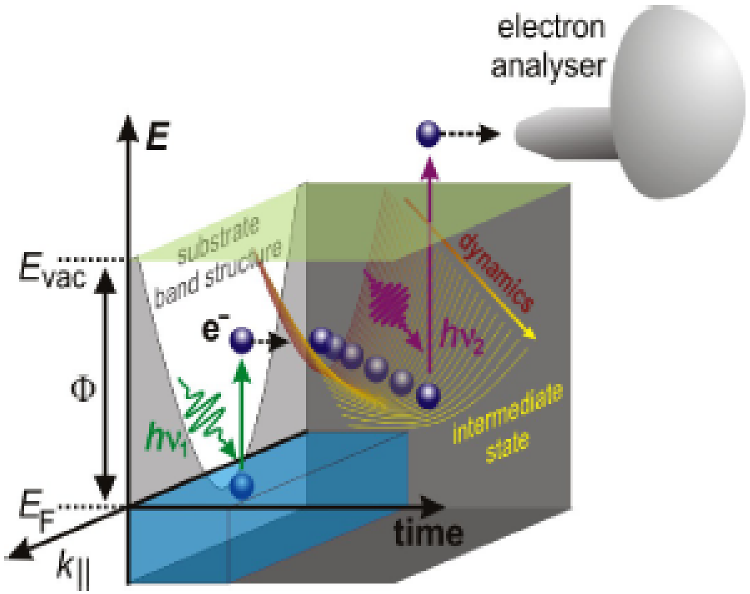


Pump and Probe experiments

Two photons photo-emission



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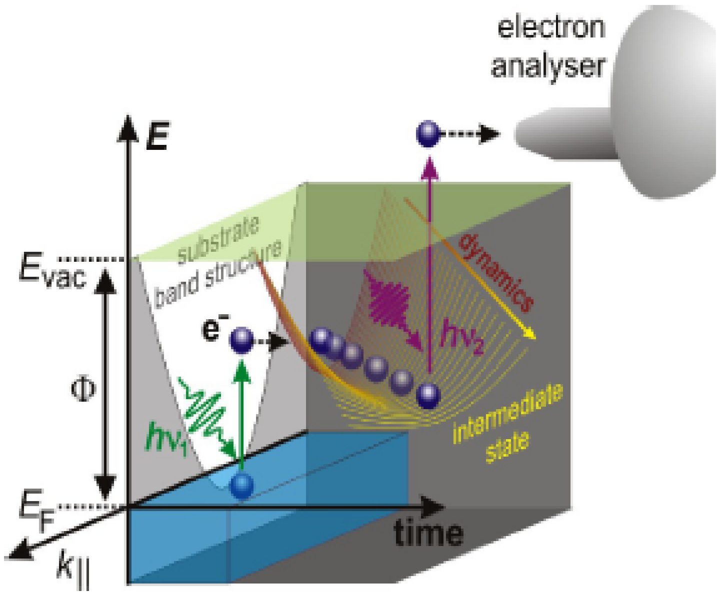

PHYSICAL REVIEW B **84**, 235210 (2011)

Ultrafast relaxation of highly excited hot electrons in Si: Roles of the L – X intervalley scattering

T. Ichibayashi, S. Tanaka, J. Kanasaki, and K. Tanimura*

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(Received 2 April 2011; revised manuscript received 29 September 2011; published 27 December 2011)

PRL **102,** 087403 (2009) PHYSICAL REVIEW LETTERS week ending 27 FEBRUARY 2009

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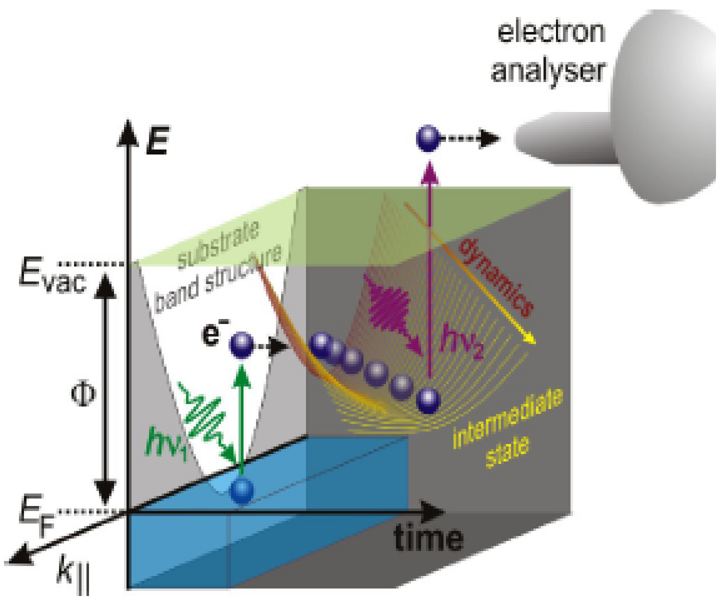

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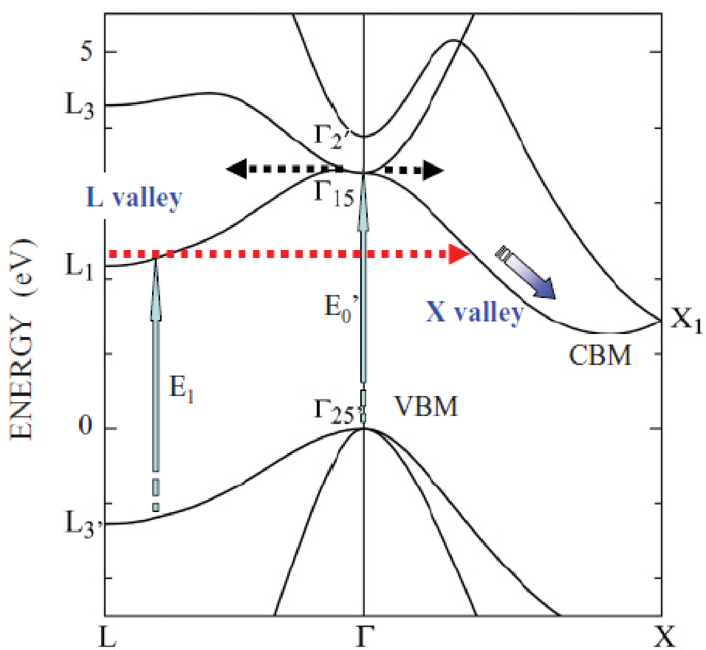

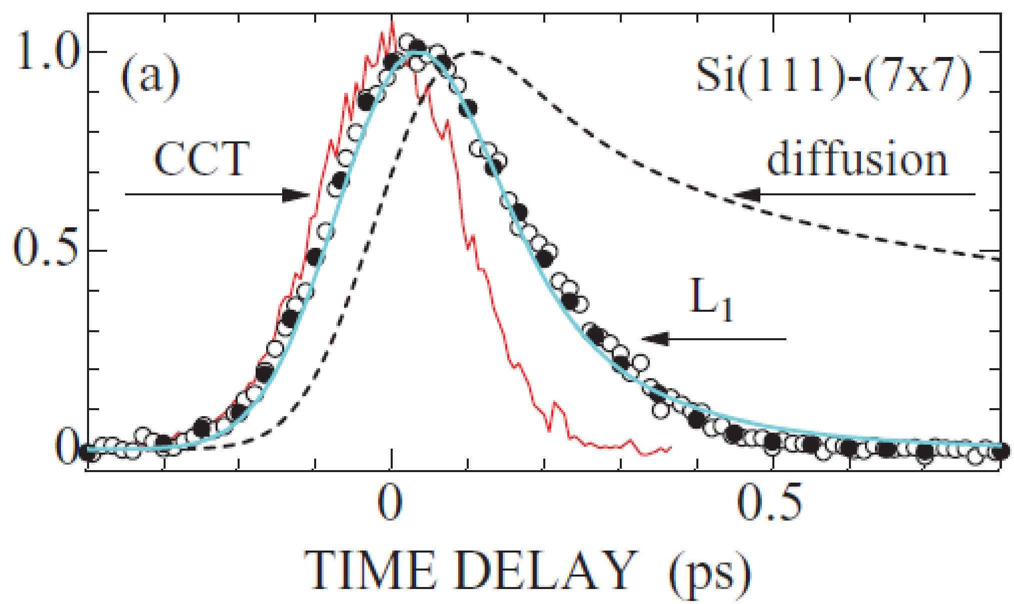

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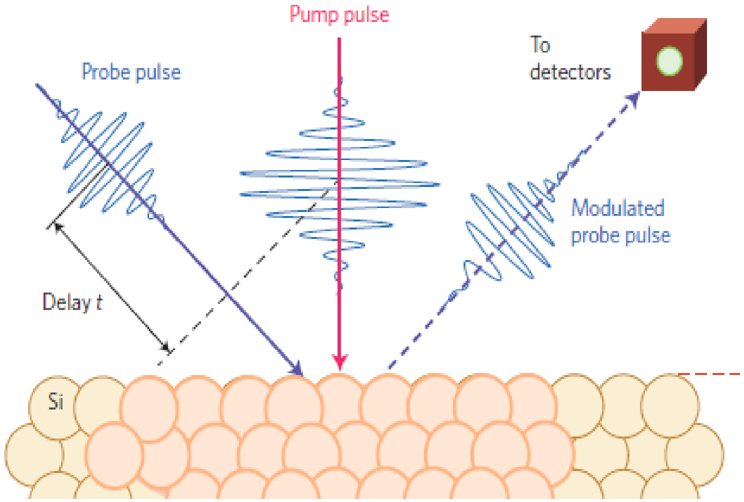

Transient absorption (reflectivity)

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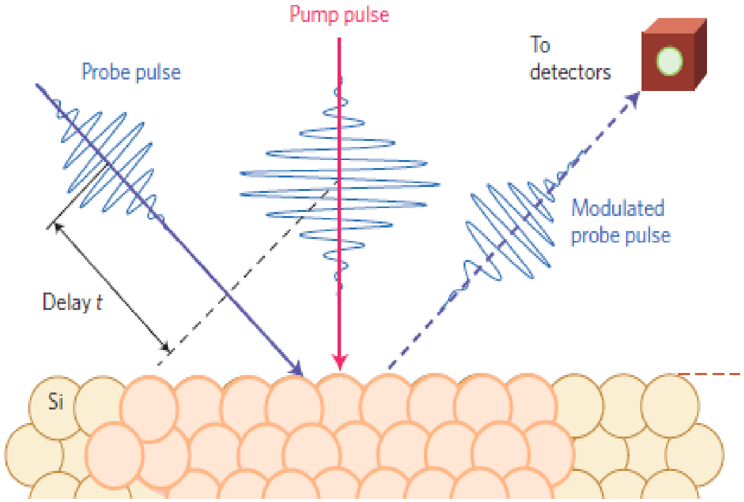

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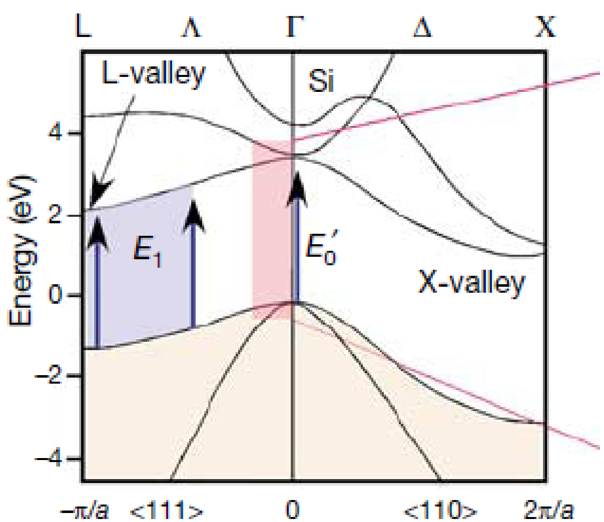

NATURE | VOL 426 | 6 NOVEMBER 2003 | www.nature.com/nature

The birth of a quasiparticle in silicon observed in time–frequency space

Muneaki Hase[1], Masahiro Kitajima[1], Anca Monia Constantinescu[2] & Hrvoje Petek[2]

nature photonics 2012 LETTERS
PUBLISHED ONLINE: 4 MARCH 2012 | DOI: 10.1038/NPHOTON.2012.35

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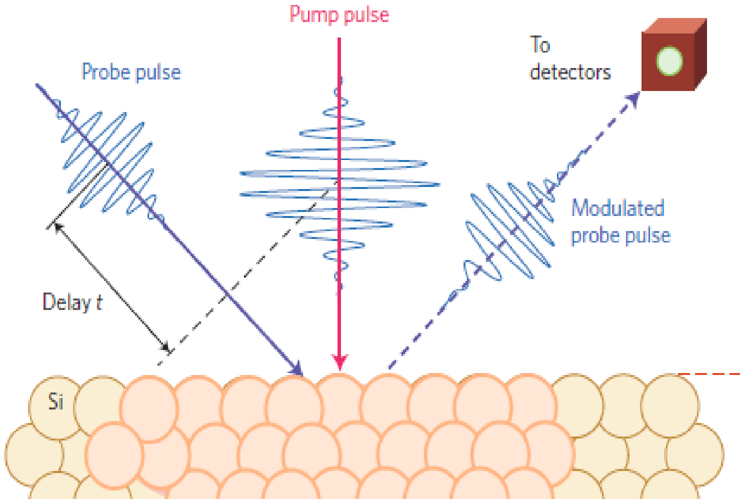

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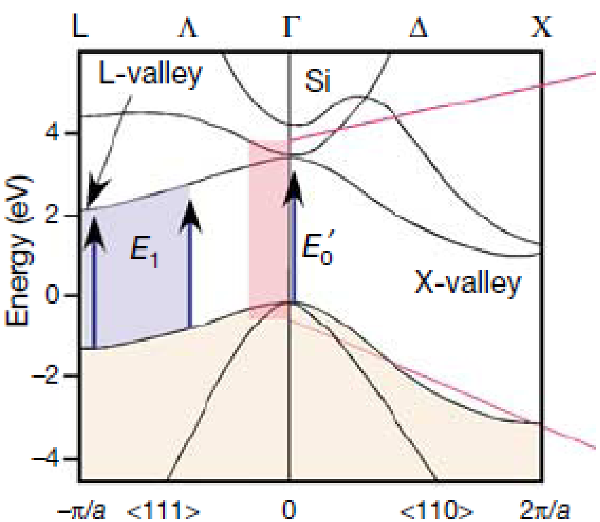

Recent measures perfomed at Politecnico in Milano

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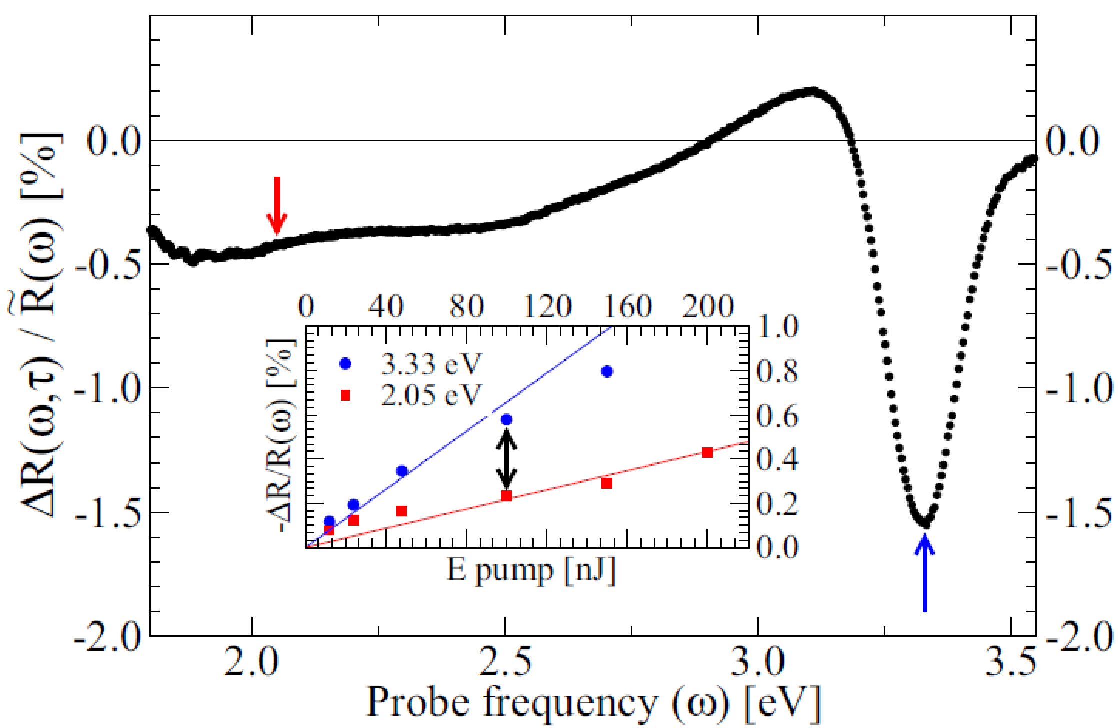
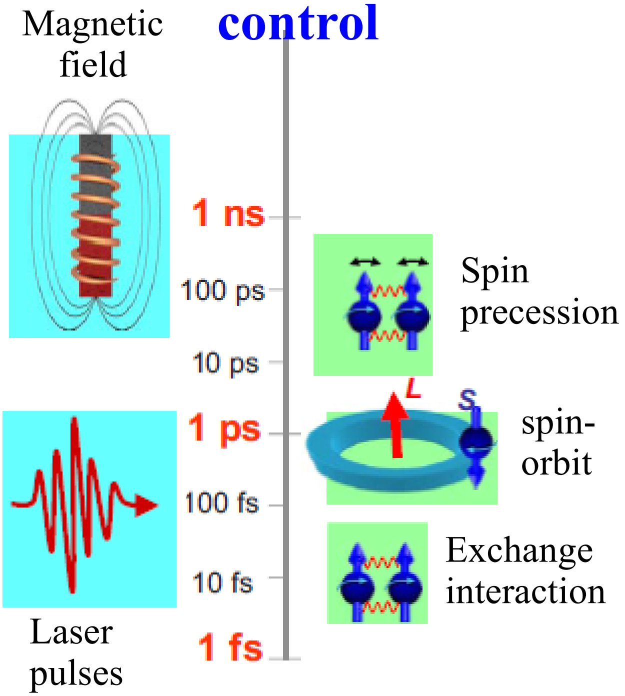


Strong technological interest

Ultra-fast magnetization control



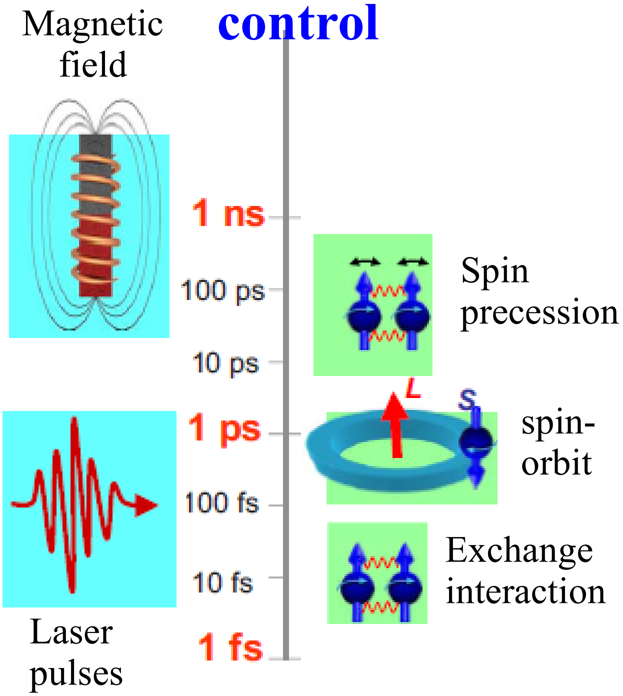
femto-magnetism

Phys. Rev. Lett. **76**, 4250 (1996)
Nature **435**, 635 (2005)
Rev. Mod. Phys. **82**, 2731 (2010)

sub-ps circularly polarized pulses

Time resolved magnetization

Ultra-fast magnetization control



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New generation magnetic recording devices

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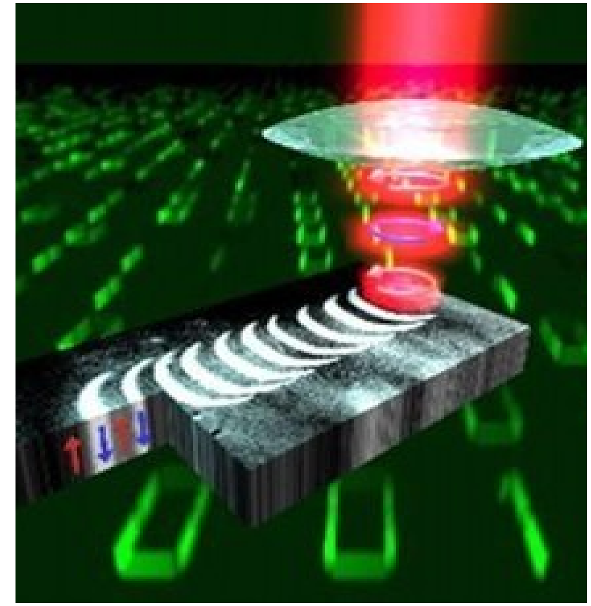
Selected for viewpoint in physics and editor's suggestion



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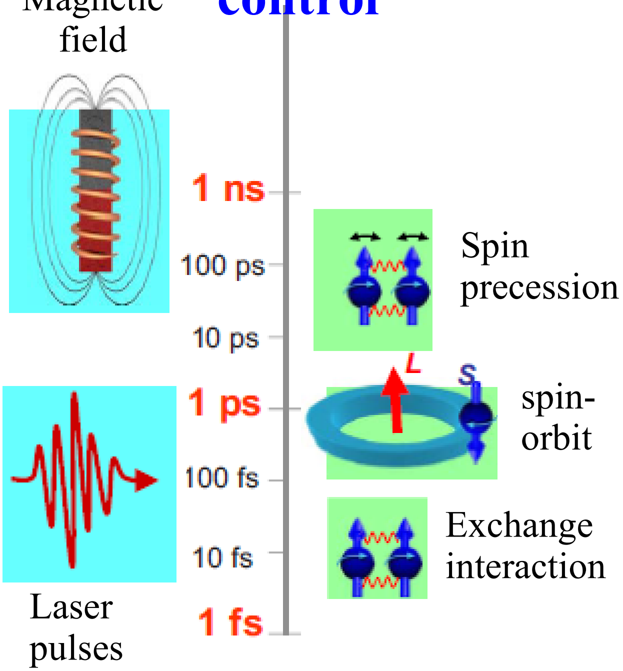

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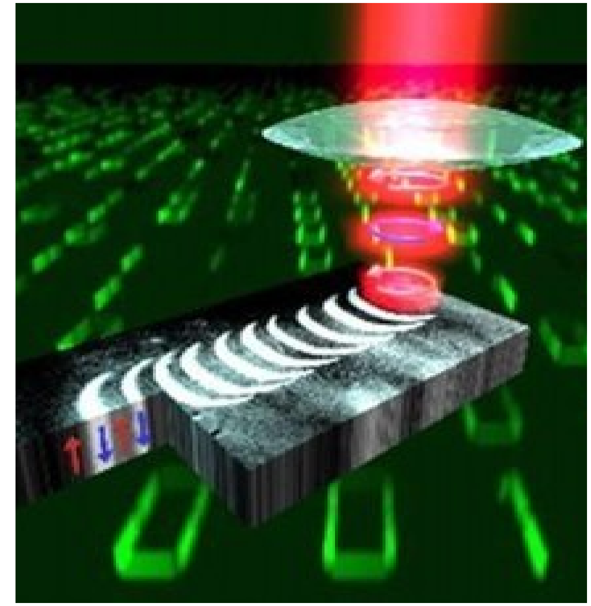


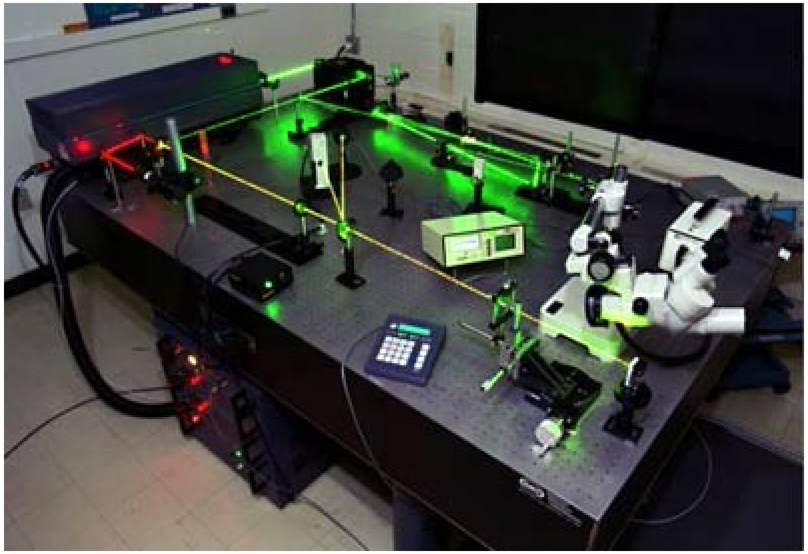
Theory ?

tem. However, a proper theoretical framework that allows an adequate description of the time-resolved pump-probe magneto-optical experiments in metals, magnetic semiconductors, and even dielectrics remains challenging, and the number of approaches is limited

Strong need of theoretical modelling

No easy interpretation of the data

Strong request for theoretical modelling
both to describe table top experiments



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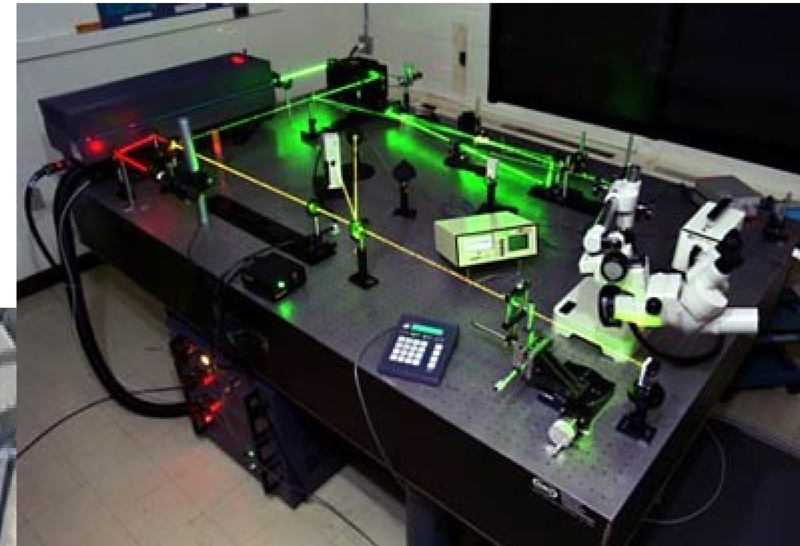
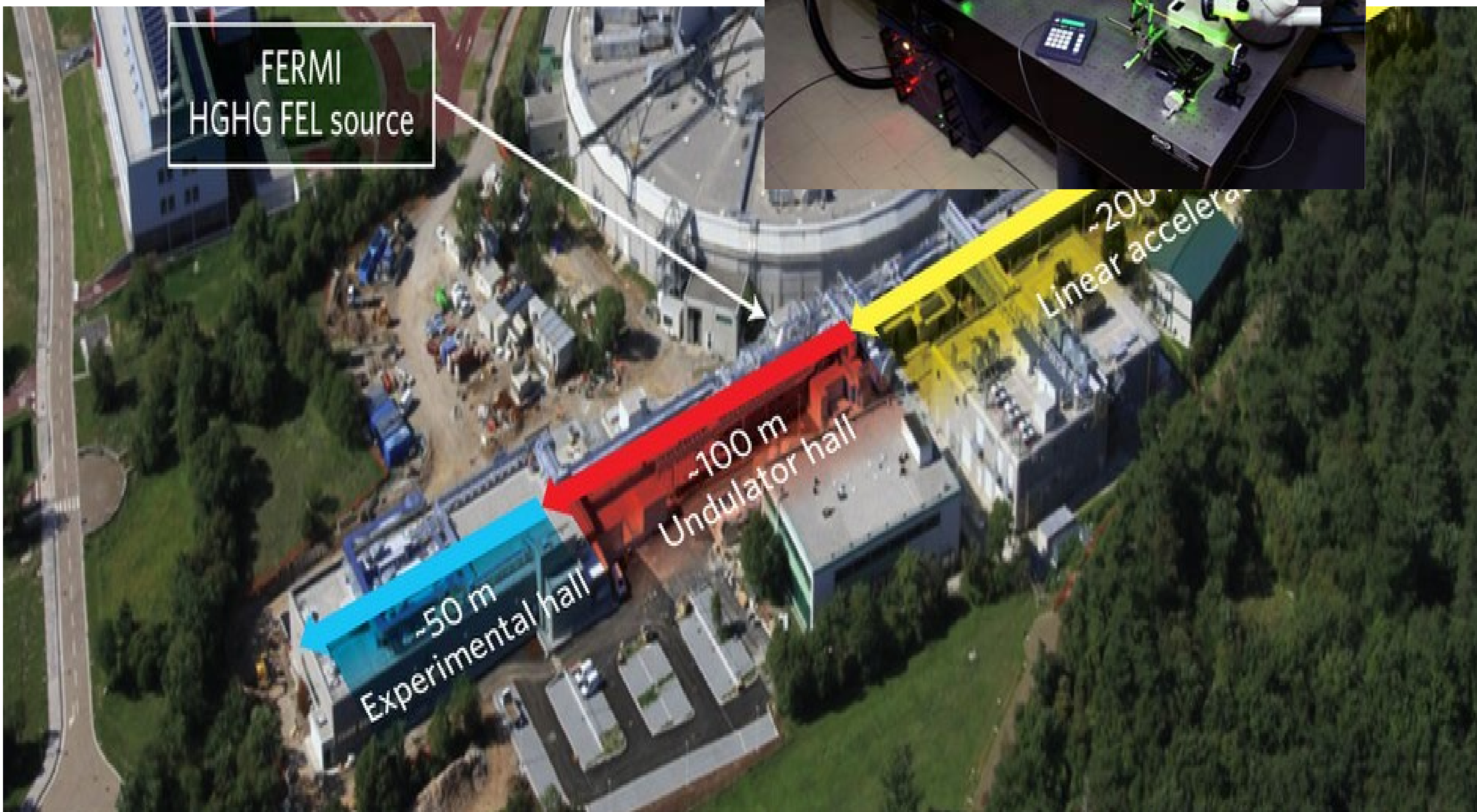
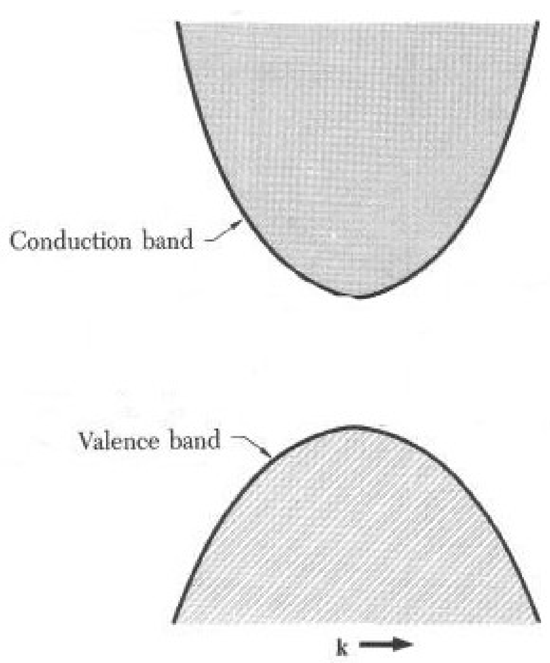




Description of pump & probe experiments

Compute the equilibrium properties of the material:
band structure, phonons, electron-phonon matrix elements



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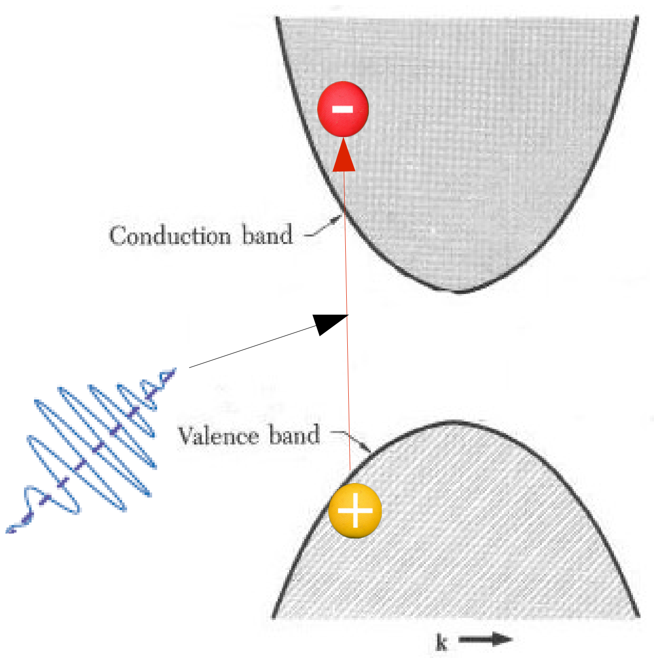

1 - Coherent evolution

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Photo-carriers excitations:
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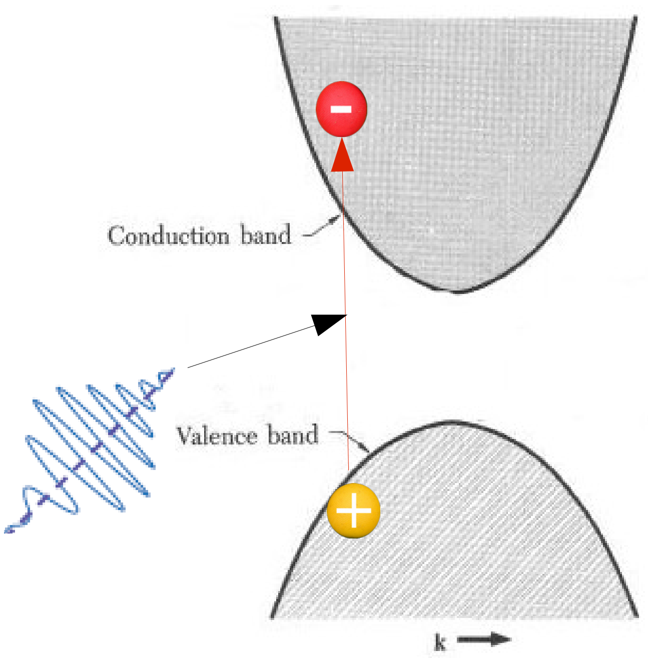
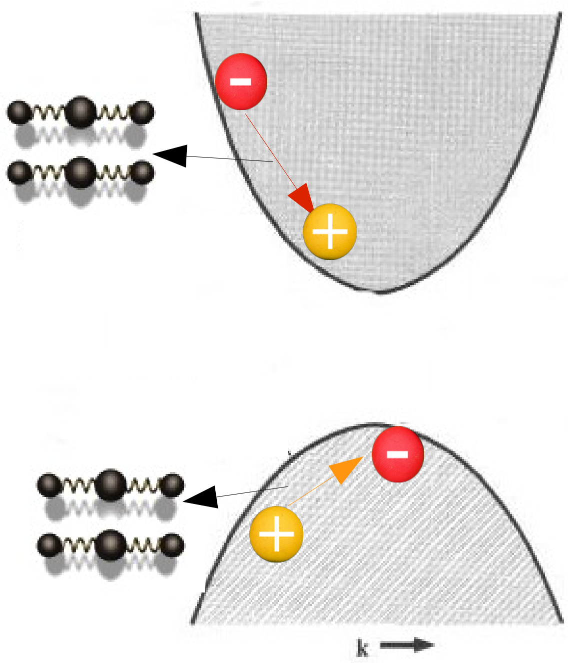
carriers relaxation:
how is the equilibrium restored?





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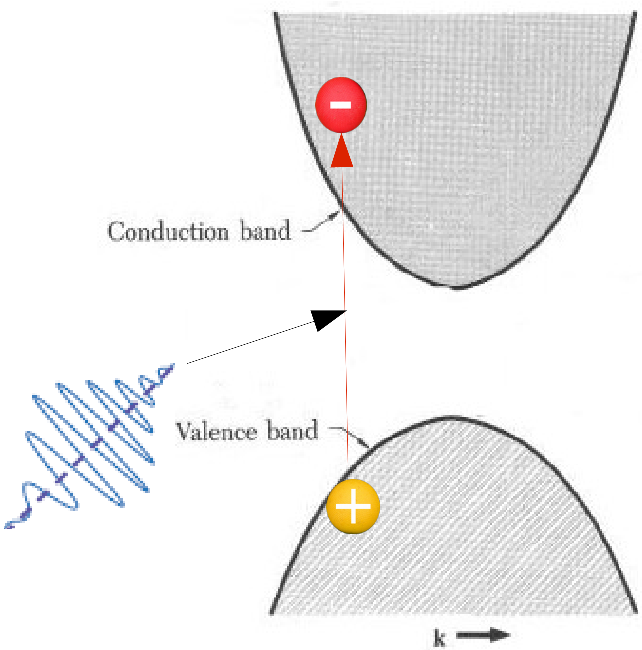

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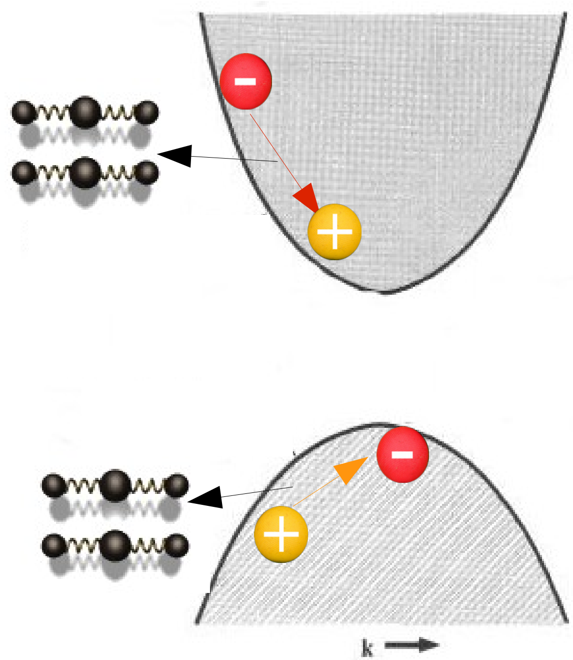
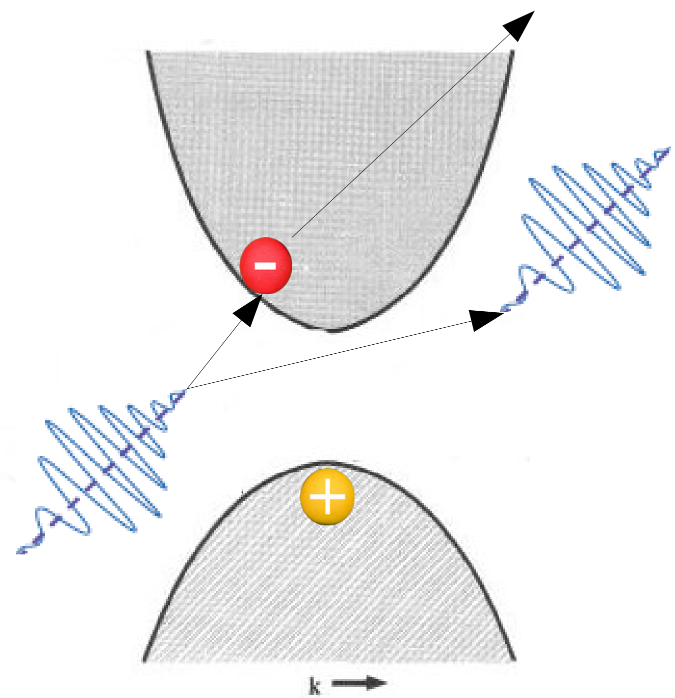


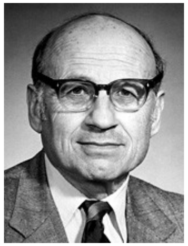
2 - Scattering term

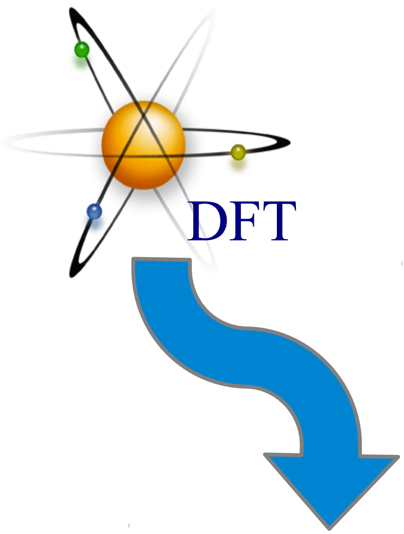
<u>Measurement process</u>



3 - Define the measured physical quantities

Ab-Initio Many-Body Perturbation Theory





AiMBPT

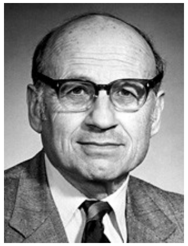
DFT

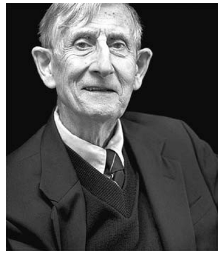
$$\left[\frac{-\nabla^2}{2} + v_s(r)\right]\psi_{nk}(r) = \epsilon_{nk}\,\psi_{nk}(r)$$

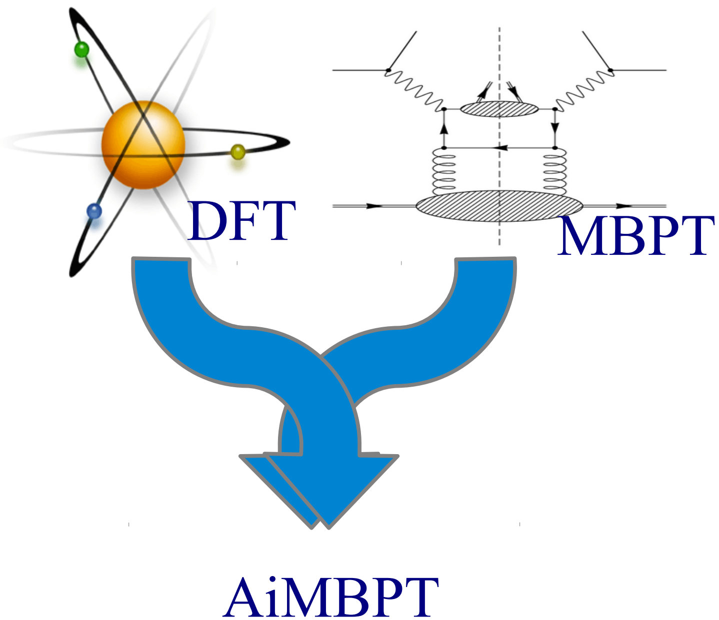
$$v_s(r) = v_{ions}(r) + v_{Hxc}[n](r)$$

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

Ab-Initio Many-Body Perturbation Theory







DFT

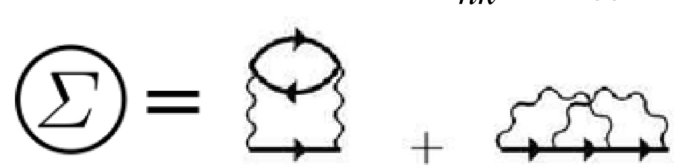
$$\left[\frac{-\nabla^2}{2}+v_s(r)\right]\psi_{nk}(r)=\epsilon_{nk}\,\psi_{nk}(r)$$

$$v_s(r)=v_{ions}(r)+v_{Hxc}[n](r)$$

+

MBPT

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



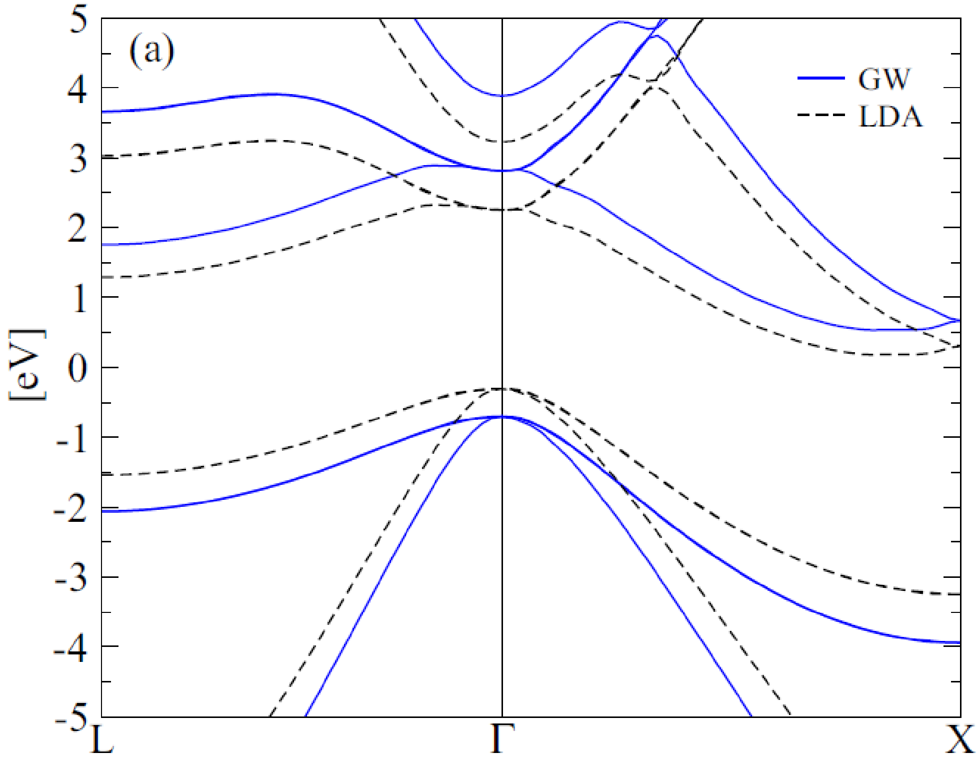
$$\epsilon^{QP}_{nk}=\epsilon^{KS}_{nk}+\langle\Sigma(\epsilon^{QP})-V_{Hxc}\rangle$$

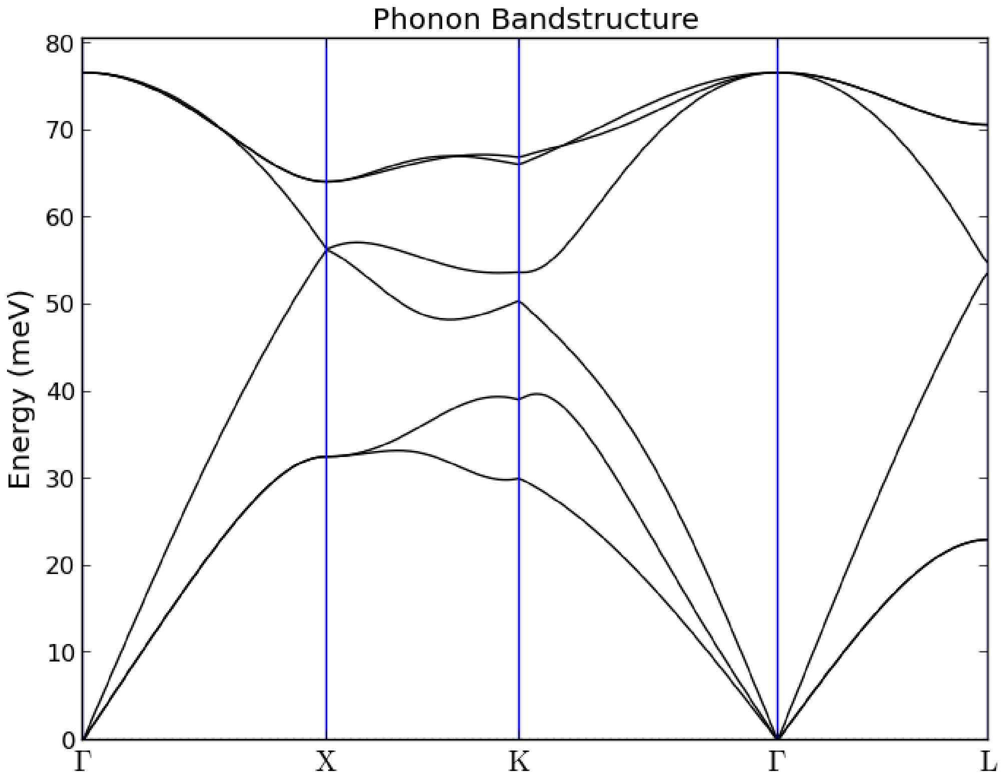
G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002)

Predictive, parameters free and accurate

Computationally very demanding

The Kadanoff Baym equation

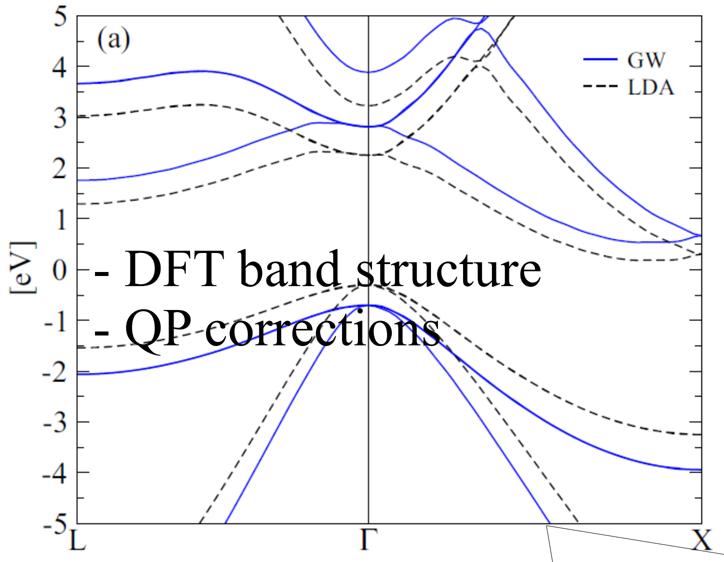




- DFT band structure
- QP corrections

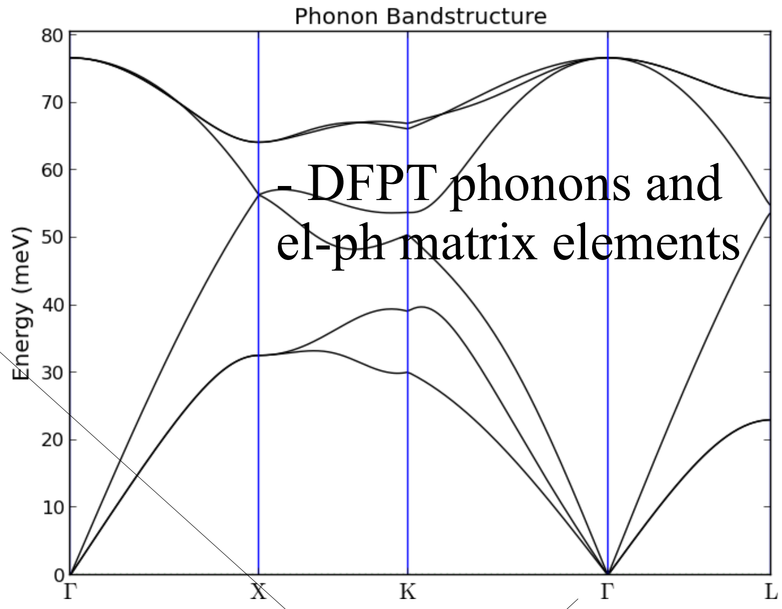
- DFPT phonons and el-ph matrix elements

The Kadanoff Baym equation



Many body effects

Pump laser pulse

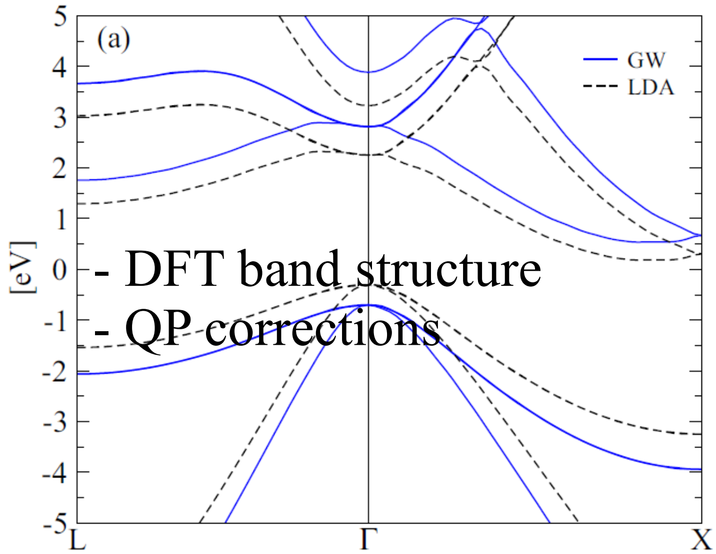


$$i\,\partial_t G^<_{nmk}(t,t) - \left[H^{eq} + \Delta V^H + \Delta\Sigma_s + U^{ext}(t), G^<(t,t) \right]_{nmk} = S_{nmk}(t)$$

Coherent evolution **Scattering term**

$$G^<_{nmk}(t) = \langle \psi_{nk} | G^<(rt, r't) | \psi_{mk} \rangle \qquad G^<_{nmk}(0) = \delta_{nm} f^{eq}_{nk}$$

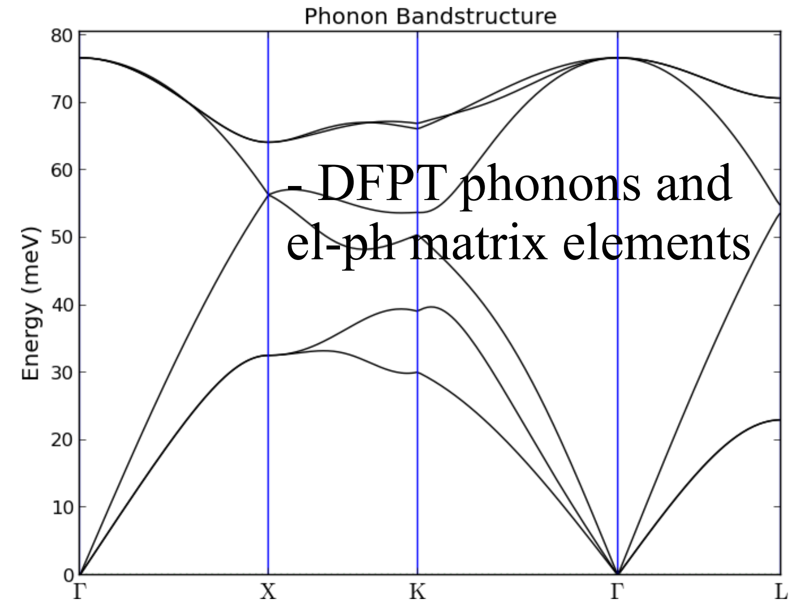
The Kadanoff Baym equation



- DFT band structure
- QP corrections

Many body effects

Pump laser pulse



- DFPT phonons and el-ph matrix elements

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

Coherent evolution

Scattering term

$$G^<_{nmk}(t) = \langle \psi_{nk} | G^<(rt, r't) | \psi_{mk} \rangle$$

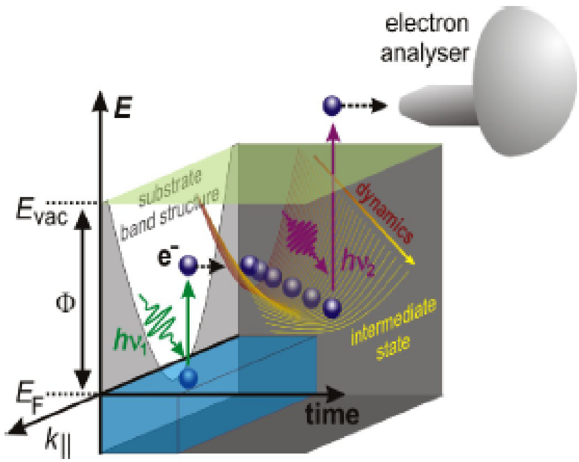
$$G^<_{nmk}(0) = \delta_{nm} f^{eq}_{nk}$$

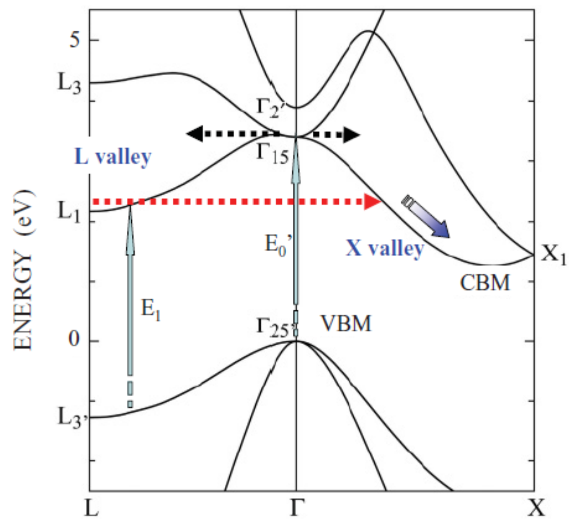
$$P(t) = -e \sum_{nmk} r_{nmk} \Delta G^<_{nmk}(t)$$

$$f_{nk}(t) = -i G^<_{nnk}(t)$$

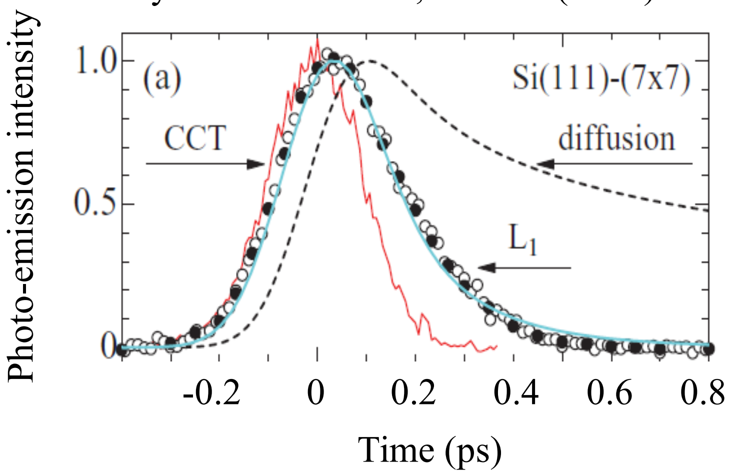
$$\chi[f_{nk}(t)](\omega)$$

Pump and probe experiments

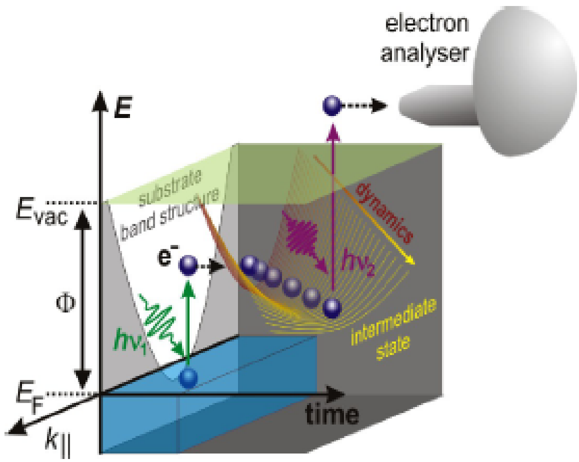


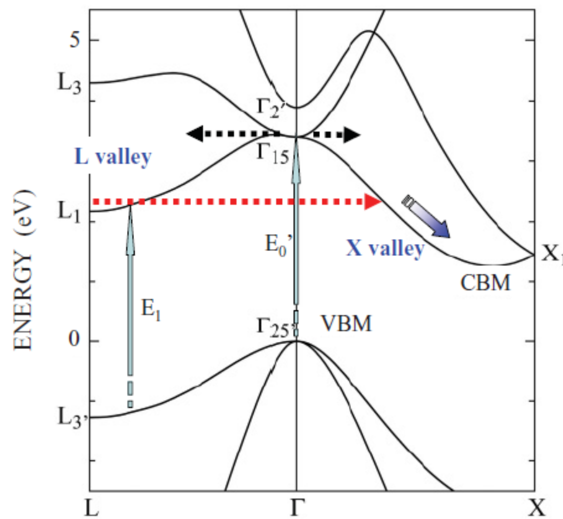


Phys. Rev. B 84, 235230 (2011)
Phys. Rev. Lett. 102, 087403 (2009)



Pump and probe experiments





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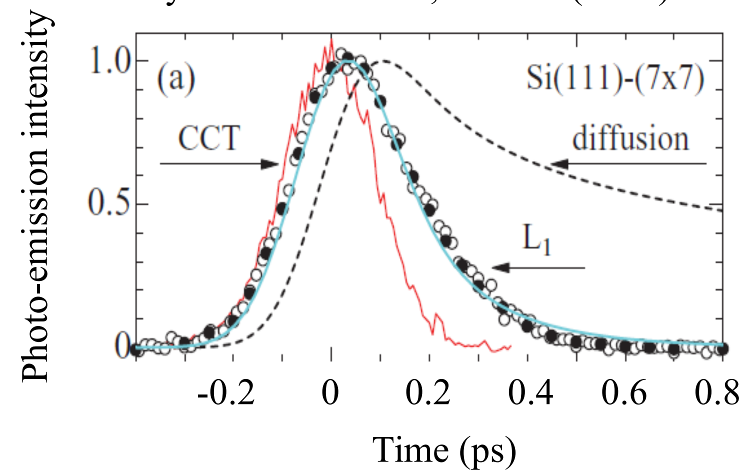
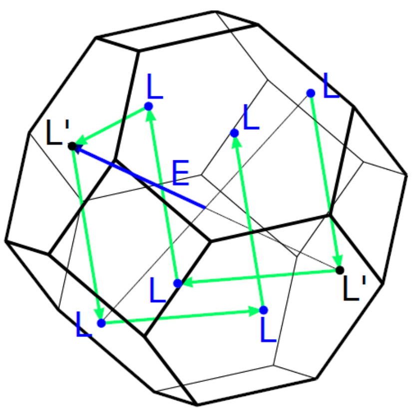
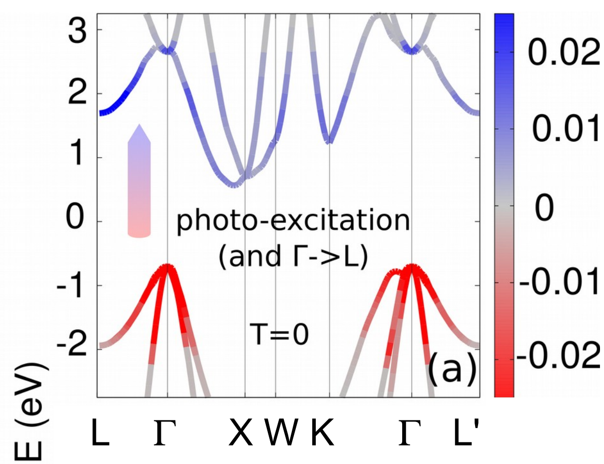
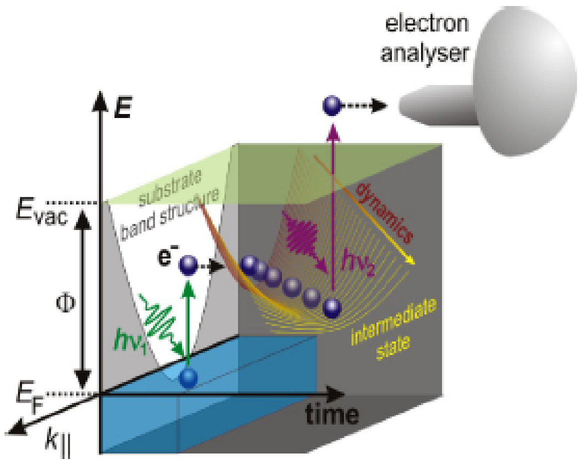


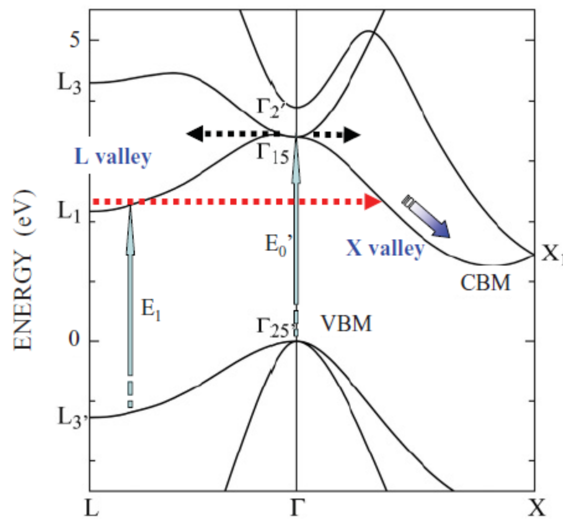




D. Sangalli, and A. Marini, Europhysics Letters 110, 47004 (2015)

Pump and probe experiments





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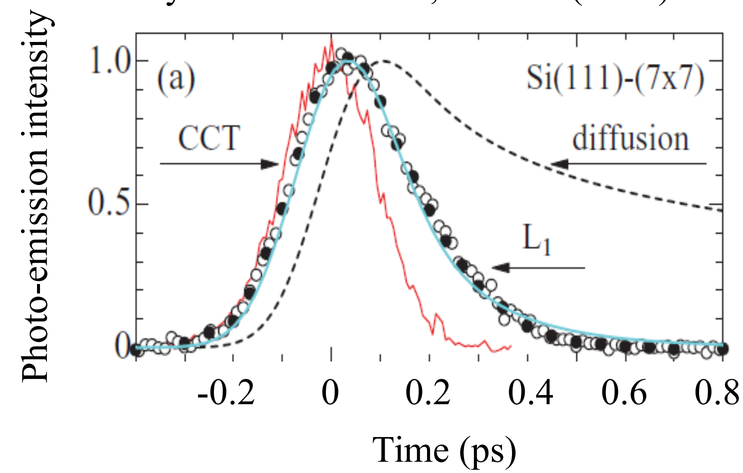
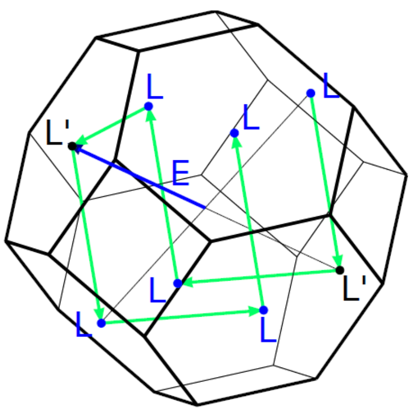
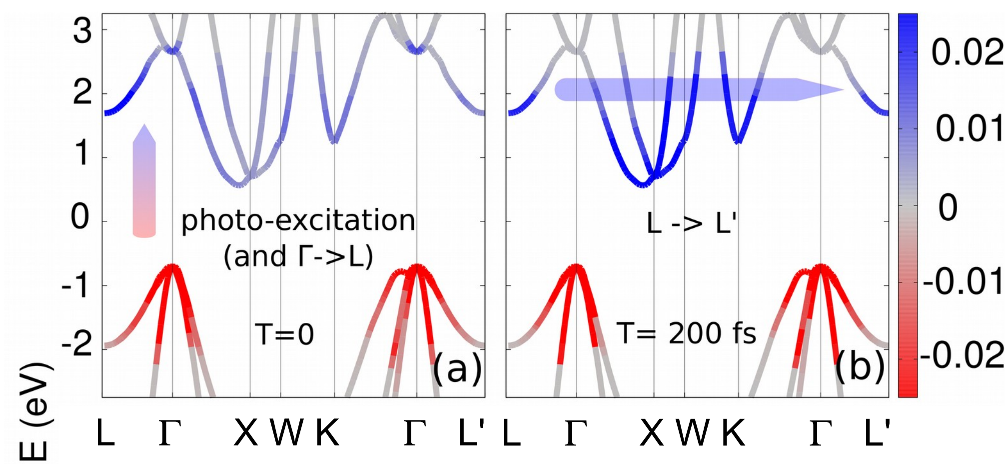
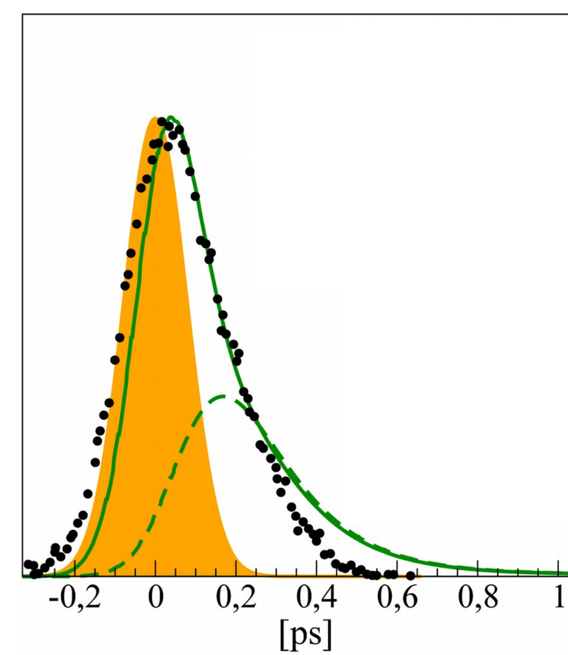


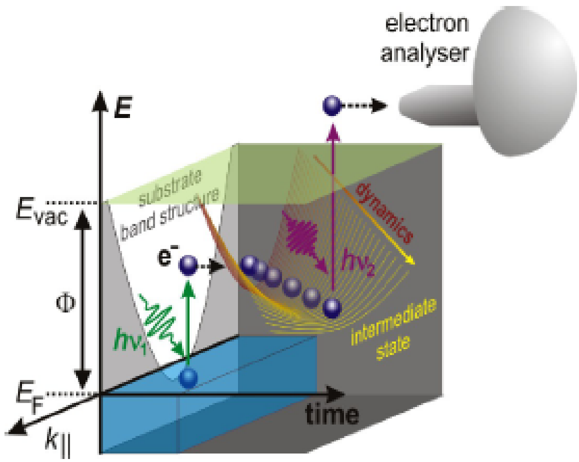


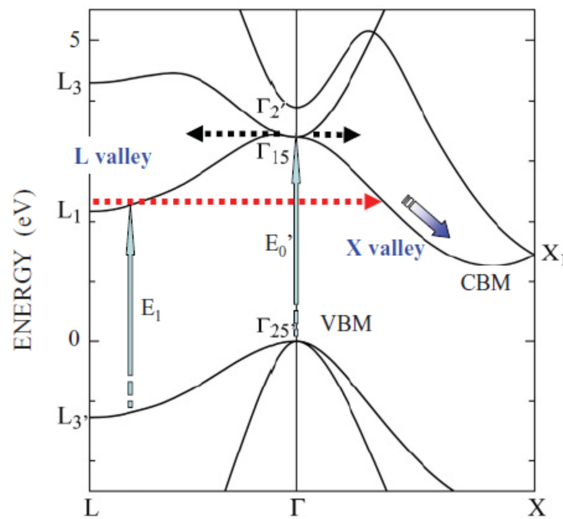




D. Sangalli, and A. Marini, Europhysics Letters 110, 47004 (2015)

Pump and probe experiments





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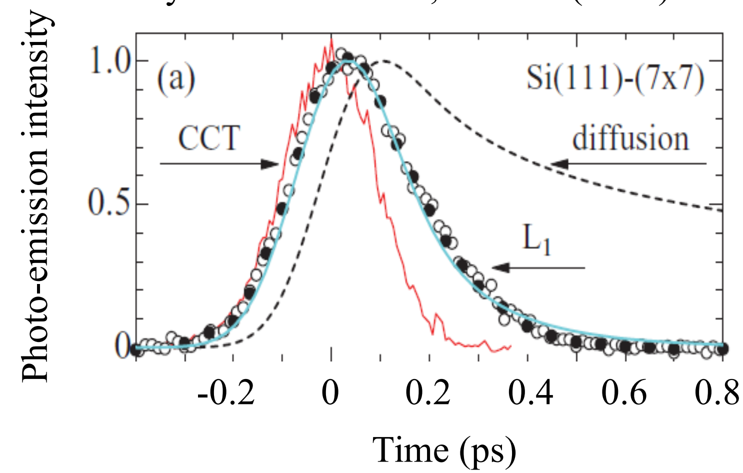
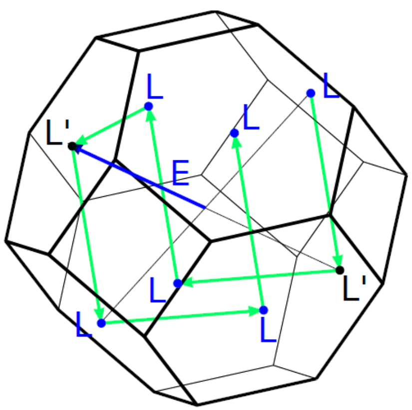
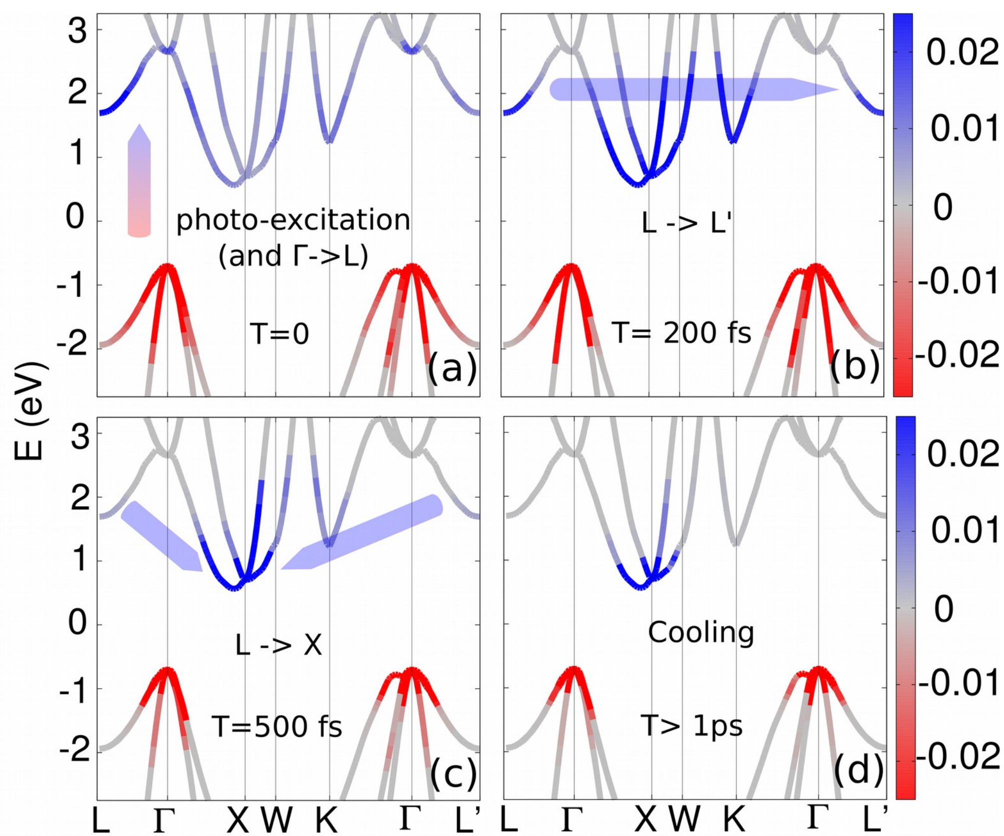
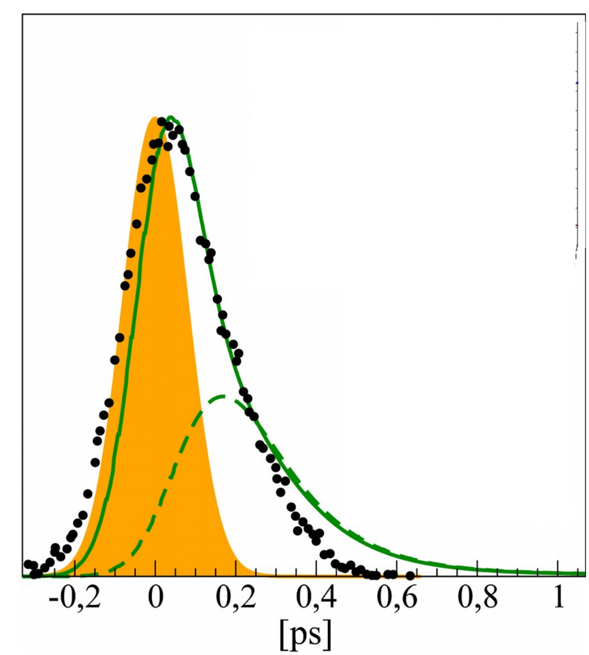






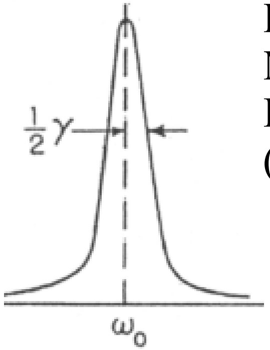


D. Sangalli, and A. Marini, Europhysics Letters 110, 47004 (2015)

Non equilibrium qp-lifetimes

$$\gamma_{nk}^{e,eq} = \Im[\Sigma_{nk}^{elph}]$$

$$f_{nk}^{(e)} = f_{nk}^{(e,0)} e^{-\gamma_{nk}^{(e,eq)} t}$$



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

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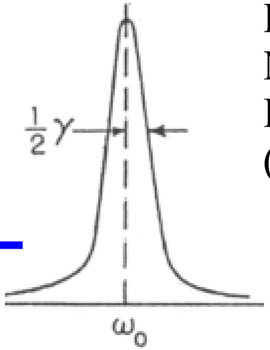
$$\gamma_{nk}^{e,eq} = \Im[\Sigma_{nk}^{elph}]$$

$$f_{nk}^{(e)} = f_{nk}^{(e,0)} e^{-\gamma_{nk}^{(e,eq)} t}$$

$$\partial_t f_{nk}^{(e)}(t) = -\gamma_{nk}^{(e,eq)} f_{nk}^{(e)}$$



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

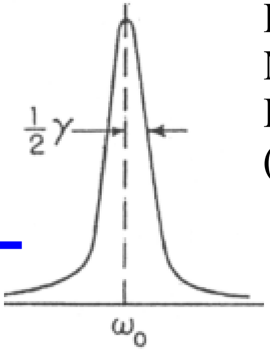
$$\partial_t f_{nk}^{(e)}(t) = \gamma_{nk}^{(h)} f_{nk}^{(h)} - \gamma_{nk}^{(e)} f_{nk}^{(e)}$$

Non equilibrium qp-lifetimes

$$\gamma_{nk}^{e,eq} = \Im[\Sigma_{nk}^{elph}]$$

$$f_{nk}^{(e)} = f_{nk}^{(e,0)} e^{-\gamma_{nk}^{(e,eq)} t}$$

$$\partial_t f_{nk}^{(e)}(t) = -\gamma_{nk}^{(e,eq)} f_{nk}^{(e)}$$



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

$$\partial_t f_{nk}^{(e)}(t) = \frac{\gamma_{nk}^{(h)} f_{nk}^{(h)} - \gamma_{nk}^{(e)} f_{nk}^{(e)}}{f_{nk}^{(e)}} f_{nk}^{(e)}$$

$$\partial_t f_{nk}^{(e)}(t) = -\overline{\gamma}_{nk}^{(e)} f_{nk}^{(e)}$$

Non equilibrium qp-lifetimes

$$\gamma_{nk}^{e,eq} = \Im[\Sigma_{nk}^{elph}]$$

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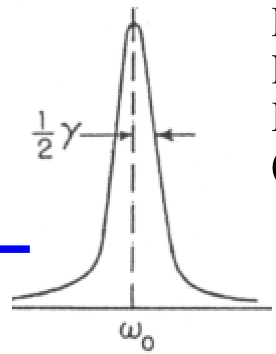

D. Sangalli, and A. Marini, Europhysics Letters 110, 47004 (2015)

$$\partial_t f_{nk}^{(e)}(t) = \frac{\gamma_{nk}^{(h)} f_{nk}^{(h)} - \gamma_{nk}^{(e)} f_{nk}^{(e)}}{f_{nk}^{(e)}} f_{nk}^{(e)}$$

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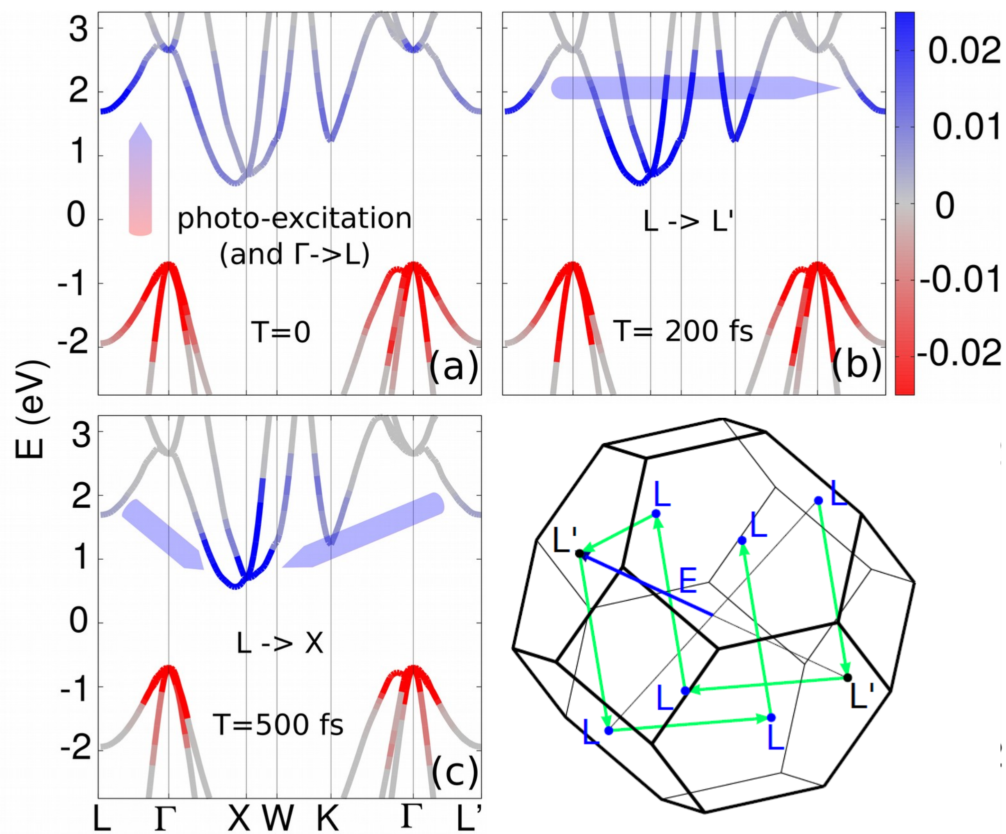
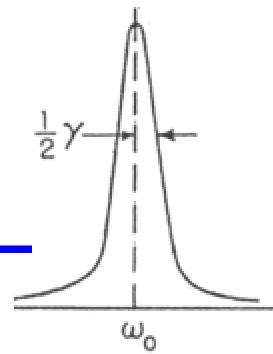


Non equilibrium qp-lifetimes

$$\gamma^{e,eq}_{nk} = \Im\left[\Sigma^{elph}_{nk}\right]$$

$$f^{(e)}_{nk} = f^{(e,0)}_{nk}\, e^{-\gamma^{(e,eq)}_{nk} t}$$

$$\partial_t f^{(e)}_{nk}(t) = -\gamma^{(e,eq)}_{nk} f^{(e)}_{nk}$$



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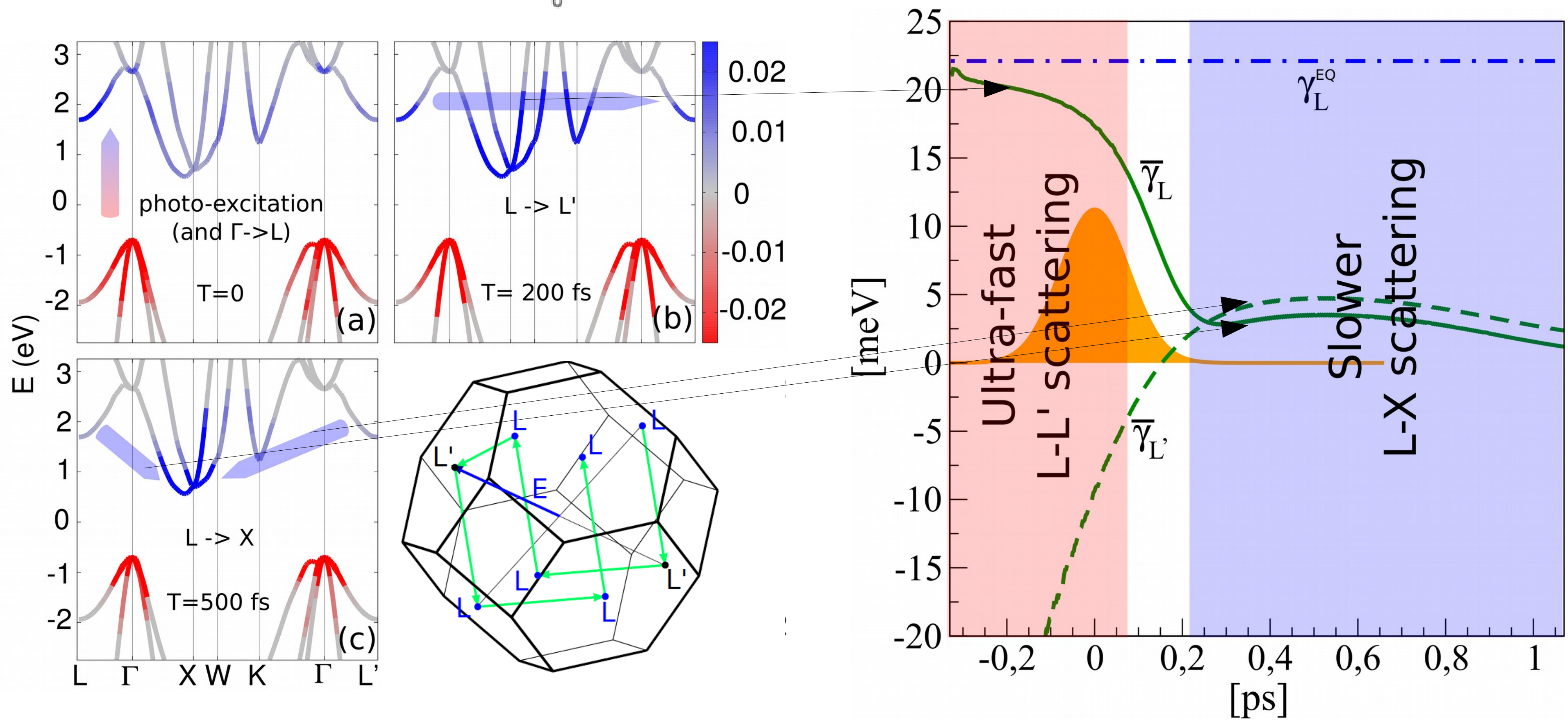
$$\partial_t f^{(e)}_{nk}(t) = \frac{\gamma^{(h)}_{nk} f^{(h)}_{nk} - \gamma^{(e)}_{nk} f^{(e)}_{nk}}{f^{(e)}_{nk}} f^{(e)}_{nk}$$

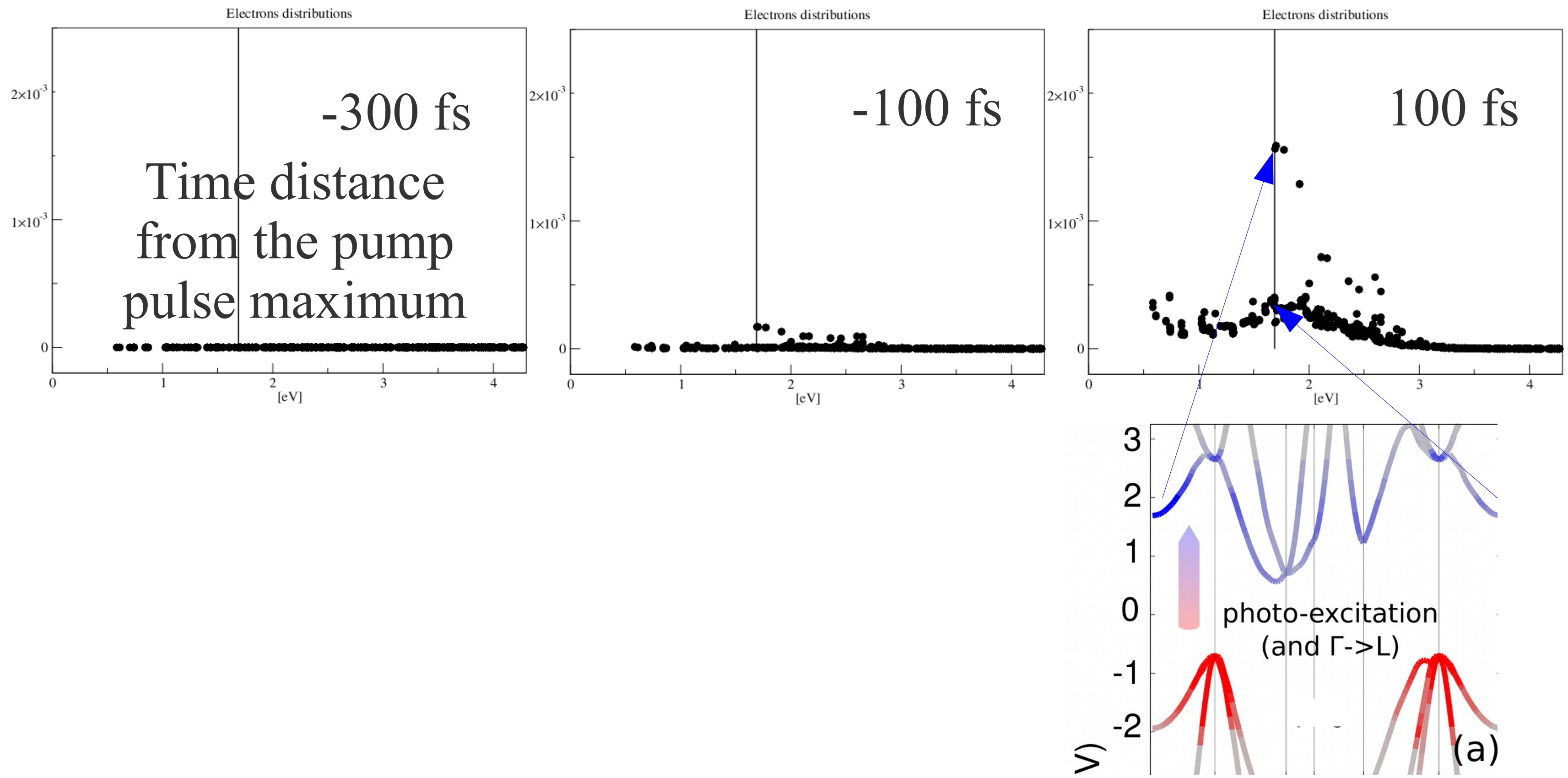
$$\partial_t f^{(e)}_{nk}(t) = -\bar{\gamma}^{(e)}_{nk} f^{(e)}_{nk}$$



$f_{nk}^{(e)}(\epsilon_{nk})$

Formation of Fermi distributions

Occupations



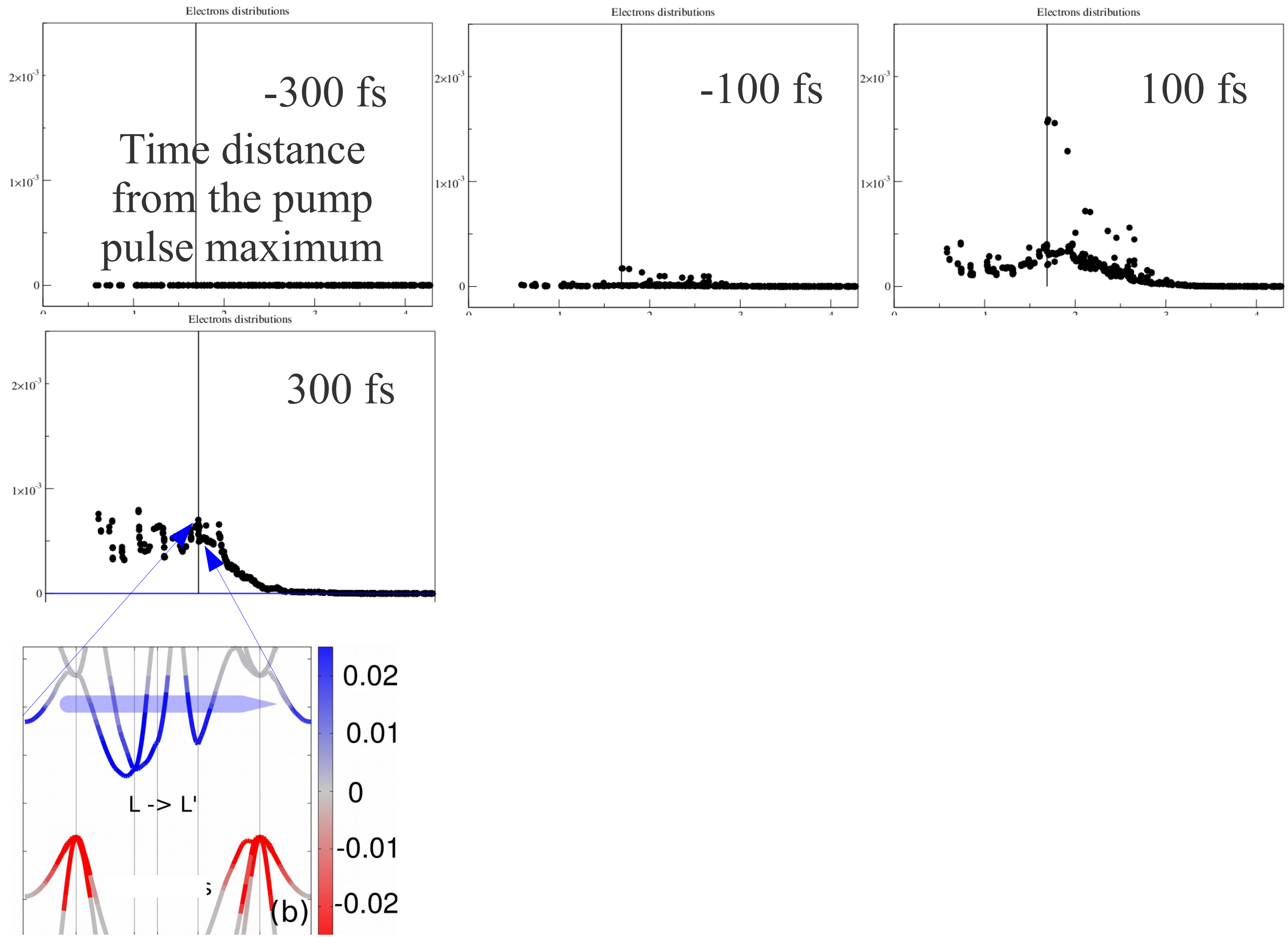
$$S_{nnk}^{<}(t)=\gamma_{nk}^{(h)} f_{nk}^{(h)}(t)-\gamma_{nk}^{(e)} f_{nk}^{(e)}(t)$$

Energy [eV]

$f_{nk}^{(e)}(\epsilon_{nk})$

Formation of Fermi distributions

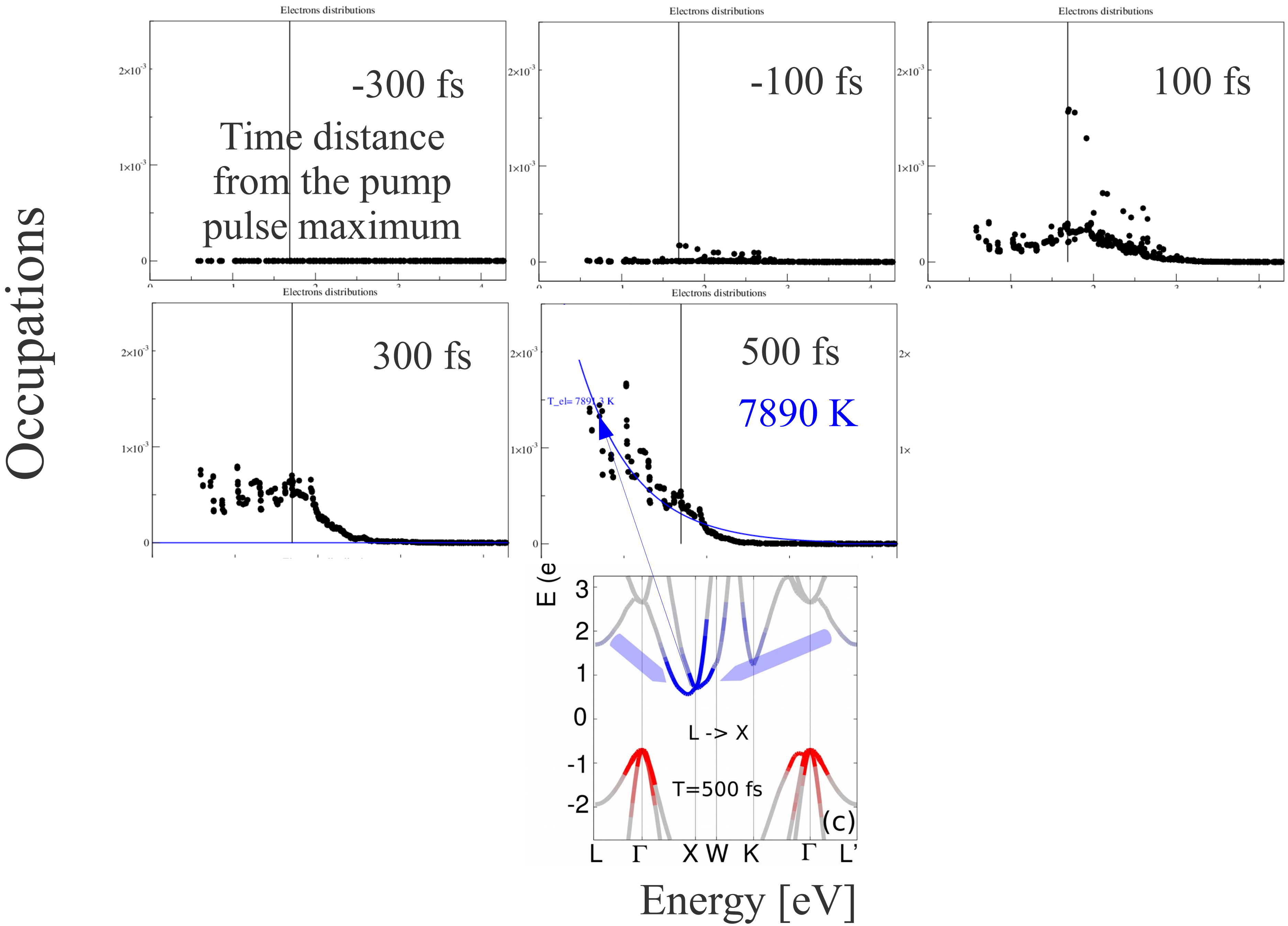
Occupations



Energy [eV]

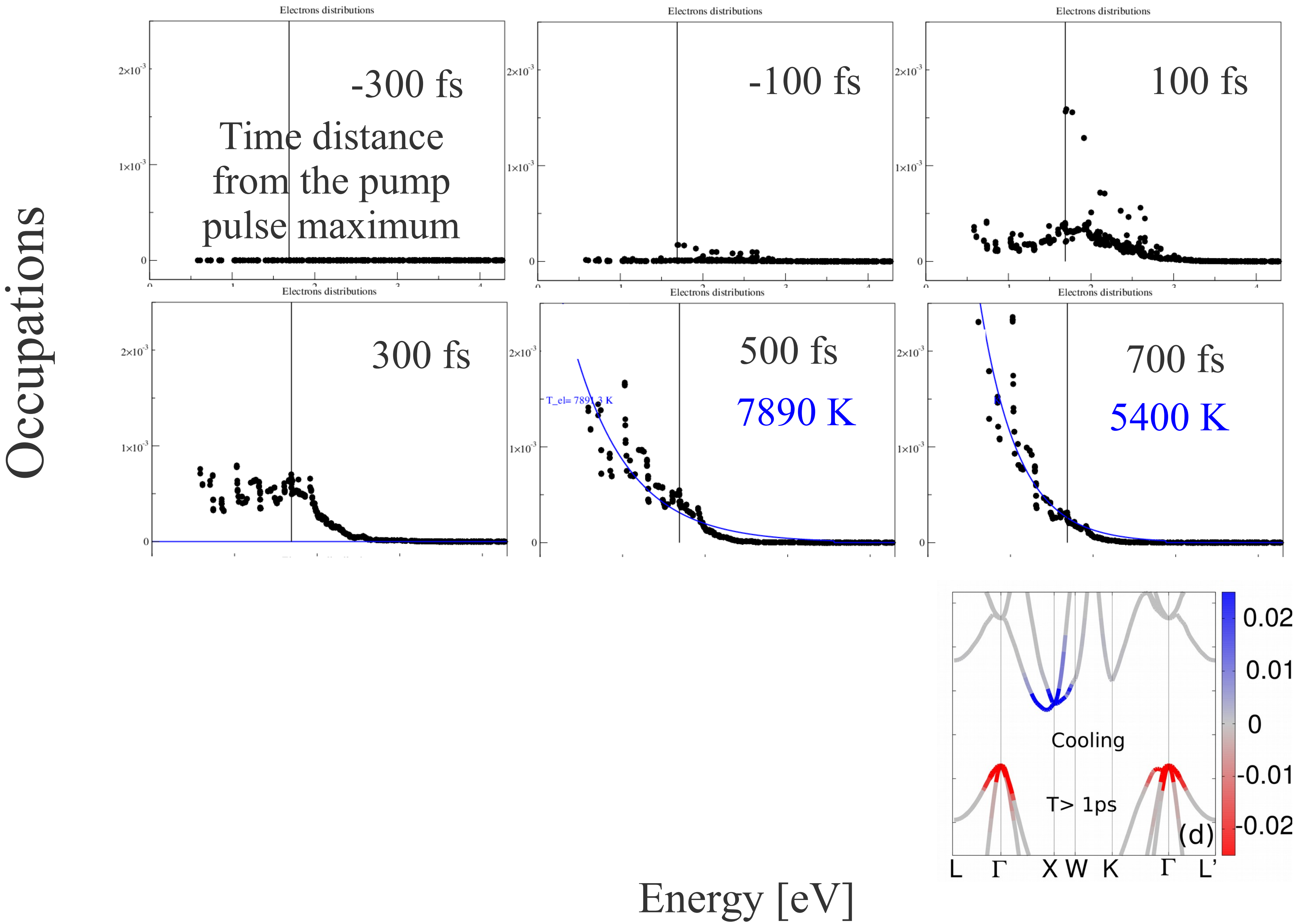
$f_{nk}^{(e)}(\epsilon_{nk})$

Formation of Fermi distributions



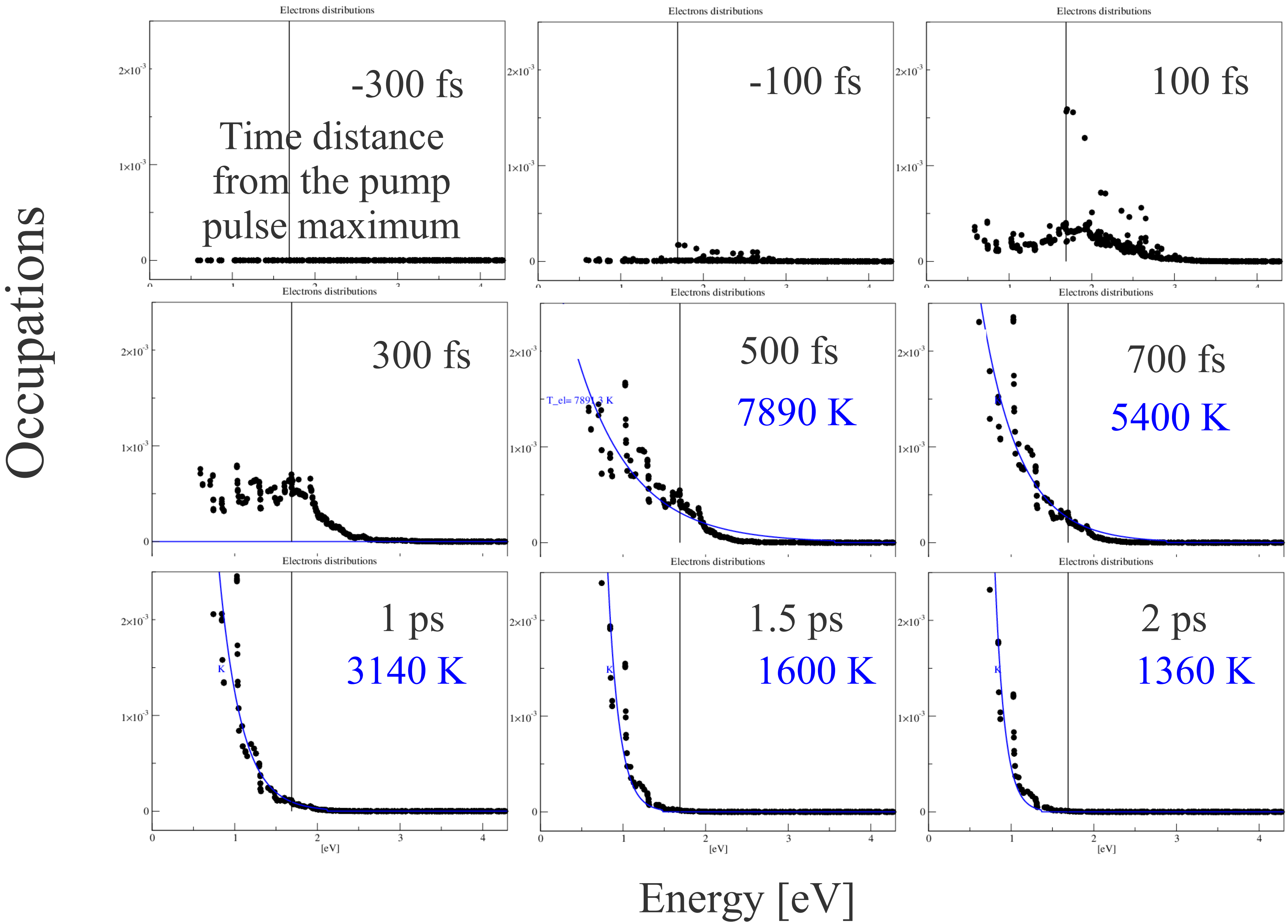
$f^{(e)}_{nk}(\epsilon_{nk})$

Formation of Fermi distributions

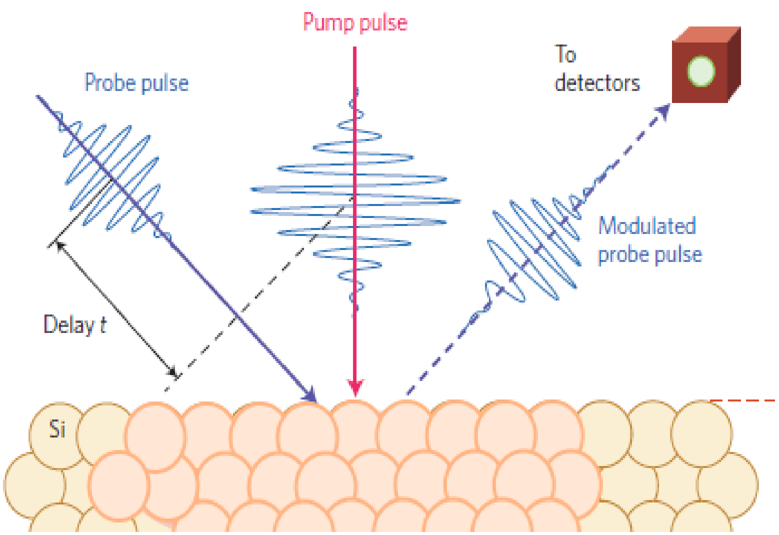


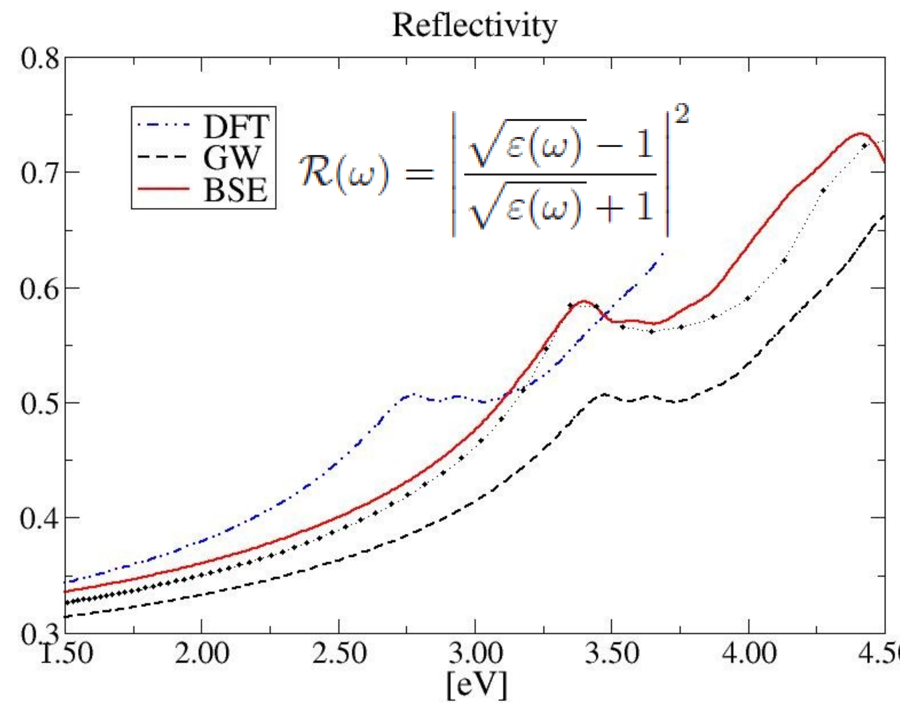
$f_{nk}^{(e)}(\epsilon_{nk})$

Formation of Fermi distributions



Transient reflectivity Silicon

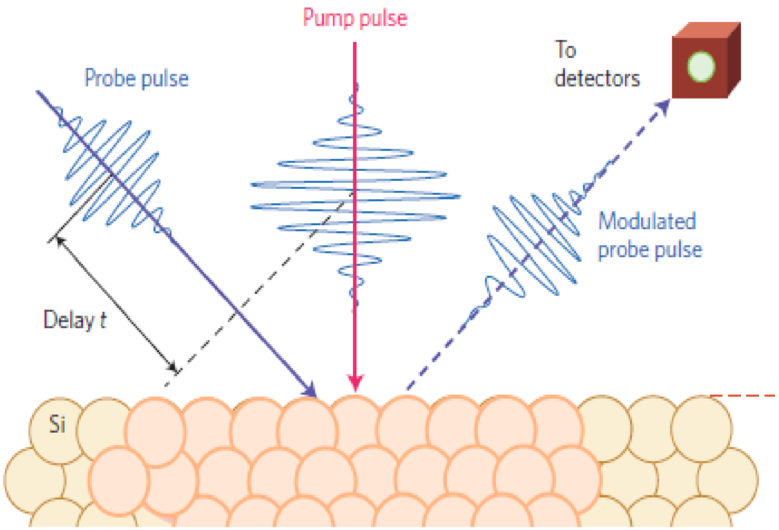


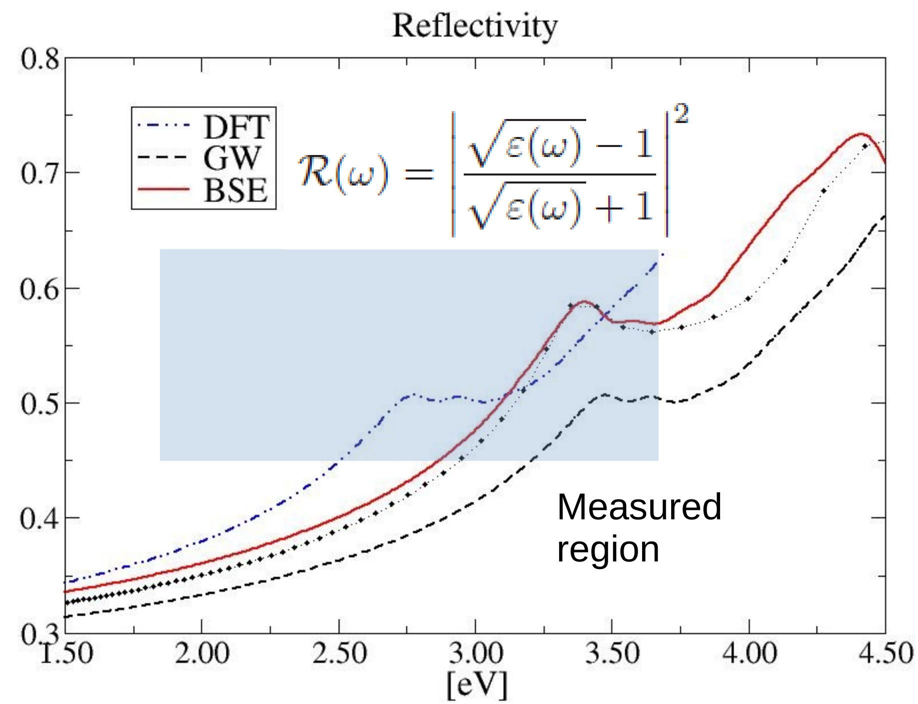


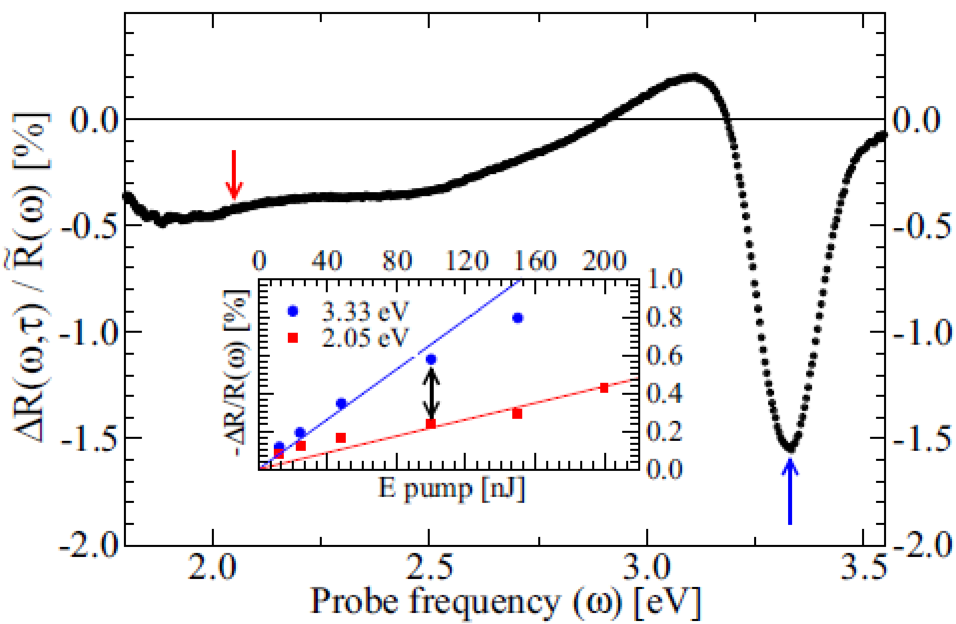
D. Sangalli, S. Dal Conte, C. Manzoni, G. Cerullo and A. Marini, PHYSICAL REVIEW B **93**, 195205 (2016)

Editor's suggestion

Transient reflectivity Silicon







Pump
Energy 3.1 eV
Fluence 12 nJ – 200 nJ

White Probe
1.7 – 3.1 eV

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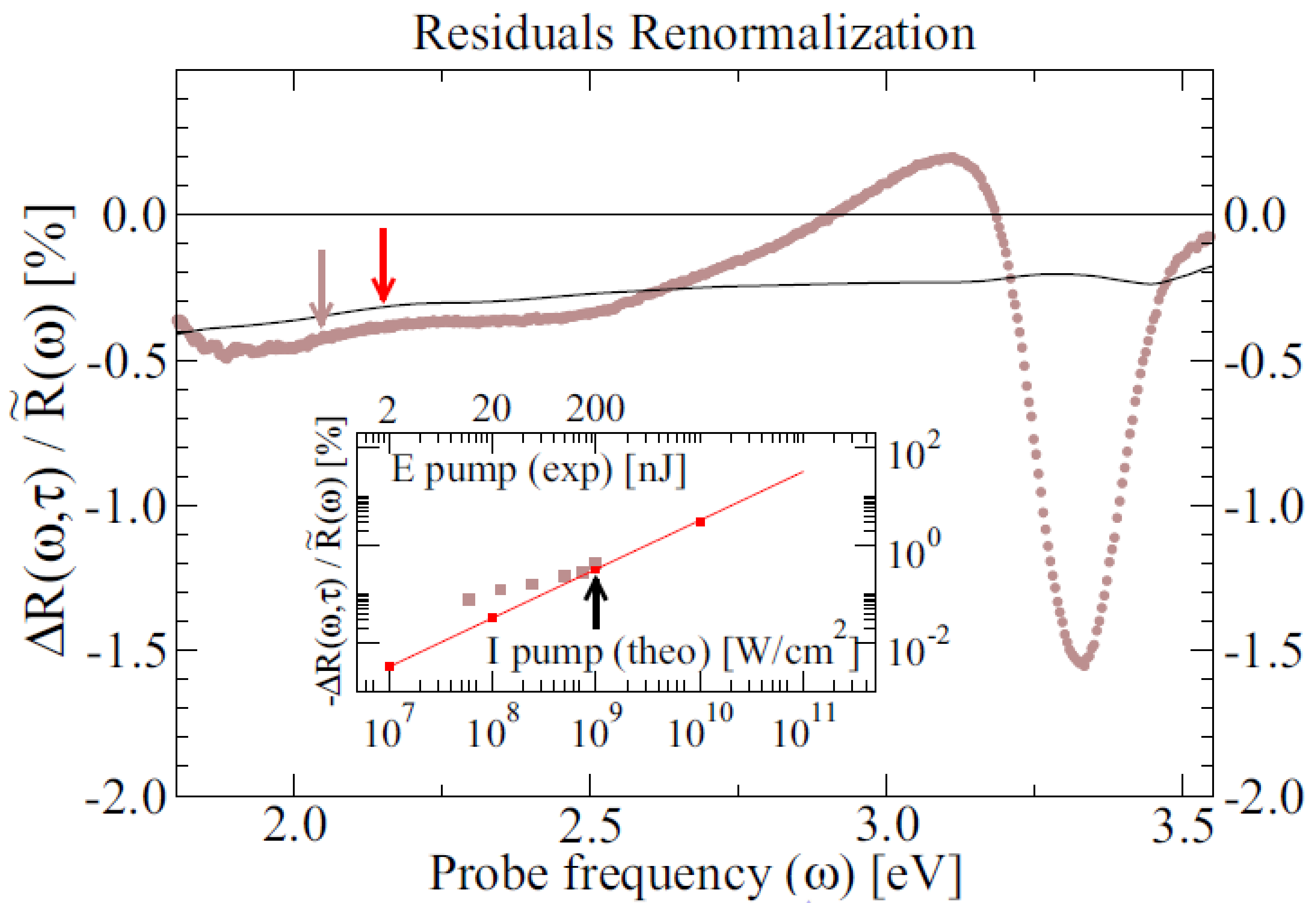
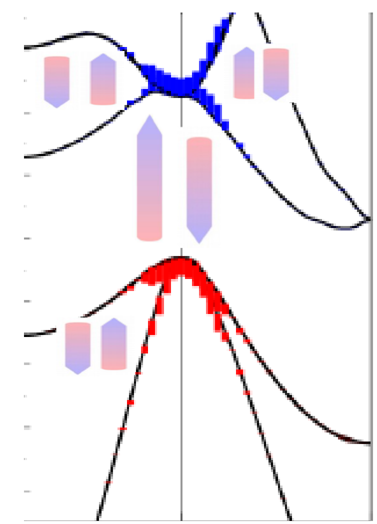
Editor's suggestion

Transient reflectivity Silicon



Bleaching,
photo-induced absorption,
stimulated emission



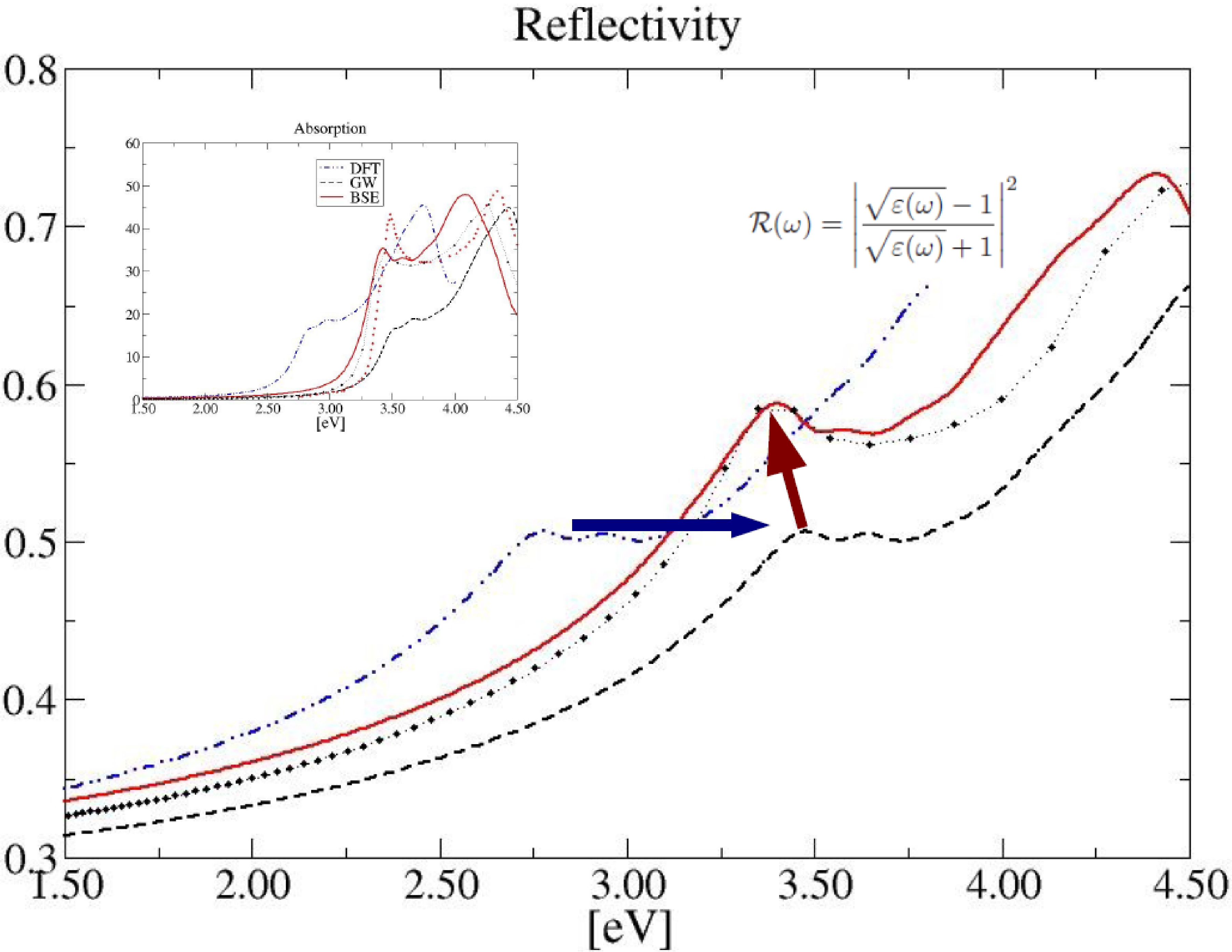
$$\epsilon(\omega,\tau) = 1 - 4\pi \sum_\lambda R^*_\lambda(\tau) L^{exc}_{\lambda\lambda}(\omega) R_\lambda(\tau) - 4\pi \sum_{ij} R^*_{ij}(\tau) L^{qp}_{ij,ij}(\omega) R_{ij}(\tau)$$

D. Sangalli, S. Dal Conte, C. Manzoni,
G. Cerullo and A. Marini,

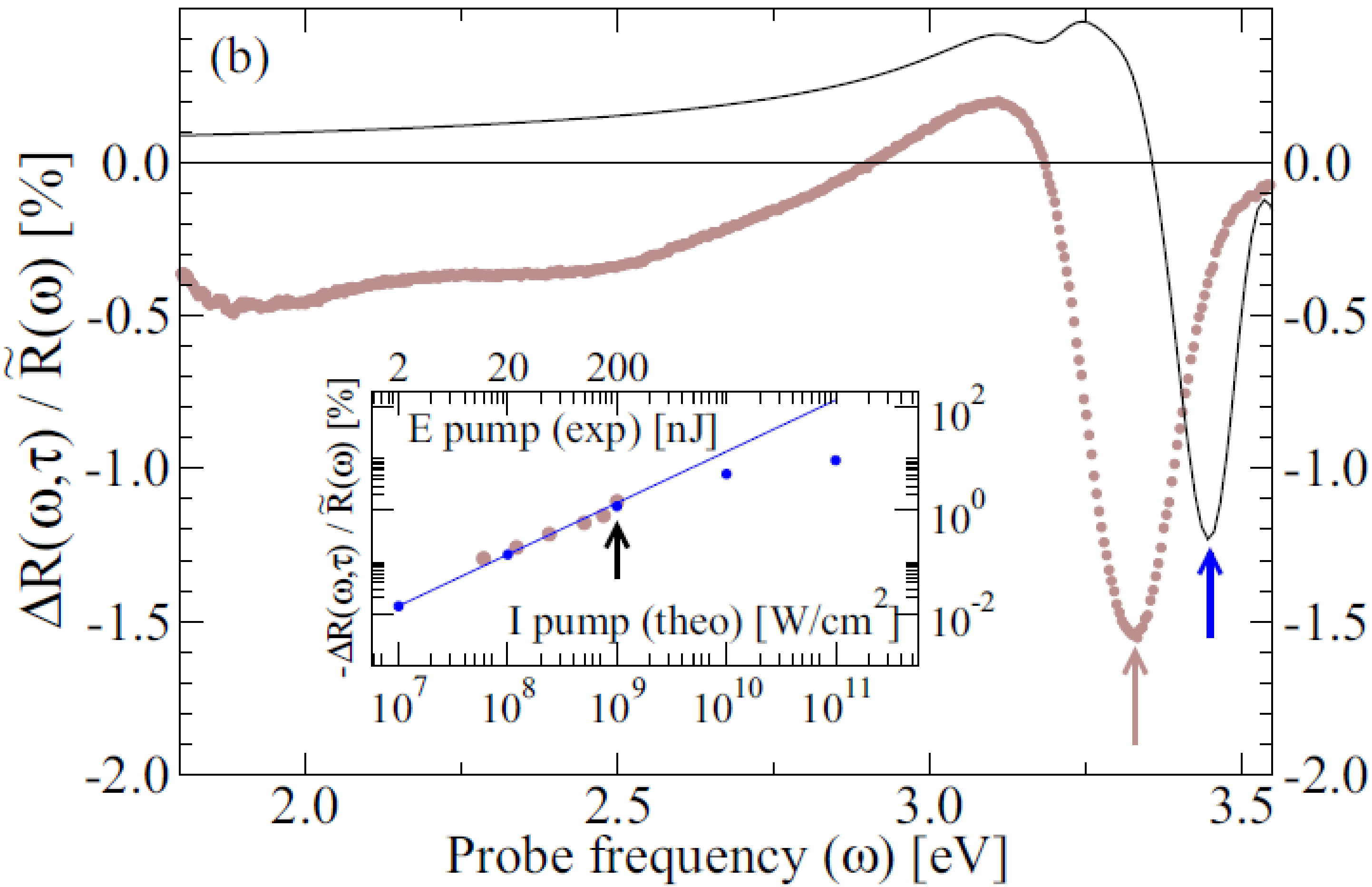
PHYSICAL REVIEW B **93**, 195205 (2016)

Editor's suggestion

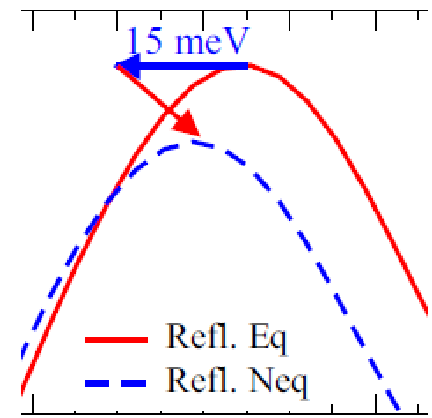
Transient reflectivity Silicon



Transient reflectivity Silicon



Screening effects



$$\epsilon(\omega,\tau) = 1 - 4\pi \Sigma_\lambda R^*_\lambda L^{exc}_{\lambda\lambda}(\omega,\tau) R_\lambda$$

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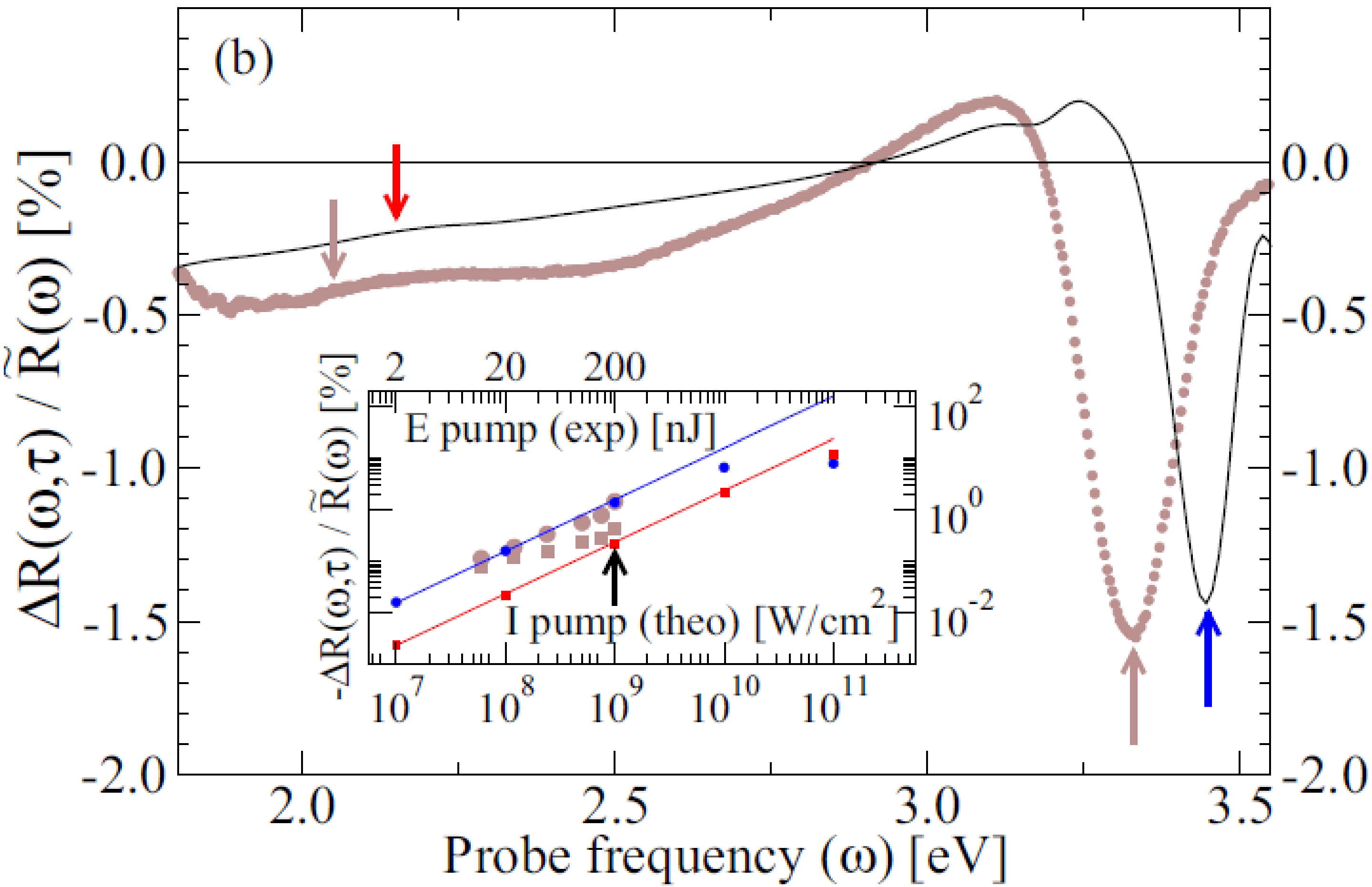
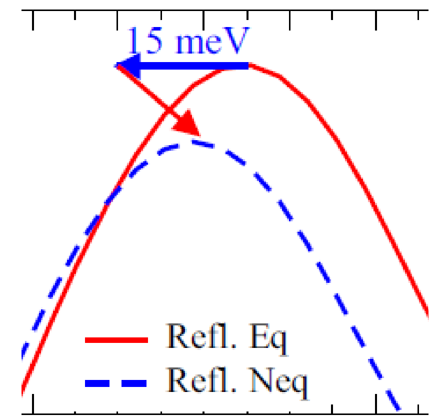
PHYSICAL REVIEW B **93**, 195205 (2016)

Editor's suggestion

Transient reflectivity Silicon

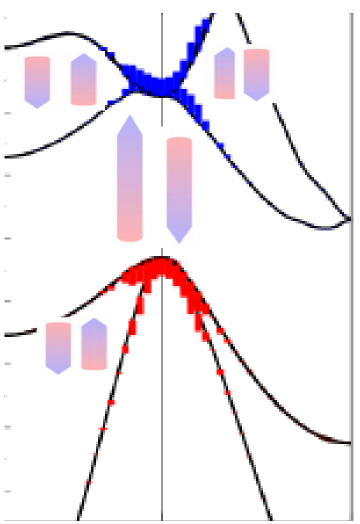


Screening effects



+

Bleaching,
stimulated emission,
photo-induced absorption



D. Sangalli, S. Dal Conte, C. Manzoni, G. Cerullo and A. Marini,

PHYSICAL REVIEW B **93**, 195205 (2016)

Editor's suggestion

The “ultra-fast” team

A. Marini
(project leader)

D. Sangalli

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

Code, theory developments, application to bulk systems:
www.yambo-code.org (part GPL / part “pre-GPL”)
https://github.com/yambo-code

E. Perfetto

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Code, theory development,
applications to models and isolated systems

The "ultra-fast" team


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Code, theory developments, application to bulk systems:
www.yambo-code.org (part GPL / part "pre-GPL")
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Yambo©

Applications to transition metal dicalcogenides

Nano Letters, **17**, 4549 (2017): *Ab Initio Calculations of Ultrashort Carrier Dynamics in Two-Dimensional Materials: Valley Depolarization in Single-Layer WSe2*

ACS nano **10**, 1182 (2016) *Photo-Induced Bandgap Renormalization Governs the Ultrafast Response of Single-Layer MoS2*


M. Marsili

Teaching

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Thank you for your attention

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The Kadanoff Baym equation

$$\underbrace{i\partial_t G^<_{nmk}(t,t) - [H^{eq} + \Delta V^H + \Delta\Sigma_s + U^{ext}(t), G^<(t,t)]_{nmk}}_{\text{Coherent evolution}} = \underbrace{S_{nmk}(t)}_{\text{Scattering term}}$$

Coherent evolution **Scattering term**

Propagate a group of small matricies, one for each k-point, "N x N".
Silicon case: N = 8; 743 matricies on a double grid in the IBZ (4x4x4 + 15x15x15)
(6x6x6 + 25x25x25)

All EOM are coupled via
a) The calculation of the density matrix (easy part)
b) The scattering processes from k -> k+q which need to be updated

Some timing on bulk silicon @(4x4x4+15x15x15):

DFT: (i) scf:	~1s	serial (coarse grid)
(ii) nscf:	33s	serial (coarse grid, 100 bands)
	5m 6s	4 cores (fine grid)
DFPT: (i) phonons and elph:	1m	4 cores (coarse grid, 10 bands)
GW:	9h 8m	4 cores (fine grid)
BSE:	1h30m	4 cores (fine grid)
SEX Kernel:	2m48s	4 cores (coarse grid)
NEGF: (t=0.01 fs)	14h38m	4 cores (double grid, scatt. 2.5 fs, 11h1m)
NEQ COHSEX:	1h51m	4 cores (fine grid)
NEQ BSE:	2h40m	4 cores (fine grid)