Ab initio approach to Spectroscopies

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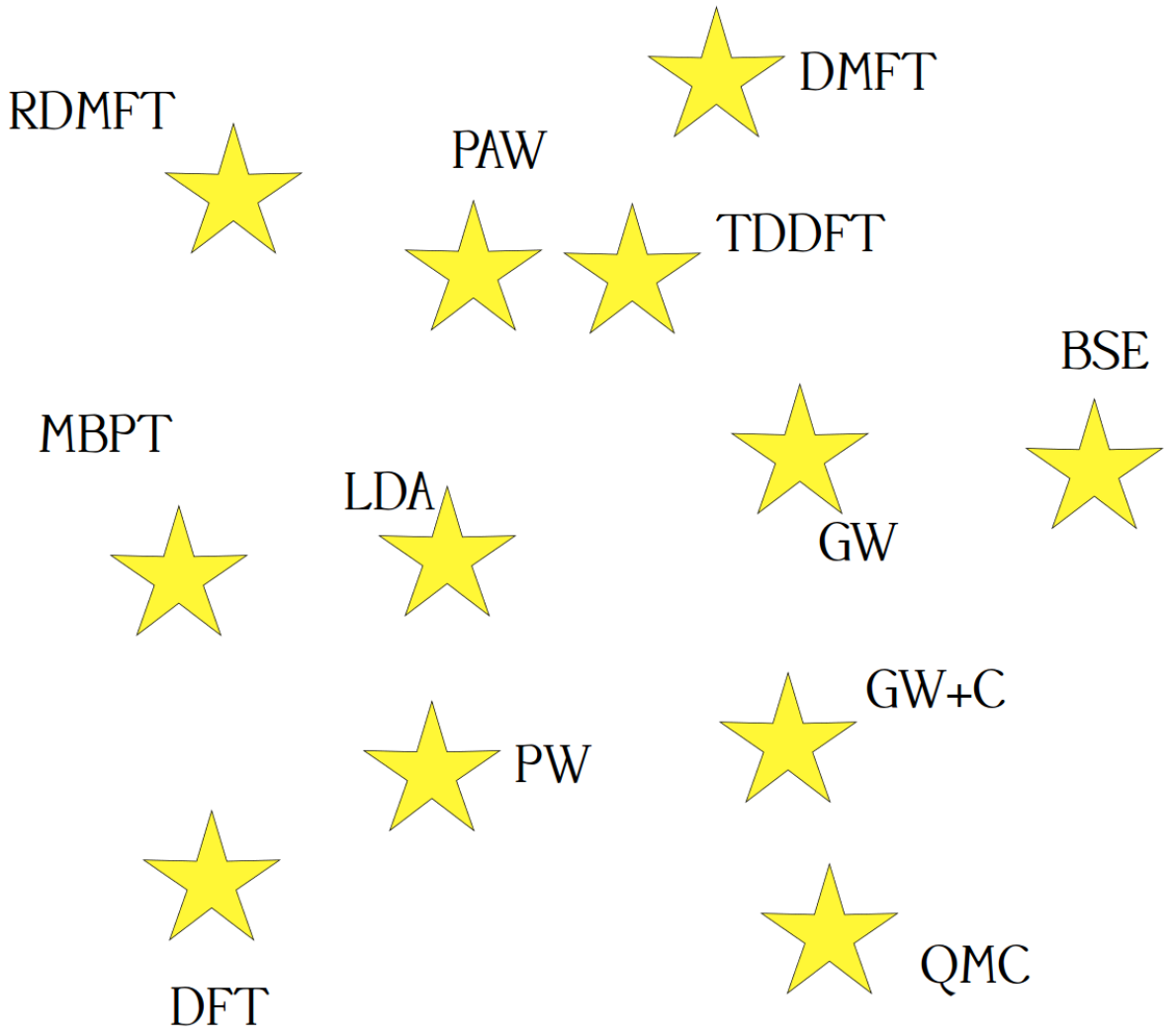
Theory Days - SOLEIL - 8 November 2016

ETSF
European Theoretical Spectroscopy Facility

LSI

ÉCOLE POLYTECHNIQUE
UNIVERSITÉ PARIS-SACLAY

Theoretical keys from an outsider



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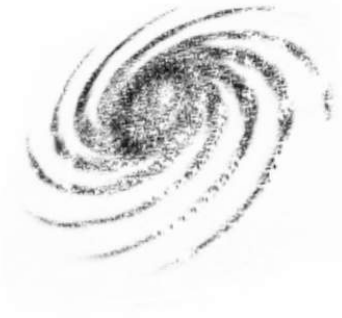
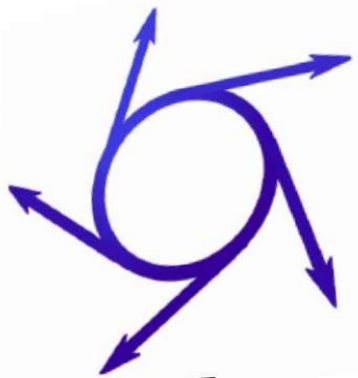




From theory(ies) to collaboration

User projects (EU)

http://www.etsf.eu/

Collaborative projects

industry projects, training projects

Collaborative projects

industry projects, training projects

- Get into contact

  Silvana Botti `silvana.botti@uni-jena.de`
  For SOLEIL :: Matteo Gatti
  Beamlines

- What is your topic and scientific question? Quick exchange
- Establish contact ⟶ possible collaboration
- Project and joint publications enter ETSF statictics

Collaborative projects

industry projects, training projects

- Get into contact

Silvana Botti

Large pool of theoreticians
keen to work with experimentalists

ETSF
European Theoretical Spectroscopy Facility

question? Quick exchange

contact → possible collaboration

- Project and joint publications enter ETSF statictics

X-ray absorption

Magnetic system

Optical absorption

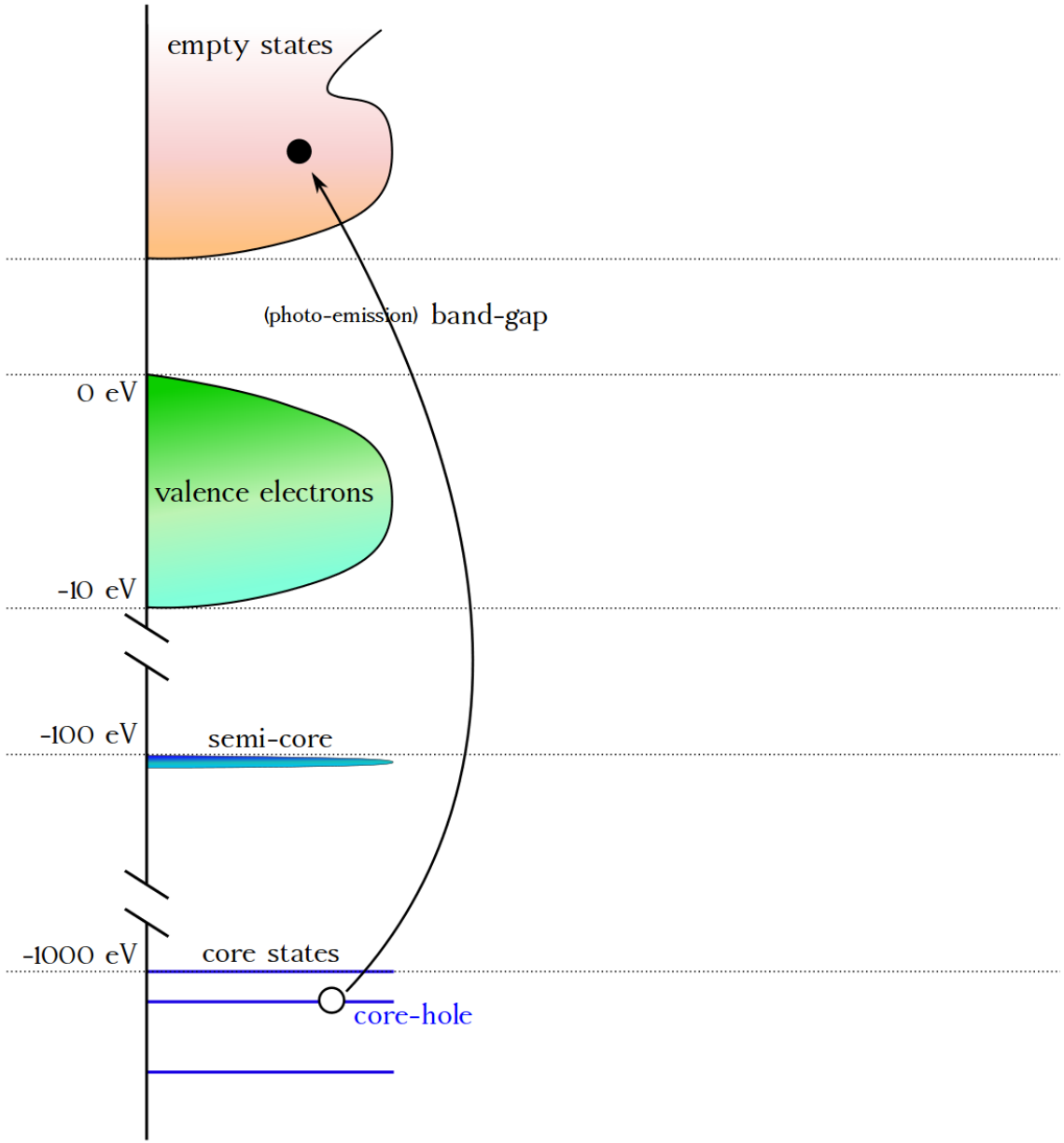
Quantum transport

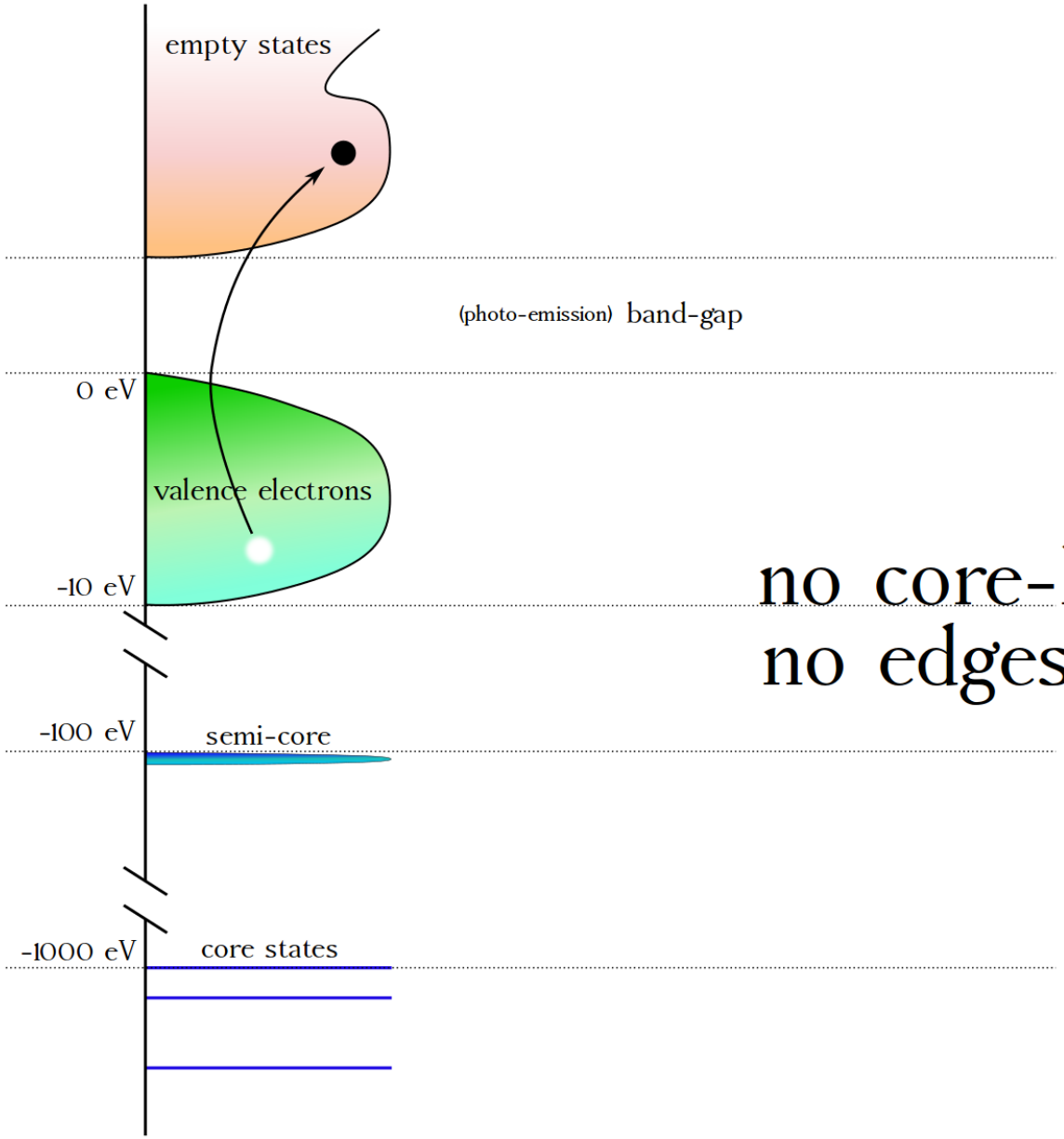
Angle-resolved Photo-emission

Raman spectra

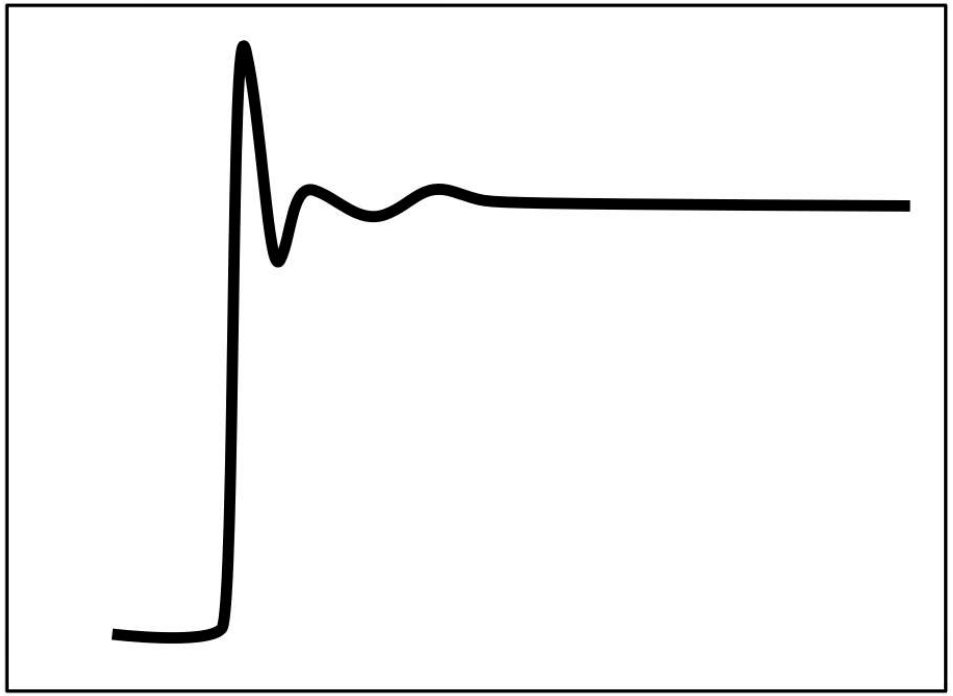
Loss spectroscopy

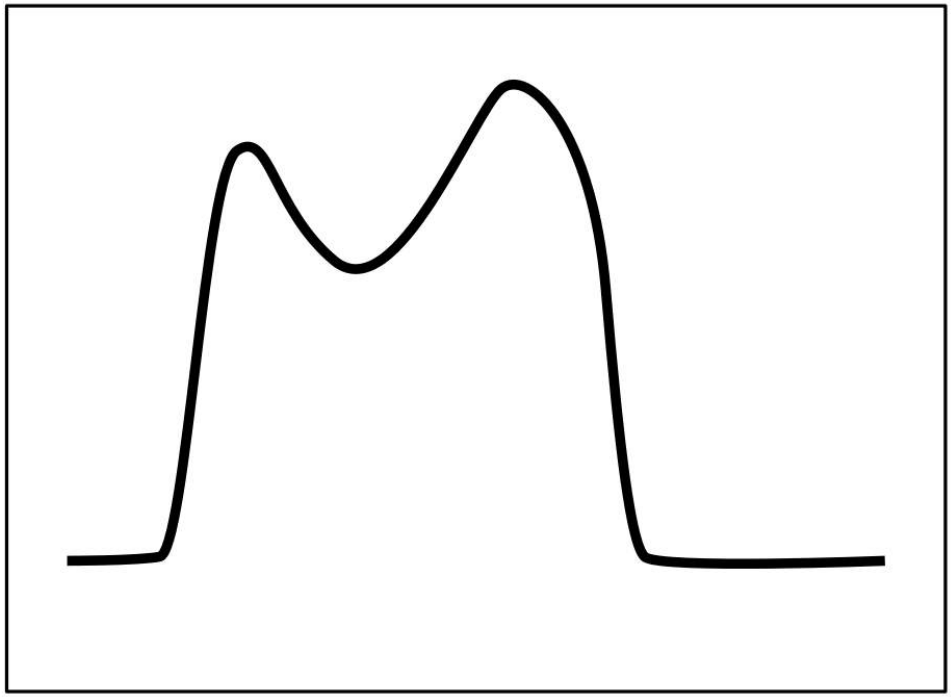
Inelastic X-ray Scattering


empty states
(photo-emission) band-gap
0 eV
valence electrons
-10 eV
-100 eV
semi-core
-1000 eV
core states
core-hole



no core-hole
no edges





REST

GDR REST

Rencontres de Spectroscopie Théorique

Two stage approach

- Ground state via Density Functional Theory
  (one-particle band-structure)

  ↳ Real space (atoms, molecules)

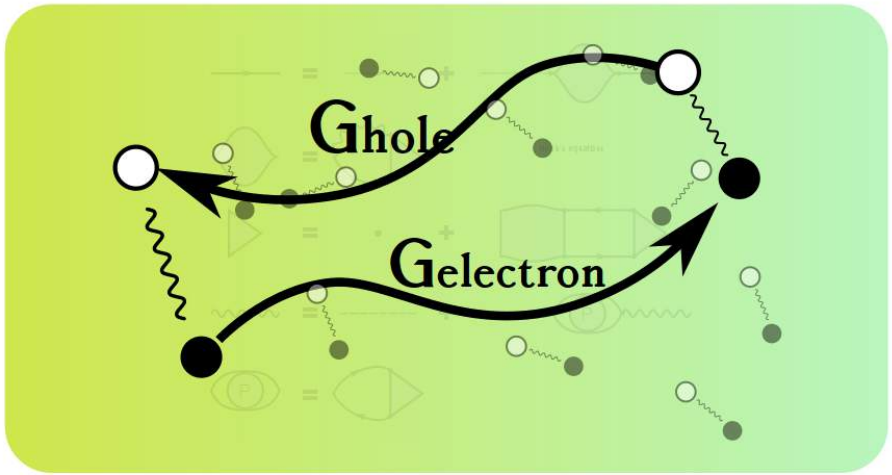
  ↳ Special (localized) basis :: Gaussians, wavelets, Slaters, ...

  ↳ Plane waves (solids) [Abinit, Espresso, VASP, ...]

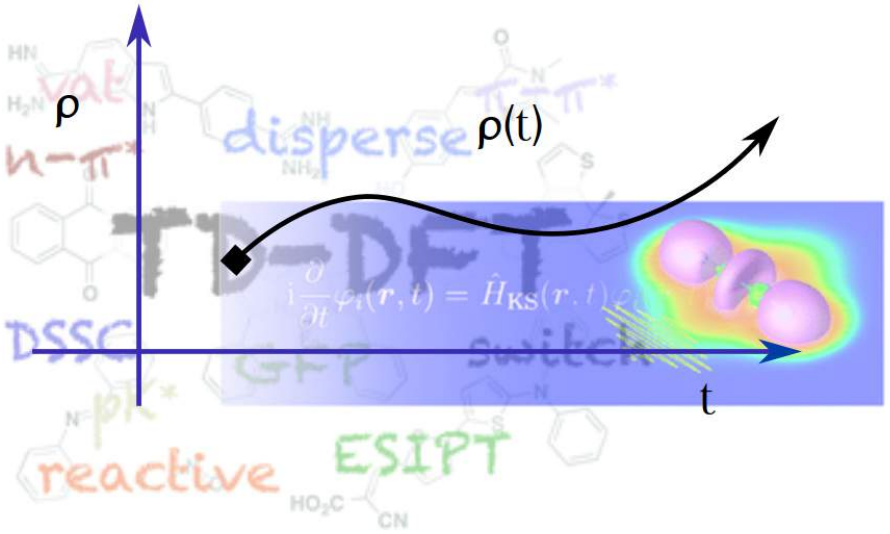
- Excited states (and spectroscopy) via ...

- Excited states (and spectroscopy) via ...

Many-body perturbation Theory



Time Dependent Density Functional Theory



2nd INTERNATIONAL SUMMER SCHOOL
IN ELECTRONIC STRUCTURE THEORY

I STPC

ELECTRON CORRELATION
IN PHYSICS & CHEMISTRY

JUNE 18th - JULY 1st

2017

Centre Paul-Langevin
Aussois – Savoie
FrAnce

Markus Reiher, ETH, Zurich, Switzerland

I STPC
2017

Looking forward to seeing you at the
ISTPC 2017 SUMMER SCHOOL!

Organizing committee:
Emmanuel Fromager, Vincent Robert,
Julien Toulouse, and Francesco Sottile.

Flash this QR-code for updates and practical informations
http://quantique.u-strasbg.fr/ISTPC

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GDR REST: **http://gdr-rest.polytechnique.fr**

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Theoretical Spectroscopy Lectures
CECAM-HQ-EPFL, Lausanne, Switzerland

European Theoretical Spectroscopy Facility

5 Days (theory and hands-on)

Density Functional Theory

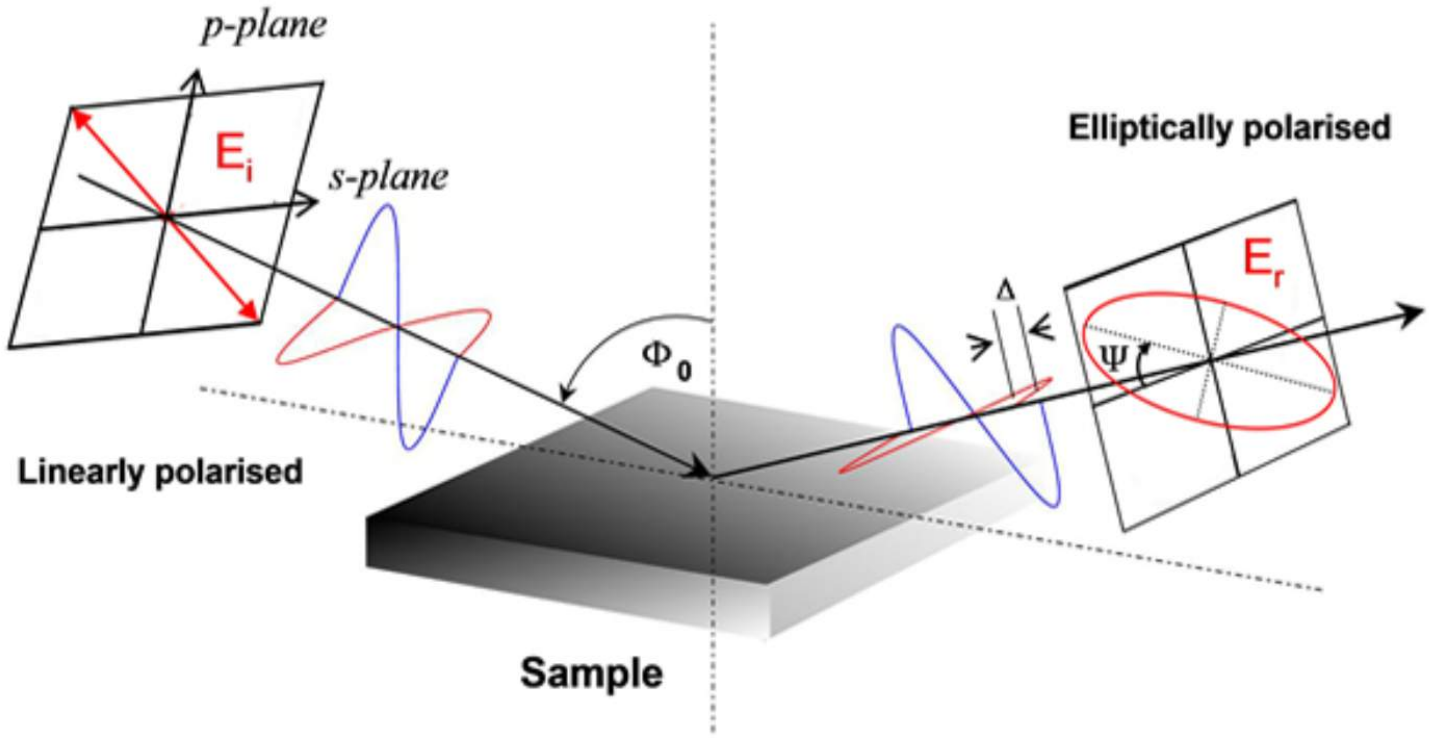
Green's Function Theory

GW approximation

Time Dependent Density Functional Theory

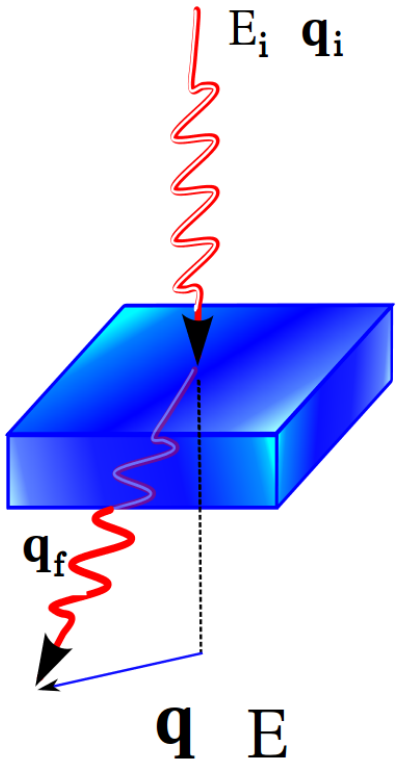
Bethe-Salpeter Equation

Optical absorption - Ellipsometry



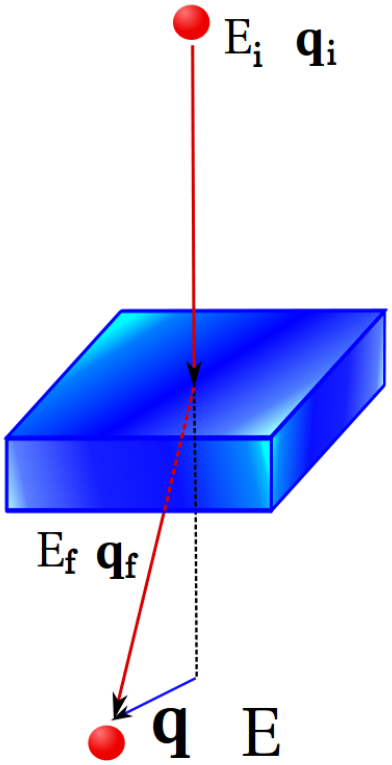
Reflcctivity, surface analysis (RAS, SDR, etc.)

Inelastic X-ray Scattering

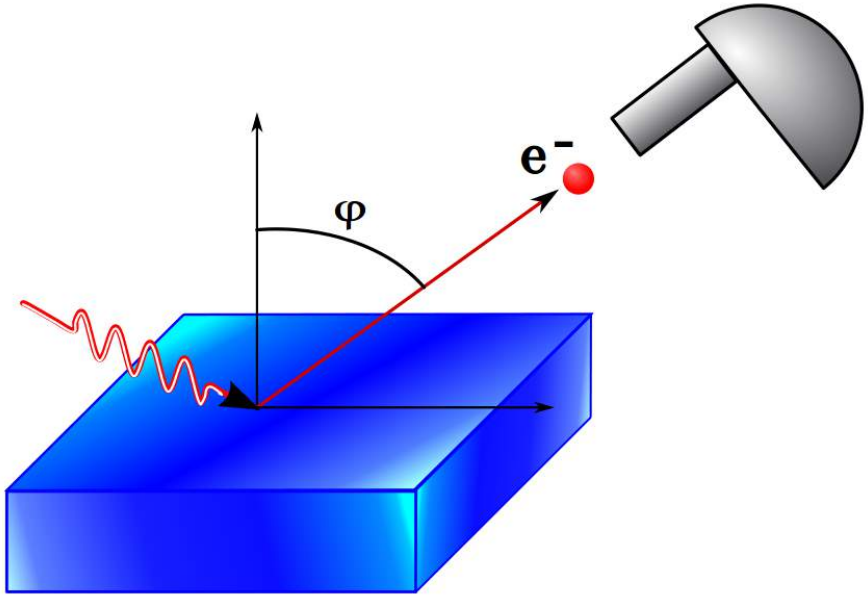


Resonant (RIXS) and non-resonant (NIXS)

Electron Energy Loss (EELS)



(angle-resolved) Photo-emission spectroscopy

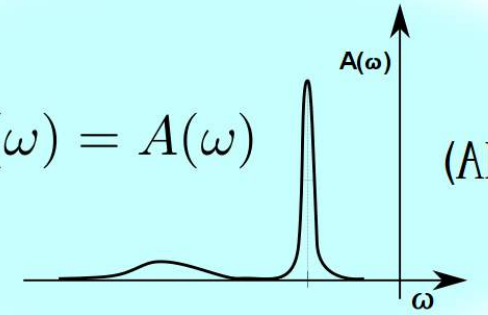


electronic band-structure

Many-body perturbation Theory

G^{el}
G^{hole} } band-gap

$\text{Im}G(\omega) = A(\omega)$



(AR)PES

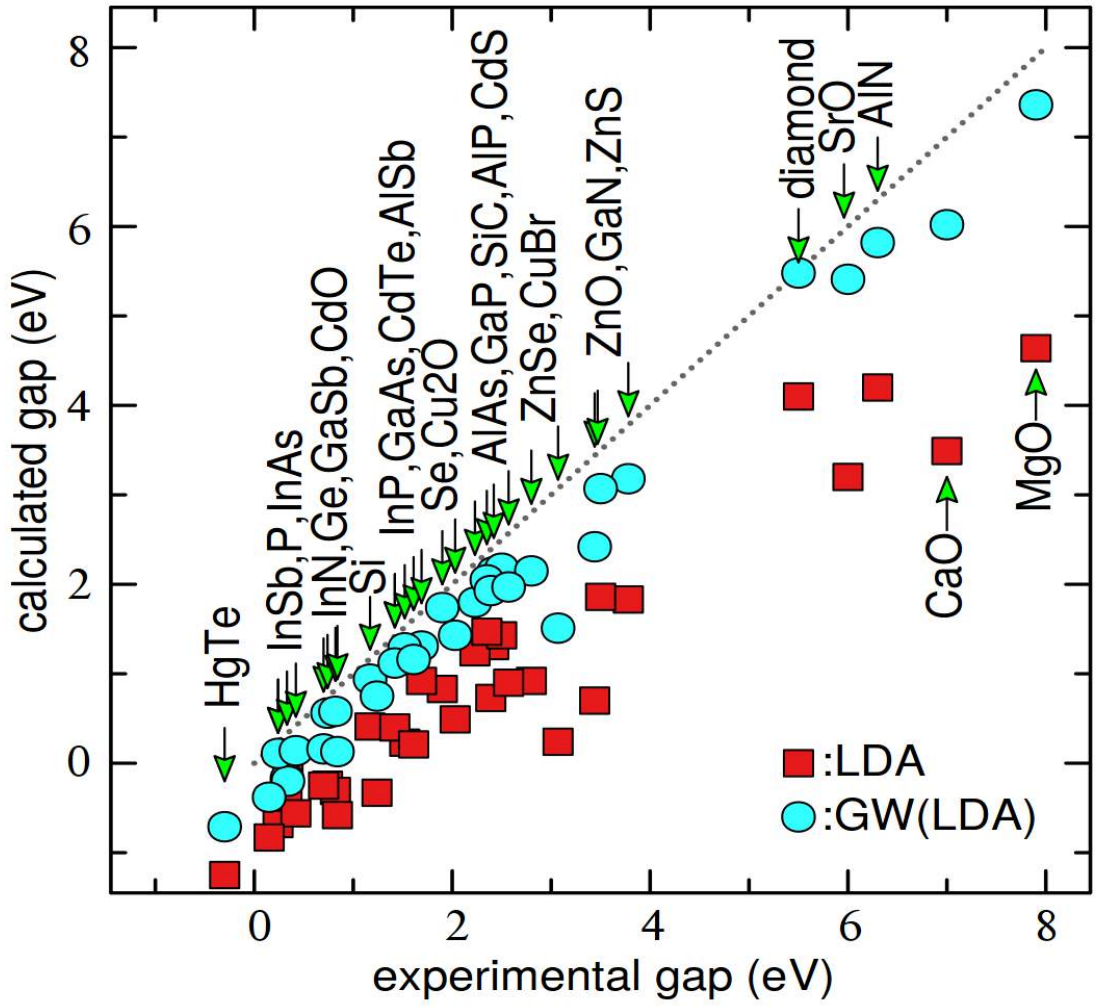
$G(\omega)$

$$G = G^0 + G^0 \Sigma G$$

unknown, to approximated

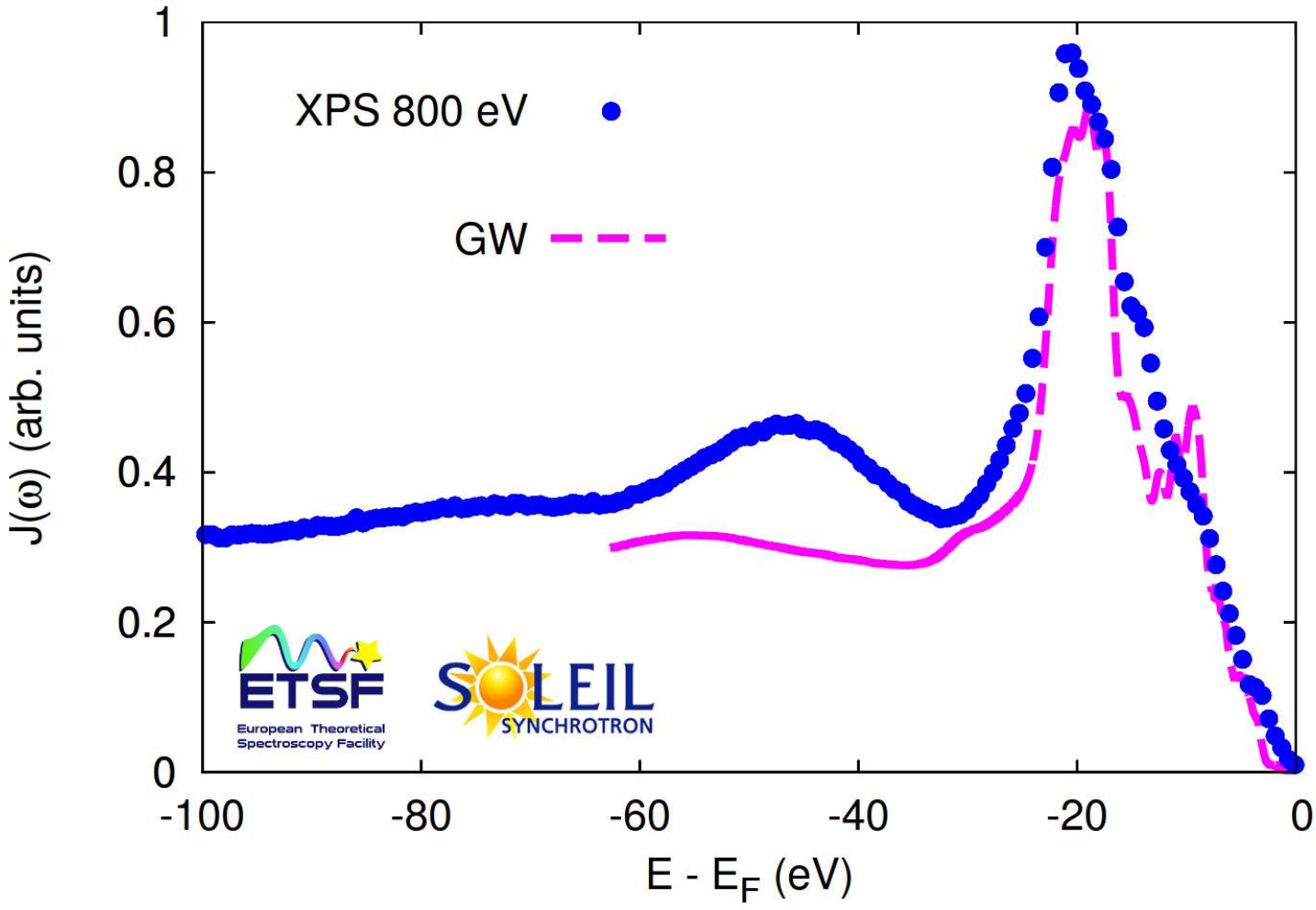
$\Sigma = GW$ approximation

Band-gaps of materials



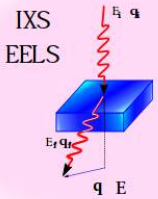
Phys. Rev. Lett. **96**, 226402 (2006)

Spectral function of Graphite vs PES experiment



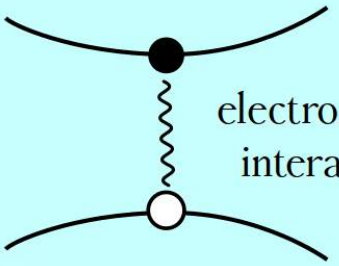
Phys. Rev. B **89**, 085425 (2014)

Many-body perturbation Theory



$$\chi \propto \frac{d^2\sigma}{d\omega d\Omega}$$

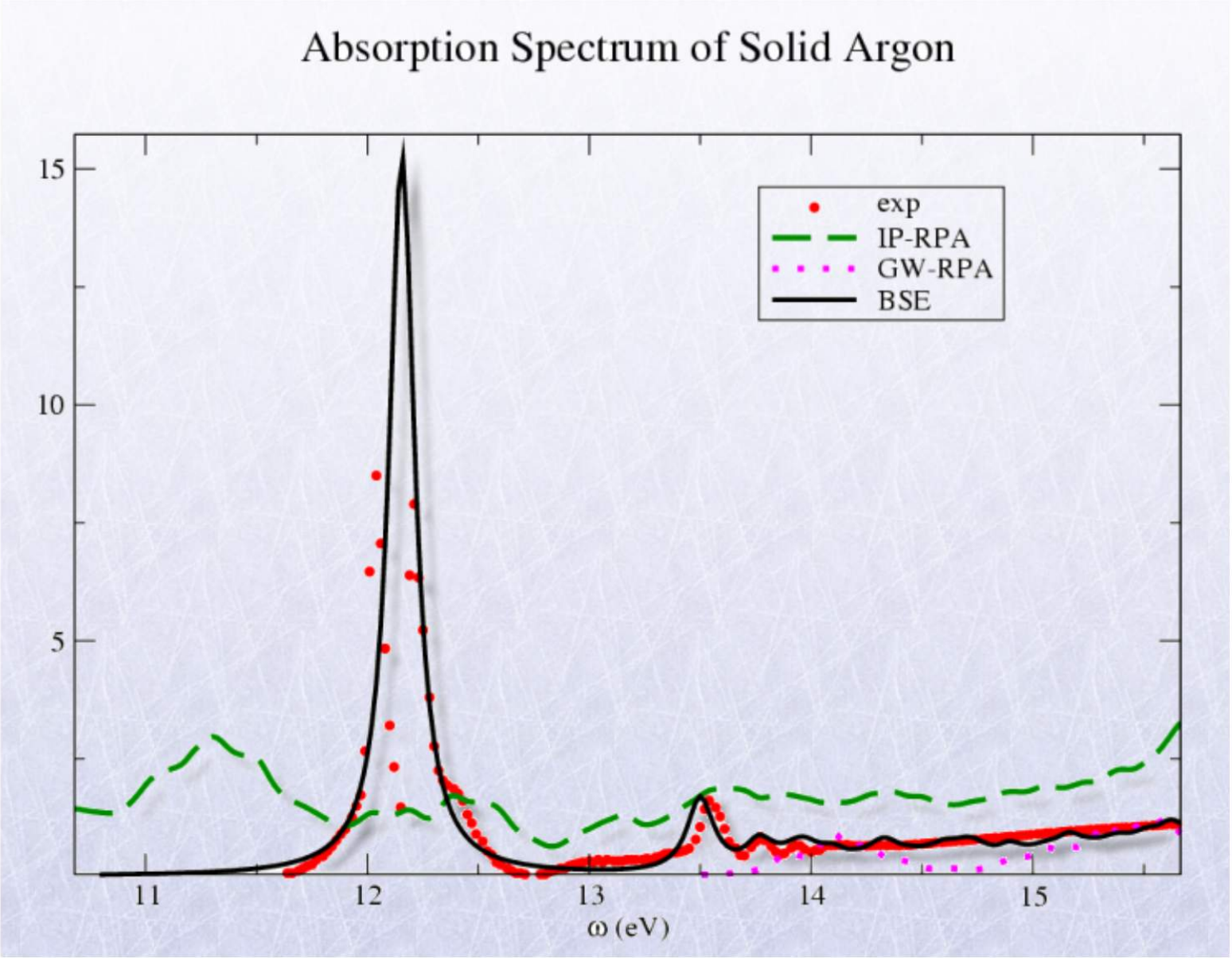
Absorption experiment



$$G^{(2)} \propto \chi(\omega)$$

$$\chi = GG + GG\frac{\delta\Sigma}{\delta G}\chi$$

Bethe-Salpeter equation



Phys. Rev. B **76**, 161103(R) (2007)

Many-body perturbation Theory

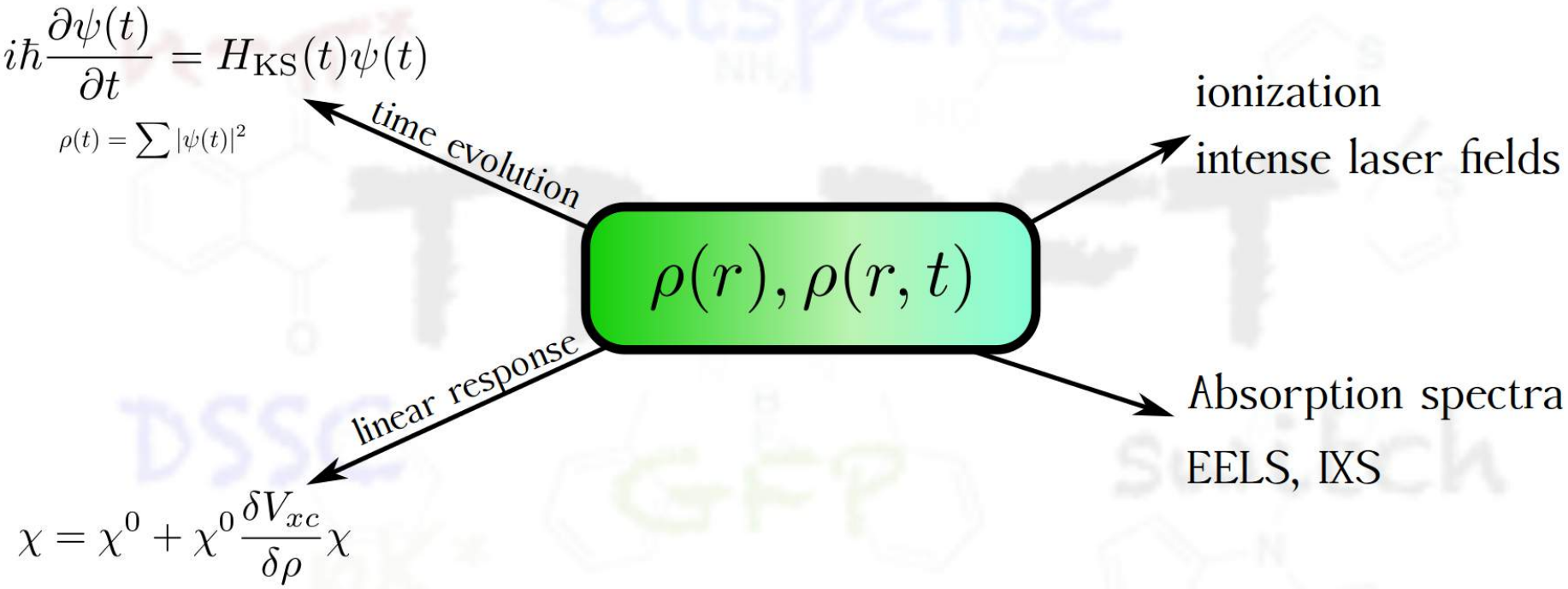
- **(AR)PES** $G, \Sigma = GW$

  scaling N_{at}^4 < 1000 atoms

- **Absorption, EELS, IXS** $\chi, \frac{\delta \Sigma}{\delta G} = W$

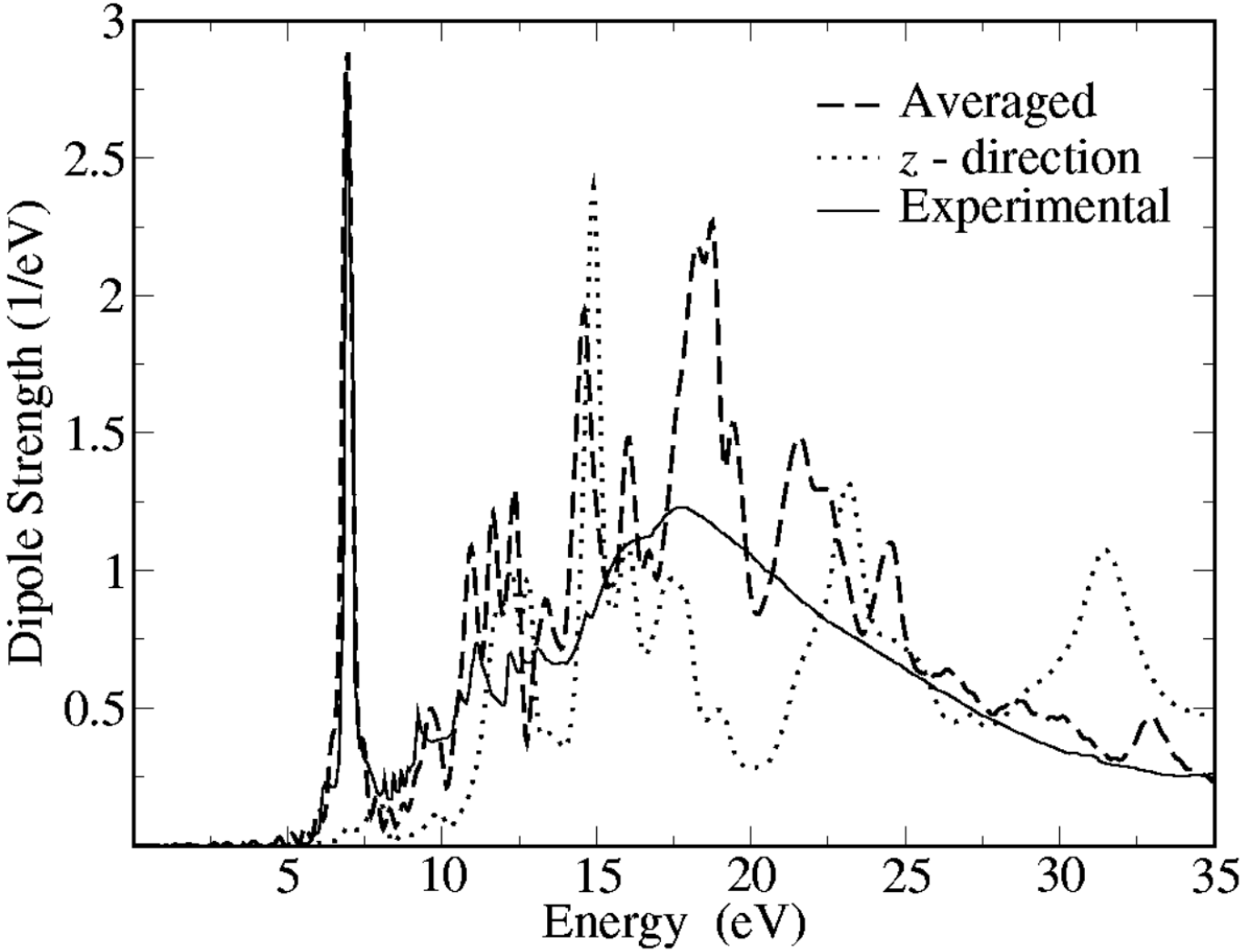
  scaling $N_{\mathrm{at}}^{4 \div 6}$ ~ 100 atoms

Time Dependent Density Functional Theory

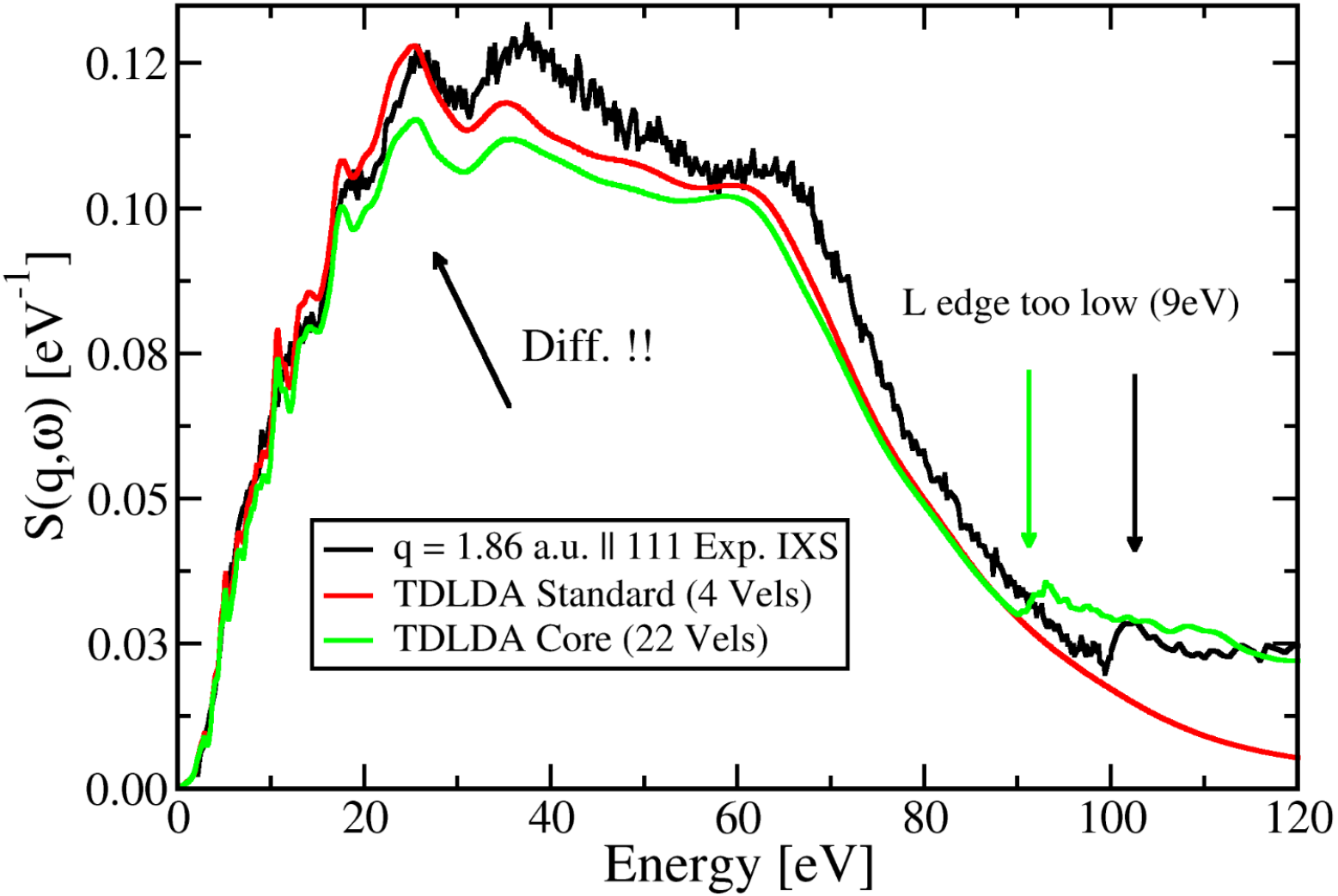


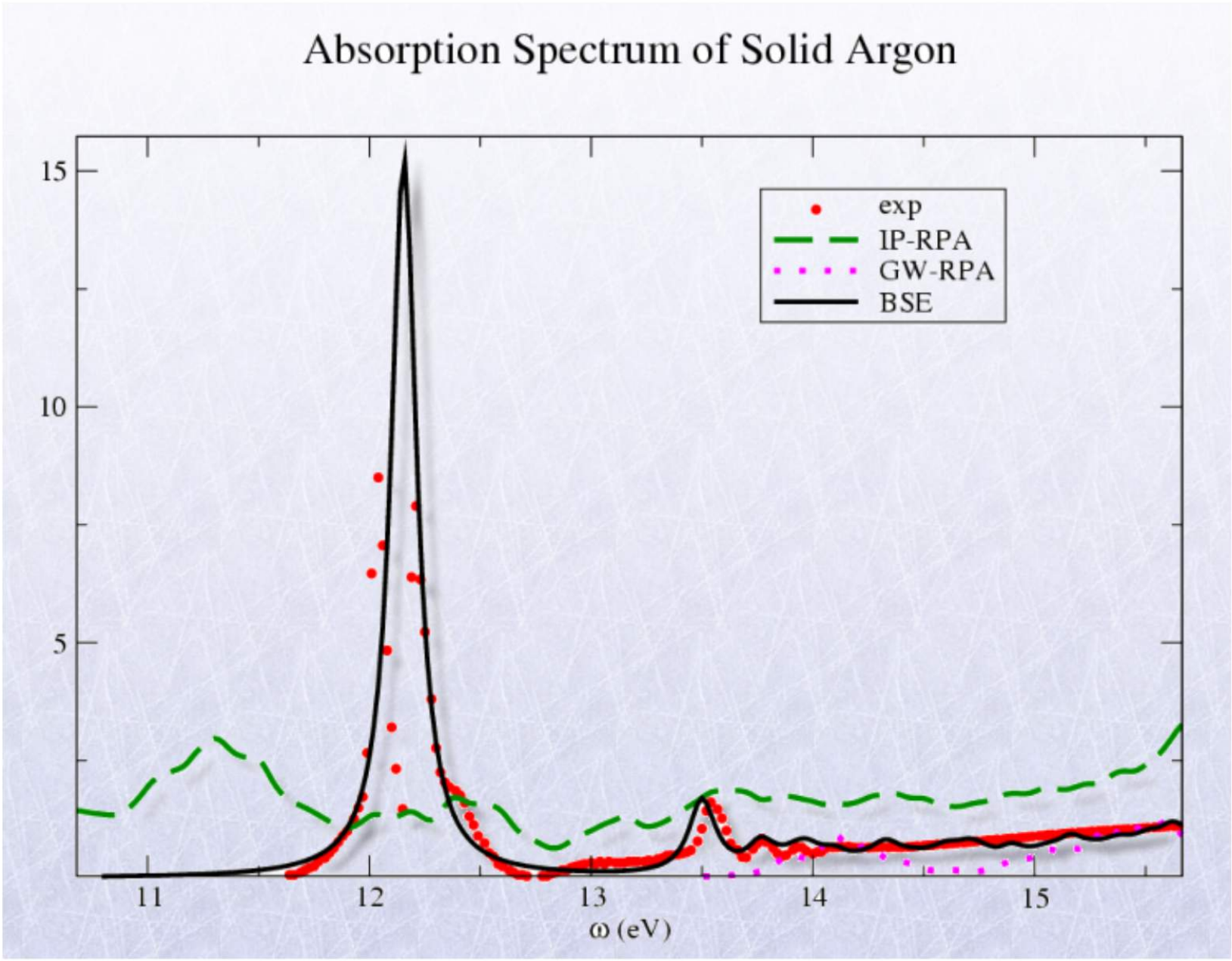
$$V_{xc}^{\mathrm{LDA,GGA}},\ f_{xc}^{\mathrm{ALDA}} = \frac{\delta V_{xc}^{\mathrm{LDA}}}{\delta\rho}$$

Absorption of Benzene



IXS of Silicon



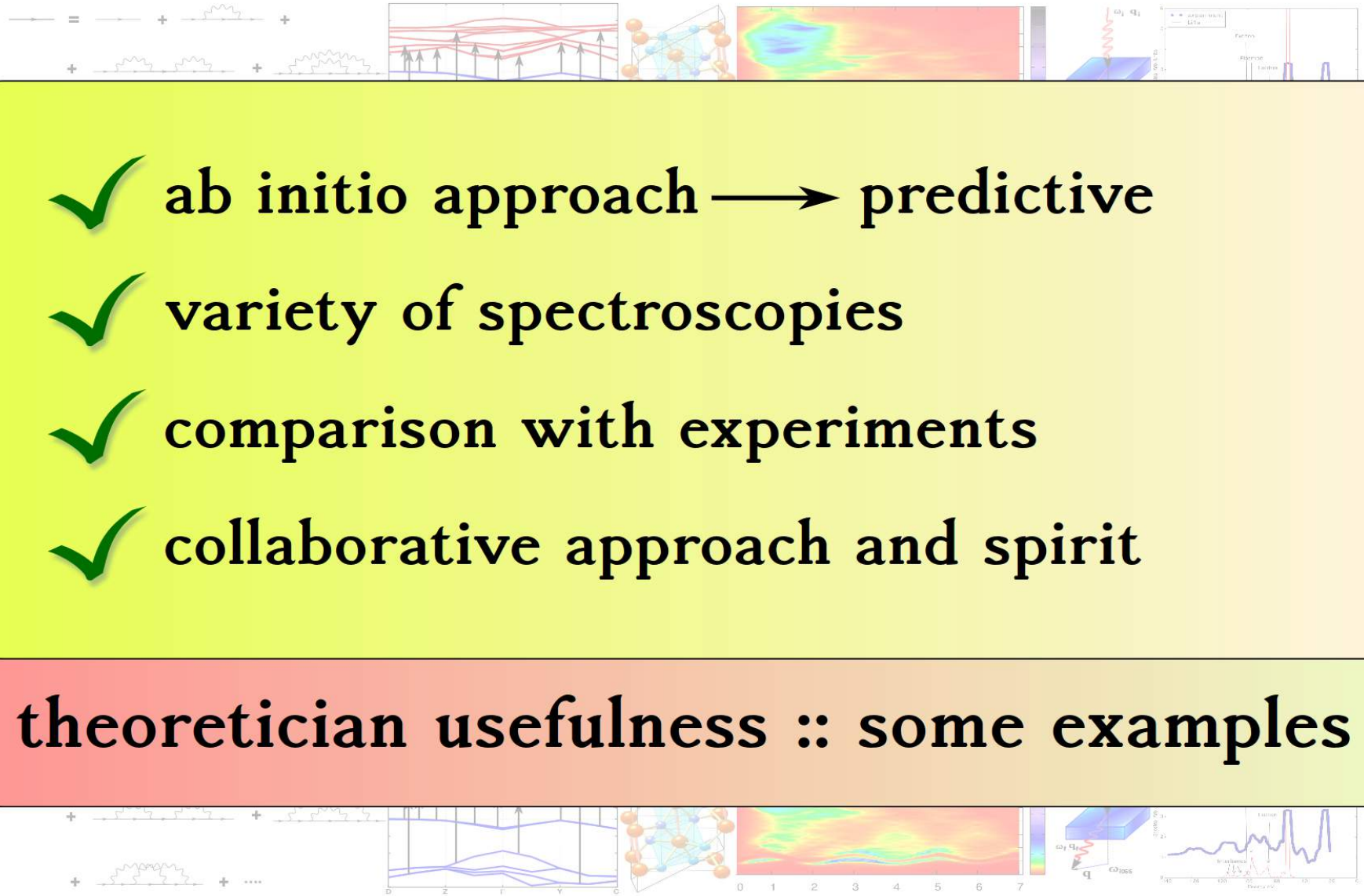

Absorption Spectrum of Solid Argon
15
10
5
11
12
13
14
15
ω (eV)
exp
IP-RPA
GW-RPA
BSE

Time Dependent Density Functional Theory

Absorption, EELS, IXS $V_{xc}^{\mathrm{LDA,GGA}}$

scaling $N_{\mathrm{at}}^{3 \div 4}$ < 10000 atoms

ab initio description of valence electron spectroscopies



- ✓ ab initio approach ⟶ predictive
- ✓ variety of spectroscopies
- ✓ comparison with experiments
- ✓ collaborative approach and spirit

theoretician usefulness :: some examples