Time Dependent Density Functional Theory

Applications, limitations and ... new frontiers

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Vienna, 19 January 2007

Outline

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PHYSICAE ET CHIMICAE SOLIDORUM AMICI

LESS 2007

Low Energy Spectrometry Symposium - January 18+19, 2007 - Vienna/Austria

Motivation

Spectrometries of the low energy region are currently a hot topic. There exist many different experimental techniques (optical absorption, resonant inelastic X-ray scattering, reflection EELS, ellipsometry, ...) as well as theoretical approaches (TDDFT, BSE, ...) to access the dielectric function. However, in praxis, there is only a little if no overlap between the research in the different fields. With this symposium we intend to bring researchers of these different fields together. To ensure that many fruitful discussions will take place, the number of participants is limited to 60.

Outline

The name of the game: TDDFT

TDDFT: density functional philosophy to the world of the systems driven out of equilibrium, by an external time-dependent perturbation.

Density Functional Concept $\Rightarrow$ 2 (important) points

1. Hohenberg-Kohn theorem

The ground-state expectation value of any physical observable of a many-electrons system is a unique functional of the electron density $n(\mathbf{r})$

$$\left\langle \varphi^0 \right| \widehat{O} \left| \varphi^0 \right\rangle = O[n]$$

P.Hohenberg and W.Kohn
Phys.Rev. **136**, B864 (1964)

Density Functional Concept $\Rightarrow$ 2 (important) points

2. Kohn-Sham equations

$$\left[-\frac{1}{2}\nabla_i^2 + V_{tot}(\mathbf{r})\right]\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

$$V_{tot}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')n(\mathbf{r}') + V_{xc}\left([n],\mathbf{r}\right)$$

$V_{xc}\left([n],\mathbf{r}\right)$ Unknown, stupidity term

W.Kohn and L.J.Sham

Phys. Rev. **140**, A1133 (1965)

The name of the game: TDDFT

DFT

Hohenberg-Kohn

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TDDFT

Runge-Gross theorem

The expectation value of any physical time-dependent observable of a many-electrons system is a unique functional of the **time-dependent** electron density $n(\mathbf{r}, t)$ and of **the initial state** $\varphi^0 = \varphi(t = 0)$

$$\left\langle \varphi(t) | \widehat{O}(t) | \varphi(t) \right\rangle = O[n, \varphi^0](t)$$

E. Runge and E.K.U. Gross
Phys.Rev.Lett. **52**, 997 (1984)

The name of the game: TDDFT

DFT

TDDFT

Kohn-Sham equations

$$\left[-\frac{1}{2}\nabla_i^2 + V_{tot}(\mathbf{r})\right]\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

$$V_{tot}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')n(\mathbf{r}') + V_{xc}\left([n],\mathbf{r}\right)$$

$$V_{xc}\left([n],\mathbf{r}\right) = \quad \text{Unknown, stupidity term}$$

Time-dependent KS equations

$$\left[-\frac{1}{2}\nabla^2 + V_{tot}(\mathbf{r},t)\right]\phi_i(\mathbf{r},t) = i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t)$$

$$V_{tot}(\mathbf{r},t) = V_{ext}(\mathbf{r},t) + \int v(\mathbf{r},\mathbf{r}')n(\mathbf{r}',t)d\mathbf{r}' + V_{xc}([n]\mathbf{r},t)$$

$$V_{xc}\left([n],\mathbf{r},t\right) = \quad \text{Unknown, (even more) stupidity term}$$

Unknown exchange-correlation potential.
V_{xc} functional of the density.

Unknown exchange-correlation time-dependent potential.
V_{xc} functional of the density **at all times** and of the **initial state**.

The name of the game: TDDFT

DFT

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TDDFT

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The name of the game: TDDFT

Demonstrations, further readings, etc.

R. van Leeuwen
Int.J.Mod.Phys. **B15**, 1969 (2001)

⏩ Linear Response

Time-Dependent Kohn-Sham equations

$$H_{KS}(\mathbf{r},t)\phi_i(\mathbf{r},t) = \imath\frac{\partial}{\partial t}\phi_i(\mathbf{r},t)$$

Practical computational scheme: Real space - time evolution

Evolution of the KS wave functions

$$H_{KS}(t)\phi(t) = \imath\frac{\partial}{\partial t}\phi(t)$$

$$\phi(t+\Delta t) = \left\{ e^{-\imath \int_t^{t+\Delta t} H(\tau)d\tau} \right\} \phi(t)$$

Approximation for the V_{xc}

Adiabatic LDA $V_{xc}^{\mathrm{ALDA}}[n(\mathbf{r},t)] = \left.\frac{de_{xc}(n)}{dn}\right|_{n=n(\mathbf{r},t)}$

Practical computational scheme: Real space - time evolution

Photo-absorption cross section σ

$$\sigma(\omega) = \frac{4\pi\omega}{c}\mathrm{Im}\alpha(\omega)$$

$$\alpha(t) = -\int d\mathbf{r} V_{ext}(\mathbf{r}, t) n(\mathbf{r}, t)$$

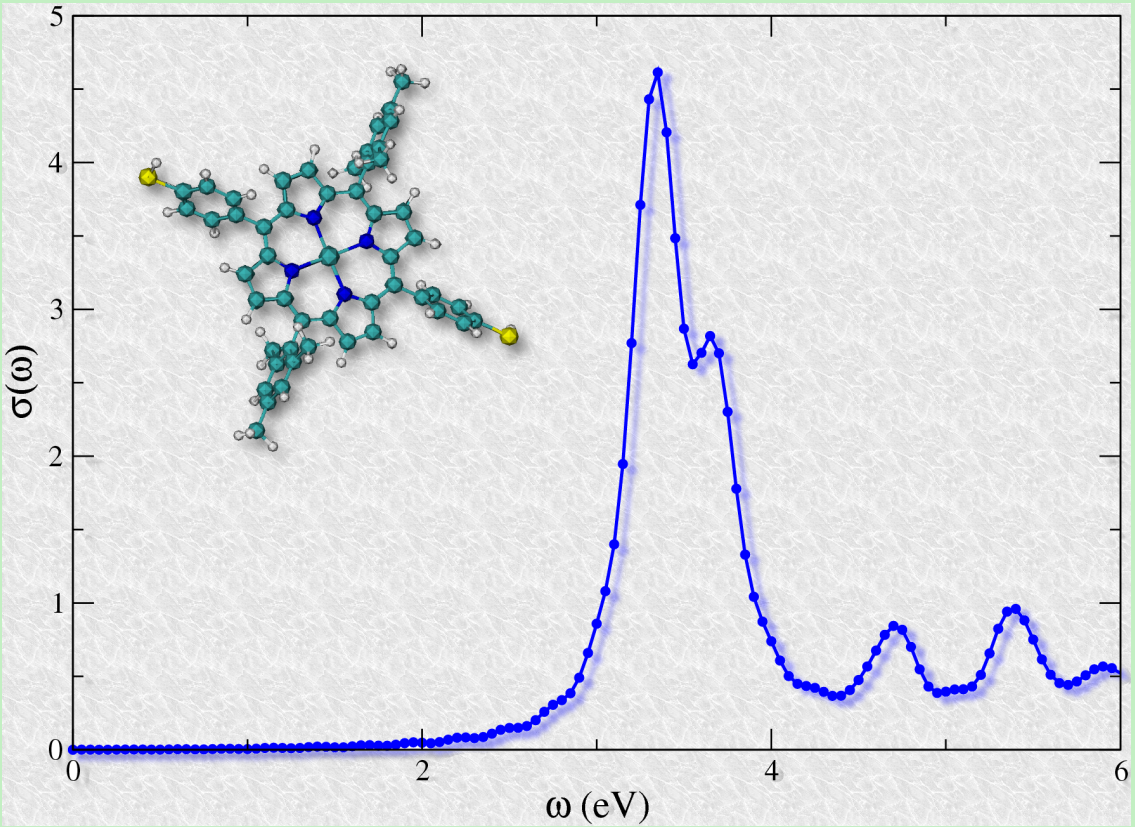
in dipole approximation ($\lambda \ggg$ dimension of the system)

$$\alpha(\omega) = -\int d\mathbf{r} z n(\mathbf{r}, \omega)$$

$$\sigma_{zz}(\omega) = -\frac{4\pi\omega}{c}\mathrm{Im}\int \mathrm{d}\mathbf{r}\ \mathrm{z}\ \mathrm{n}(\mathbf{r}, \omega)$$

Practical computational scheme: Real space - time evolution

Photo-absorption cross section σ: porphyrin



- octopus (GPL) http://www.tddft.org/programs/octopus/

Practical computational scheme: Real space - time evolution

Other observables

Multipoles

$$M_{lm}(t) = \int d\mathbf{r} r^l Y_{lm}(r) n(\mathbf{r}, t)$$

Angular momentum

$$L_z(t) = -\sum_i \int d\mathbf{r} \phi_i(\mathbf{r}, t)\, \imath\, (\mathbf{r} \times \nabla)_z\ \phi_i(\mathbf{r}, t)$$

Real space - Time evolution approach

Advantages

- Direct application of KS equations
- Advantageous scaling
- Optimal scheme for finite systems
- All orders automatically included

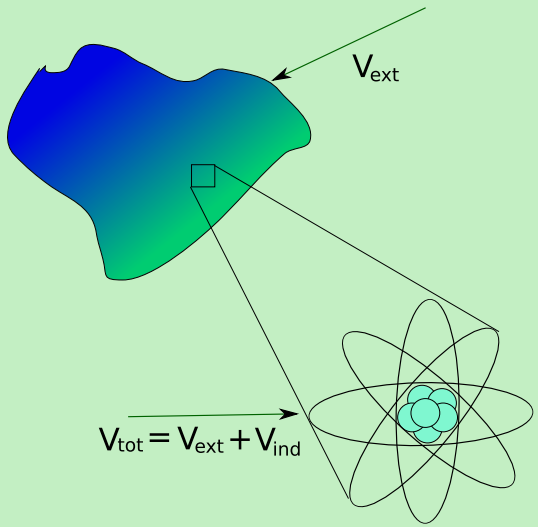
Shortcomings

- Difficulties in approximating the $V_{xc}[n](\mathbf{r}, t)$ functional of the history of the density
- Real space not necessarily suitable for solids
- Does not explicitly take into account a "small" perturbation. Interesting quantities (excitation energies) are contained in the linear response function!

Outline

Linear Response Approach

System submitted to an external perturbation



Linear Response Approach

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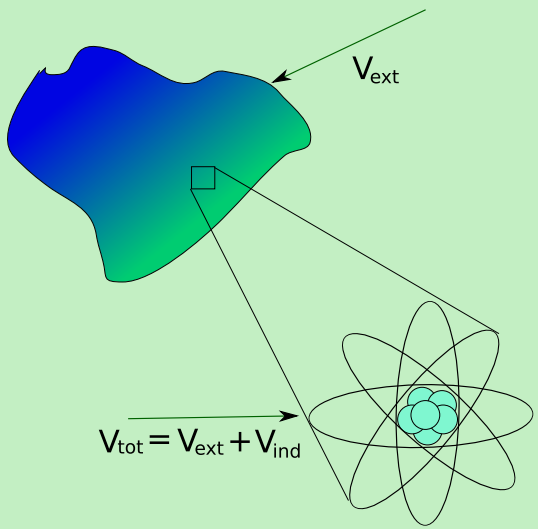

$$V_{tot} = \varepsilon^{-1} V_{ext}$$

$$V_{tot} = V_{ext} + V_{ind}$$

Linear Response Approach

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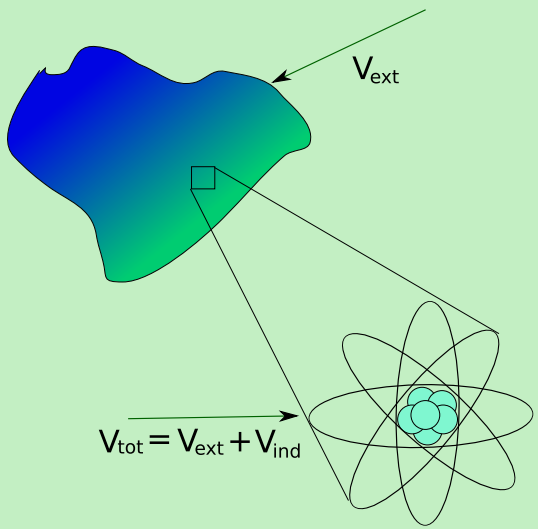

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$$\mathbf{E} = \varepsilon^{-1} \mathbf{D}$$

Linear Response Approach

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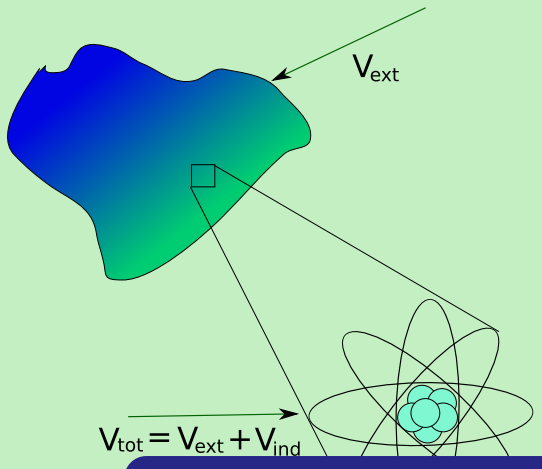

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Dielectric function ε

$$\varepsilon$$

Linear Response Approach

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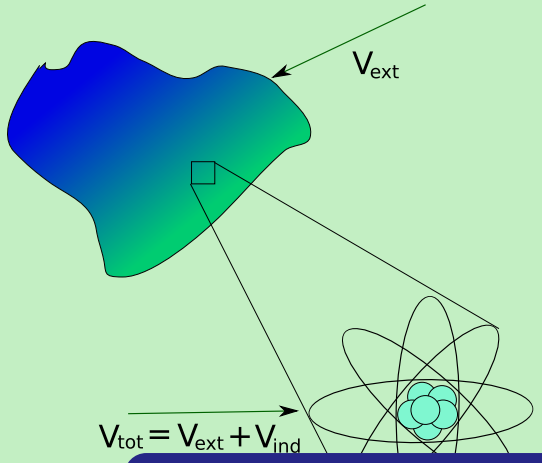

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Dielectric function ε

ε

Abs

Linear Response Approach

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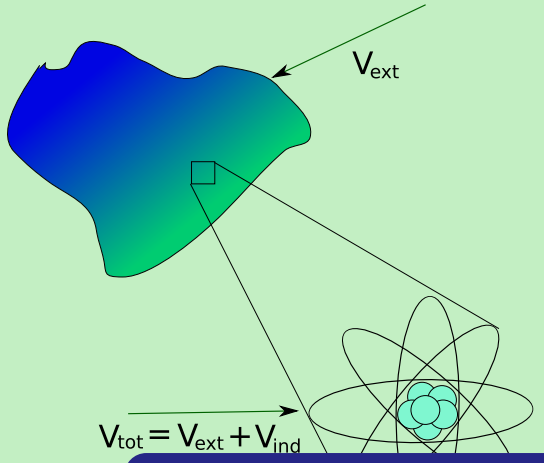

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Dielectric function ε

EELS

ε

Abs

Linear Response Approach

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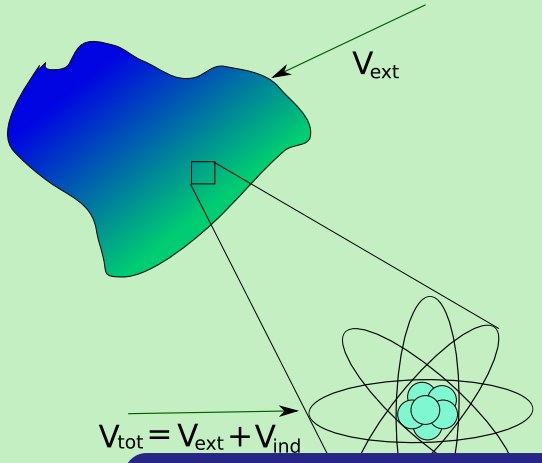

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Dielectric function ε

EELS

ε

Abs

X-ray

Linear Response Approach

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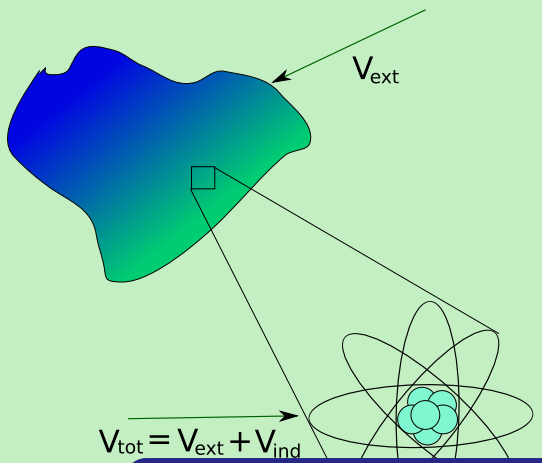

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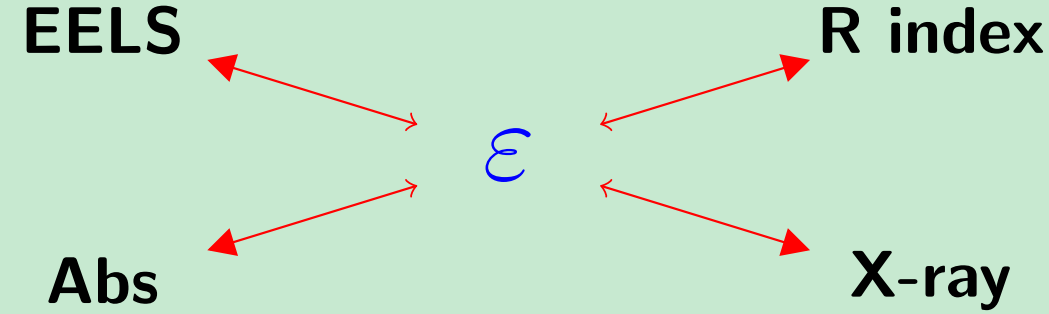

Linear Response Approach

Definition of polarizability

$$\varepsilon^{-1} = 1 + v\chi$$

χ is the polarizability of the system

Linear Response Approach

Polarizability

$$\text{interacting system} \quad \delta n = \chi \delta V_{ext}$$

$$\text{non-interacting system} \quad \delta n_{n-i} = \chi^0 \delta V_{tot}$$

Linear Response Approach

Polarizability

$$\text{interacting system} \quad \delta n = \chi \delta V_{ext}$$

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Single-particle polarizability

$$\chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j)}$$

hartree, hartree-fock, dft, etc.

G.D. Mahan *Many Particle Physics* (Plenum, New York, 1990)

Linear Response Approach

Polarizability

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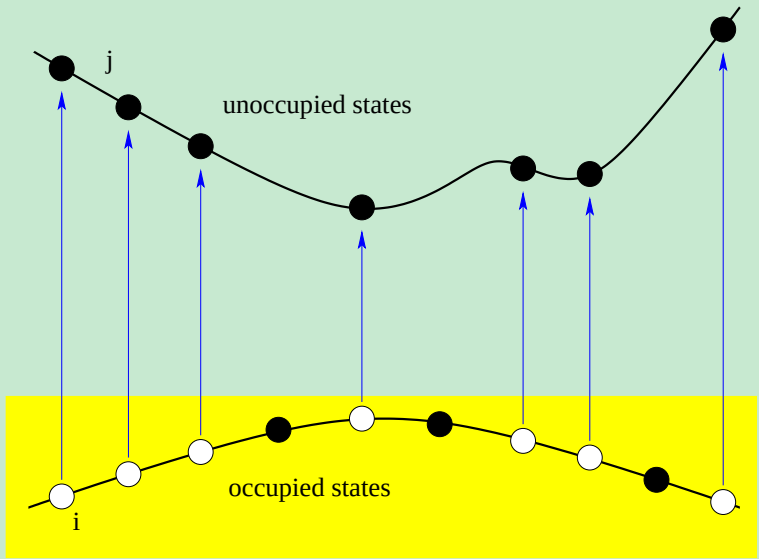

Linear Response Approach

Polarizability

interacting system $\quad \delta n = \chi \delta V_{ext}$

non-interacting system $\quad \delta n_{n-i} = \chi^0 \delta V_{tot}$

$$\Updownarrow$$

Density Functional Formalism

$$\delta n = \delta n_{n-i}$$

$$\delta V_{tot} = \delta V_{ext} + \delta V_H + \delta V_{xc}$$

Linear Response Approach

Polarizability

$$\chi = \chi^0 + \chi^0 \left(v + f_{xc} \right) \chi$$

with $f_{xc} = \frac{\delta V_{xc}}{\delta n}$ **exchange-correlation kernel**

with $v = \frac{\delta V_H}{\delta n}$ **coulomb interaction**

Linear Response Approach

Polarizability

$$\chi = \left[1 - \chi^0 \left(v + f_{xc}\right)\right]^{-1} \chi^0$$

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Linear Response Approach

Polarizability χ in TDDFT (DFT + Linear Response)

1. DFT ground-state calc. $\longrightarrow$ ϕ_i, ϵ_i $[V_{xc}]$
2. $\phi_i, \epsilon_i \longrightarrow \chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega-(\epsilon_i-\epsilon_j)}$
3. $\left.\begin{array}{l} \frac{\delta V_H}{\delta n} = v \\ \frac{\delta V_{xc}}{\delta n} = f_{xc} \end{array}\right\}$ variation of the potentials
4. $\chi = \chi^0 + \chi^0 (v + f_{xc}) \chi$

A comment

- $f_{xc} = \left\{ \begin{array}{l} \frac{\delta V_{xc}}{\delta n} \\ \text{“any” other function} \end{array} \right.$

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Linear Response Approach

Approximation for f_{xc}

$$f_{xc} = 0 \qquad \text{RPA}$$

$$f_{xc} = \frac{\delta V_{xc}^{LDA}}{\delta n} \qquad \text{ALDA}$$

EXX, MT, etc.

▸ Measurables

Solids

Reciprocal Space - Frequency domain

$$f(\mathbf{r}) \rightarrow f_{\mathbf{G}}(\mathbf{q}) = \frac{1}{\Omega} \int d\mathbf{r} f(\mathbf{r}) e^{\imath(\mathbf{q}+\mathbf{G})\dot{\mathbf{r}}}$$

G =reciprocal lattice vector

$\mathbf{q} \in 1BZ$ momentum transfer of the perturbation

$$\chi^0(\mathbf{r}, \mathbf{r}', \omega) \longrightarrow \chi^0_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega)$$

$$\chi^0_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega) = \sum_{vc\mathbf{k}} \frac{\left\langle \phi_{v\mathbf{k}} | e^{\imath(\mathbf{q}+\mathbf{G})\mathbf{r}} | \phi^*_{c\mathbf{k}+\mathbf{q}} \right\rangle \left\langle \phi_{c\mathbf{k}+\mathbf{q}} | e^{-\imath(\mathbf{q}+\mathbf{G}')\mathbf{r}'} | \phi^*_{v\mathbf{k}} \right\rangle}{\omega - (\epsilon_{c\mathbf{k}+\mathbf{q}} - \epsilon_{v\mathbf{k}}) + \imath\eta}$$

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Solids

Reciprocal Space - Frequency domain

$$\chi_{GG'}(\mathbf{q},\omega) = \left[1 - \chi^0 \left(v + f_{xc}\right)\right]^{-1} \chi^0$$

$$\varepsilon^{-1}_{GG'}(\mathbf{q},\omega) = \delta_{GG'} + v_G(\mathbf{q})\chi_{GG'}(\mathbf{q},\omega)$$

$$\mathrm{ELS}(\mathbf{q},\omega) = -\mathrm{Im}\varepsilon^{-1}_{00}(\mathbf{q},\omega)$$

$$\mathrm{Abs}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Im}\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)} \; ; \; \mathrm{Refrac.}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Re}\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)}$$

▸ alt. form.

S.L.Adler, Phys.Rev **126**, 413 (1962); N.Wiser Phys.Rev **129**, 62 (1963)

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Solids

Reciprocal Space - Frequency domain

$$\chi_{\mathbf{GG'}}(\mathbf{q},\omega) = \left[1 - \chi^0 \left(v + f_{xc}\right)\right]^{-1} \chi^0$$

$$\varepsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega) = \delta_{\mathbf{GG'}} + v_{\mathbf{G}}(\mathbf{q})\chi_{\mathbf{GG'}}(\mathbf{q},\omega)$$

$$\mathrm{ELS}(\mathbf{q},\omega) = -\mathrm{Im}\varepsilon^{-1}_{00}(\mathbf{q},\omega)$$

$$\mathrm{Abs}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Im}\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)} \; ; \; \mathrm{Refrac.}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Re}\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)}$$

▸ alt. form.

S.L.Adler, Phys.Rev **126**, 413 (1962); N.Wiser Phys.Rev **129**, 62 (1963)

Some measurable quantities

The macroscopic dielectric function

$$\chi_0, f_{xc} \Rightarrow \chi \Rightarrow \varepsilon_M$$

Abs, loss function, refraction index

$$\mathrm{ELS} = -\mathrm{Im}\left\{\frac{1}{\varepsilon_\mathrm{M}}\right\}$$

$$\mathrm{Abs} = \mathrm{Im}\left\{\varepsilon_\mathrm{M}\right\}$$

$$\mathrm{R_{index}} = \mathrm{Re}\left\{\varepsilon_\mathrm{M}\right\}$$

Outline

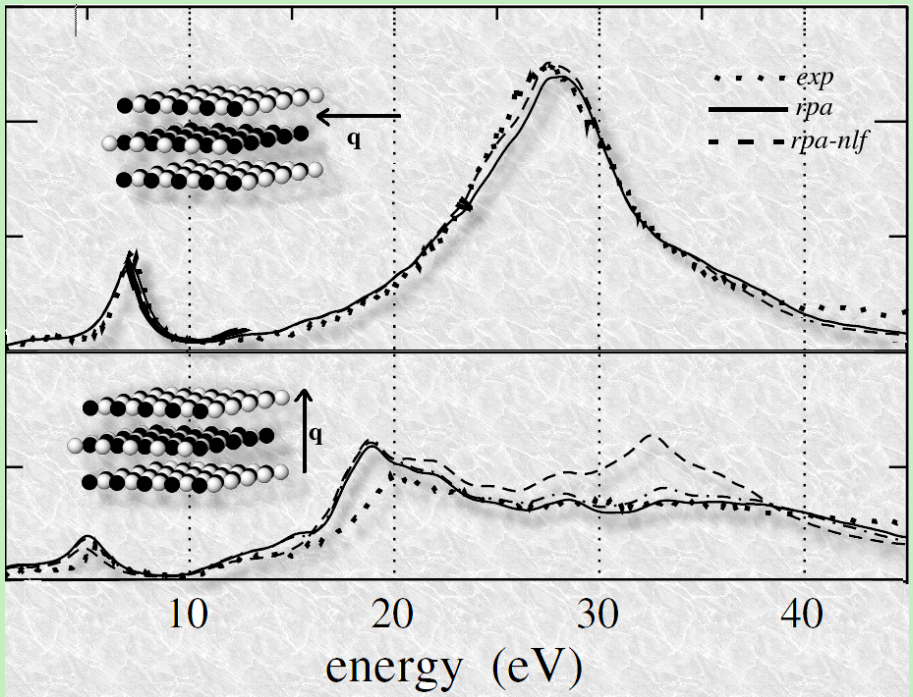
Outline

ALDA: Achievements and Shortcomings

Electron Energy Loss Spectrum of Graphite

$$\text{EELS} = -\text{Im}\left\{\frac{1}{\varepsilon_{\text{M}}}\right\}$$

RPA (w and w/o LF)
vs
Experiment



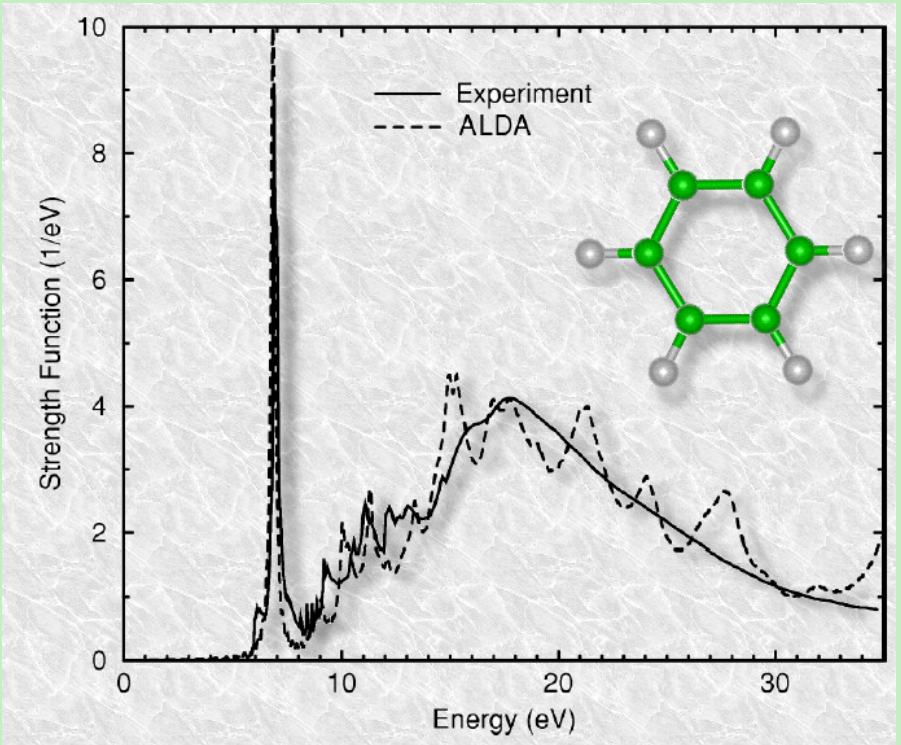
A.Marinopoulos, T.Pichler, *et al.* Phys.Rev.Lett **89**, 76402 (2002)

ALDA: Achievements and Shortcomings

Photo-absorption cross section of Benzene

ALDA vs Experiment

$$\text{Abs} = -\frac{4\pi\omega}{c}\text{Im}\int \text{d}\mathbf{r}\ \text{z}\ \text{n}(\text{r},\omega)$$



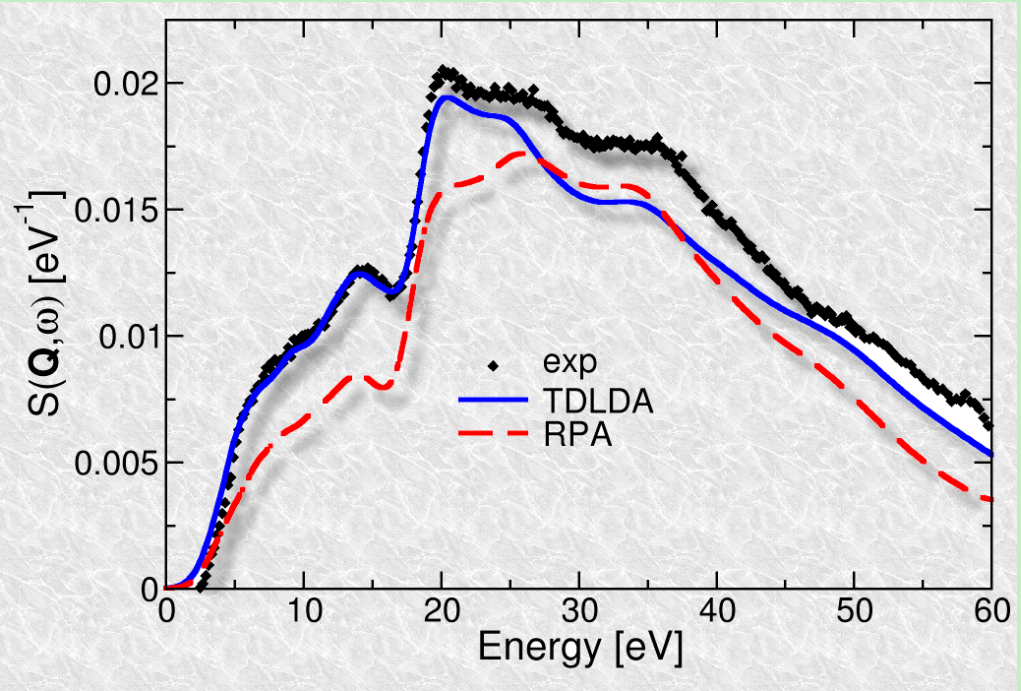
K.Yabana and G.F.Bertsch Int.J.Mod.Phys.**75**, 55 (1999)
E.E.Koch and A.Otto, Chem. Phys. Lett. **12**, 476 (1972)

ALDA: Achievements and Shortcomings

Inelastic X-ray scattering of Silicon

ALDA vs RPA vs Experiment

$$S(\mathbf{q},\omega) \propto \mathrm{Im}\left\{\frac{1}{\varepsilon_M}\right\}$$



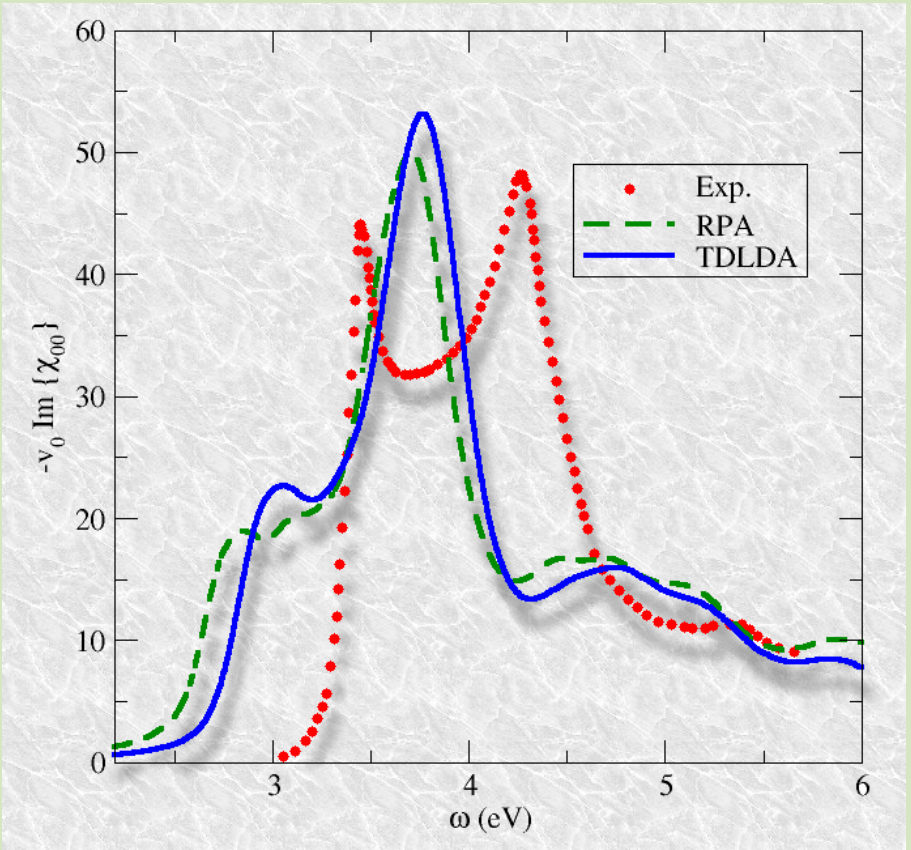
H-C.Weissker, J.Serrano *et al.* Phys.Rev.Lett. **97**, 237602 (2006)

ALDA: Achievements and Shortcomings

Absorption Spectrum of Silicon

ALDA vs RPA vs Experiment

$$\text{Abs} = \text{Im}\left\{\varepsilon_{\text{M}}\right\}$$



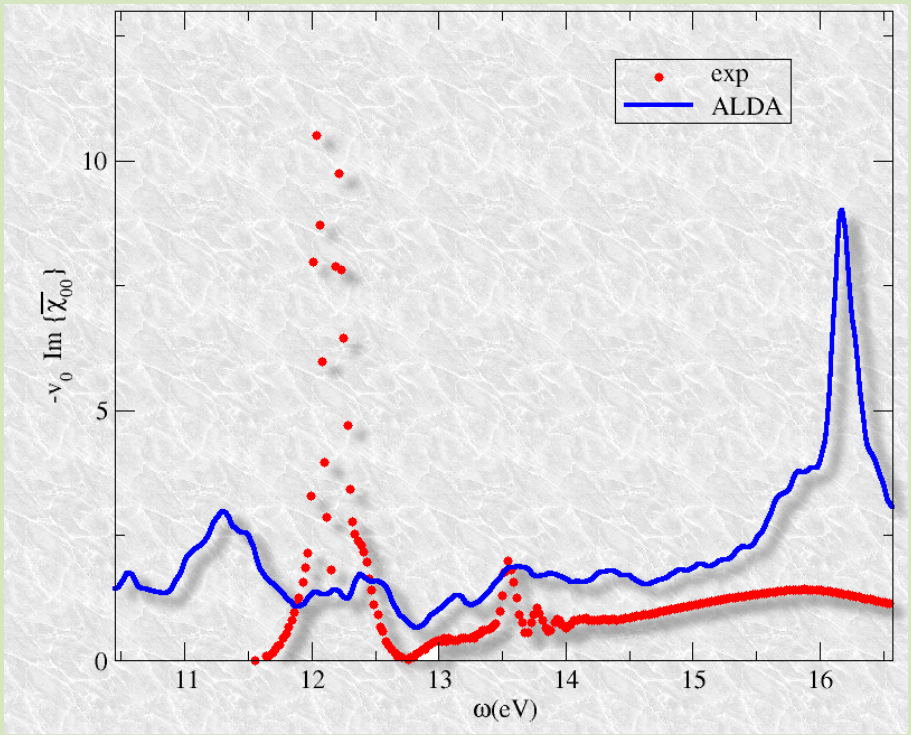
P.Lautenschlager *et al.* Phys. Rev. B **36**, 4821 (1987)

ALDA: Achievements and Shortcomings

Absorption Spectrum of Argon

ALDA vs Experiment

$$\text{Abs} = \text{Im}\left\{\varepsilon_{\text{M}}\right\}$$



V.Saile *et al.* Appl. Opt. **15**, 2559 (1976)

ALDA: Achievements and Shortcomings

Good results

- Photo-absorption of simple molecules
- ELS of solids

Bad results

- Absorption of solids

Why?

f_{xc}^{ALDA} is short-range

$$f_{xc}(\mathbf{q} \to 0) \sim \frac{1}{q^2}$$

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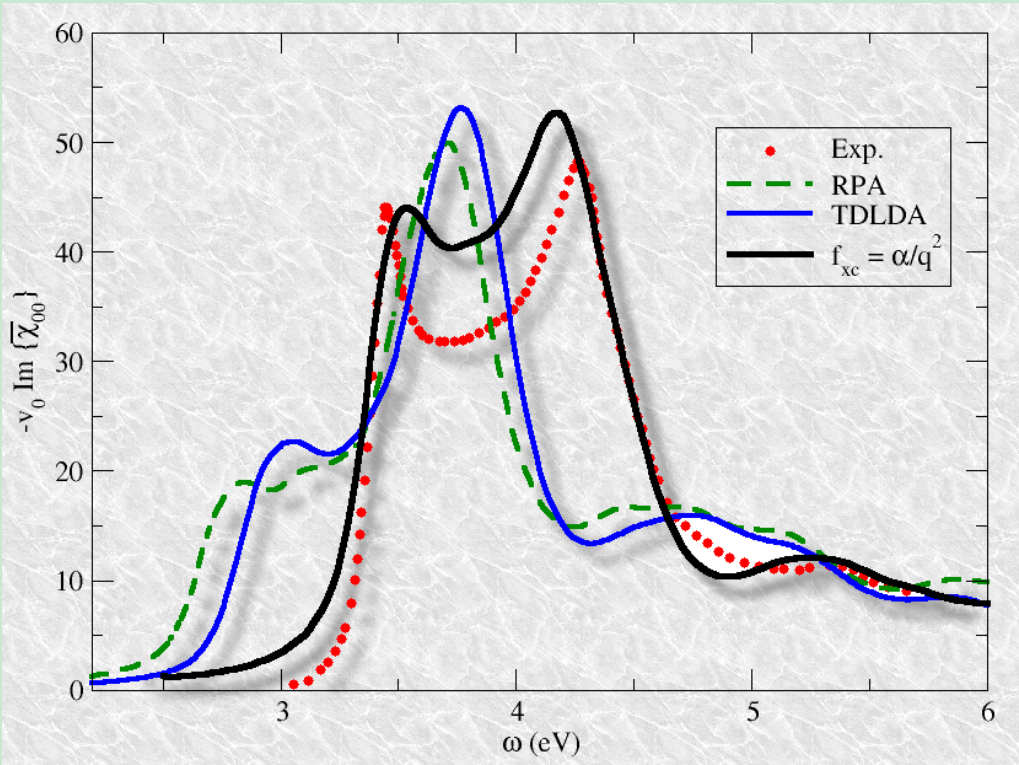
ALDA: Achievements and Shortcomings

Absorption of Silicon $f_{xc} = \frac{\alpha}{q^2}$

ALDA vs RPA vs $\frac{\alpha}{q^2}$ vs Experiment

$$\text{Abs} = \text{Im}\varepsilon_{\text{M}}$$

$$\chi = \chi_0 + \chi_0 \left(v + \frac{\alpha}{q^2} \right) \chi$$



L.Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)

Outline

Beyond ALDA approximation

The problem of Abs in solids. Towards a better understanding

- Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)
  Long-range kernel
- de Boeij *et al.* J.Chem.Phys. **115**, 1995 (2002)
  Polarization density functional. Long-range.
- Kim and Görling Phys.Rev.Lett. **89**, 96402 (2002)
  Exact-exchange
- Sottile *et al.* Phys.Rev.B **68**, 205112 (2003)
  Long-range and contact exciton.
- Botti *et al.* Phys. Rev. B **72**, 125203 (2005)
  Dynamic long-range component

Parameters to fit to experiments.

Beyond ALDA approximation

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Parameters to fit to experiments.

Beyond ALDA approximation

Abs in solids. Insights from MBPT

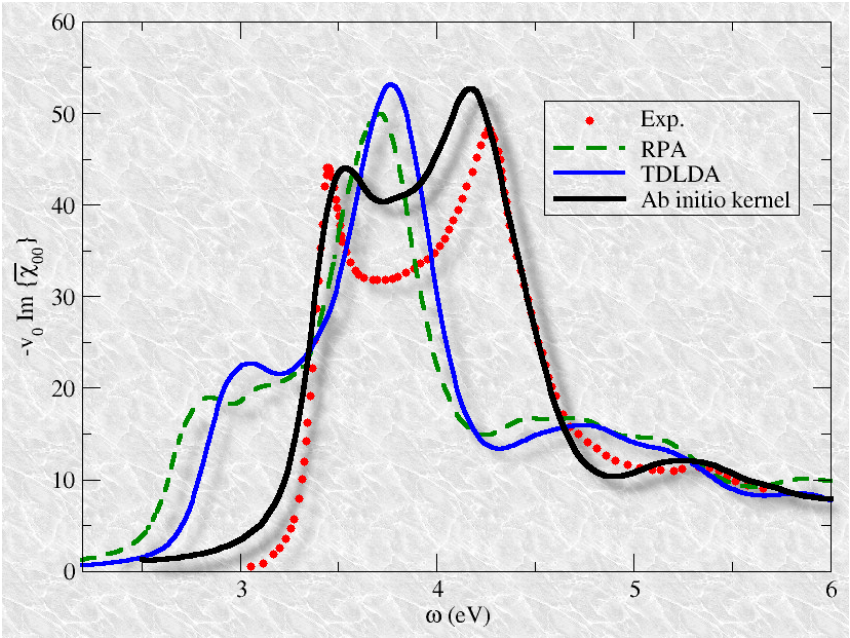
Parameter-free Ab initio kernels

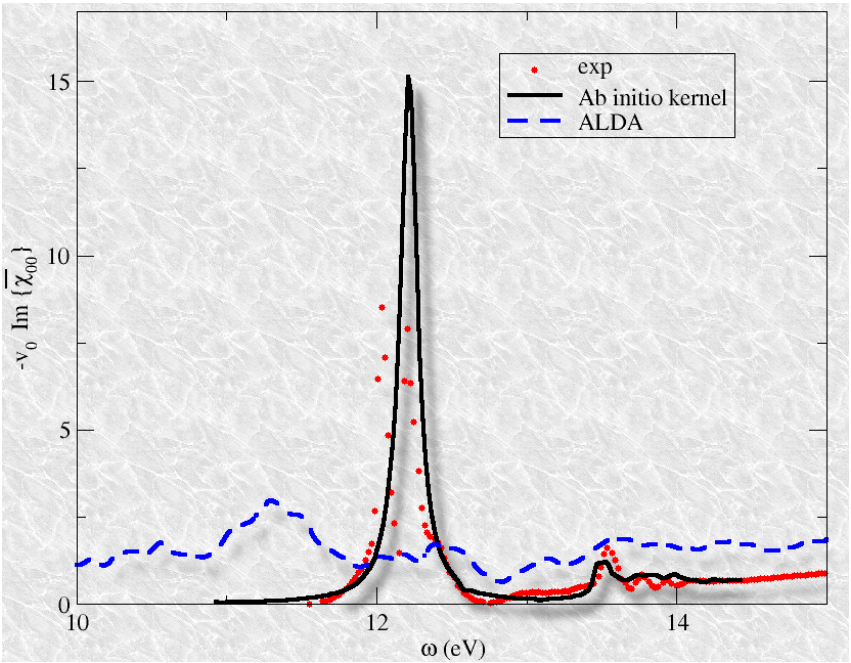

Sottile *et al.* Phys.Rev.Lett. **91**, 56402 (2003)
Full many-body kernel. Mapping Theory.


Marini *et al.* Phys.Rev.Lett. **91**, 256402 (2003)
Full many-body kernel. Perturbation Theory.

$$f_{xc} = \chi_0^{-1} GGWGG \chi_0^{-1}$$

Beyond ALDA approximation





Sottile *et al.* Phys.Rev.Lett. **91**, 56402 (2003) ; Sottile *et al.* submitted.

Beyond ALDA approximation

Abs in solids. Full Many-Body Kernel

Tested also on absorption of SiO_2, DNA bases, Ge-nanowires, RAS of diamond surface, and EELS of LiF.

- Marini *et al.* Phys.Rev.Lett. **91**, 256402 (2003).
- Bruno *et al.* Phys.Rev.B **72** 153310, (2005).
- Palummo *et al.* Phys.Rev.Lett. **94** 087404 (2005).
- Varsano *et al.* J.Phys.Chem.B **110** 7129 (2006).

▸ Refraction index

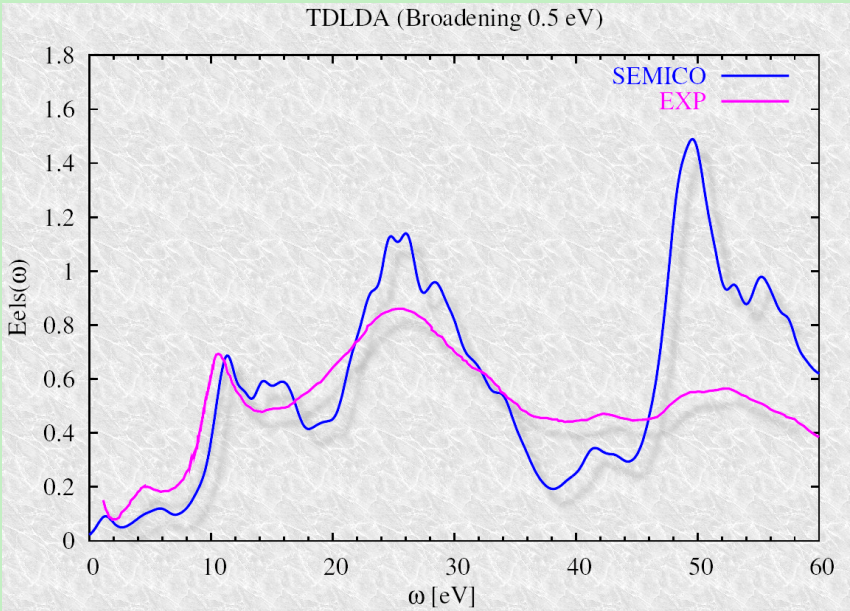
Low-energy Spectroscopy

TDDFT is the method of choice

- √ Absorption spectra of simple molecules
- √ Electron energy loss spectra
- √ Inelastic X-ray scattering spectroscopy
- √ Absorption of Solids (BSE-like scaling)
- √ Refraction indexes (BSE-like scaling)

Towards new applications

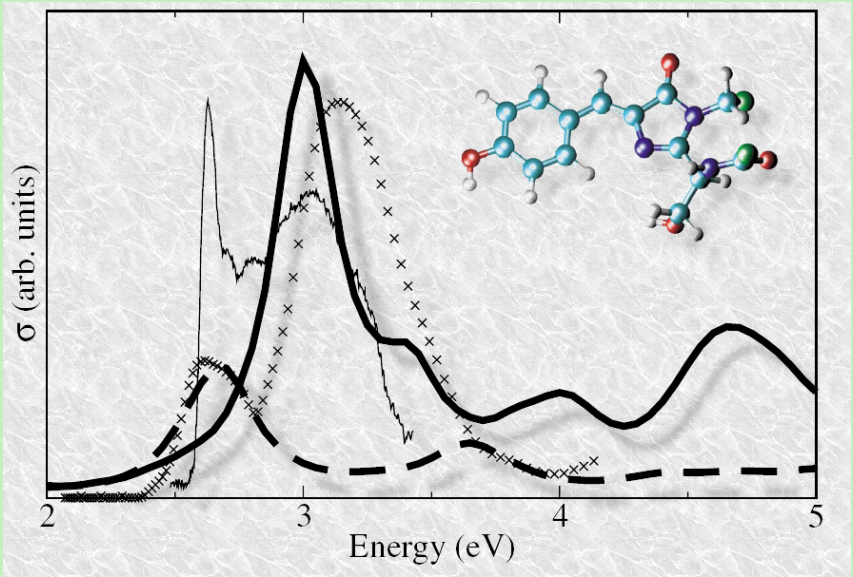
Strongly correlated systems



EEL spectrum of VO_2

M.Gatti, preliminary results

Biological systems



Abs spectrum of Green Fluorescent Protein

M.Marques *et al.* Phys.Rev.Lett **90**, 258101 (2003)

Low-energy Spectroscopy

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- √ Absorption spectra of simple molecules
- √ Electron energy loss spectra
- √ Inelastic X-ray scattering spectroscopy
- √ Absorption of Solids
- √ Refraction indexes

Open problems

- open-shell atoms
- charge-transfer excitations
- efficient calculations of solids

approximation for f_{xc}

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Open problems

- open-shell atoms
- charge-transfer excitations
- efficient calculations of solids

approximation for f_{xc}

The quest for the *good(s)* functional

Actual challenge

f_{xc} easy to calculate and accurate for any kind of system

Non-adiabatic f_{xc}

- current DFT
- deformation theory

Orbital Dependent f_{xc}

- Exact Exchange
- Meta-GGA
- OEP

Insights from MBPT

- Mapping Theory
- Diagrammatic expansion

Outline

The DP code

An open-source project: DP

- TDDFT in linear response approach
- RPA, ALDA, $\frac{\alpha}{q^2}$, Full Many-Body kernel
- TammDancoff approximation or full coupling
- Parallel version available.
- Actual developments: spin, adiabatic-connection formula, non-linear response
- `http://theory.polytechnique.fr/codes` (to be updated)
- Authors: V. Olevano, L.Reining, F.Sottile
- Contributors: F.Bruneval, M.Marsili

V.Olevano, L.Reining, and F.Sottile, *The DP code* ©1998-2007.

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Outline

New Frontiers

Excited-State Dynamics

TDDFT-MD, Ehrenfest dynamics, quantum effects of the ions, non-adiabaticity, etc.

Sugino and Miyamoto, Phys.Rev.B **59**, 2579 (1999)

Transport

New Frontiers

TDDFT concept into MBPT

$$\Sigma = GW\Gamma$$

i.e. a promising path to go beyond GW approx through TDDFT

F.Bruneval *et al.* Phys.Rev.Lett **94**, 186402 (2005)

New Frontiers

Quantum Transport in TDDFT

$$I(t) = -e \int_{\mathcal{V}} d\mathbf{r} \frac{d}{dt} n(\mathbf{r}, t)$$

total current through a junction

G.Stefanucci *et al.* Europhys.Lett. **67**, 14 (2004)

New Frontiers

Let's go back to Ground-State

Total energies calculations via TDDFT

$$E = T_{KS} + V_{ext} + E_H + E_{xc}$$

$$E_{xc} \propto \int d\mathbf{r} d\mathbf{r}' \int_0^1 d\lambda \int_0^\infty du \chi^\lambda(\mathbf{r}, \mathbf{r}', iu)$$

adiabatic connection fluctuation-dissipation theorem

D.C.Langreth *et al.* Solid State Comm. **17**, 1425 (1975)

Outline

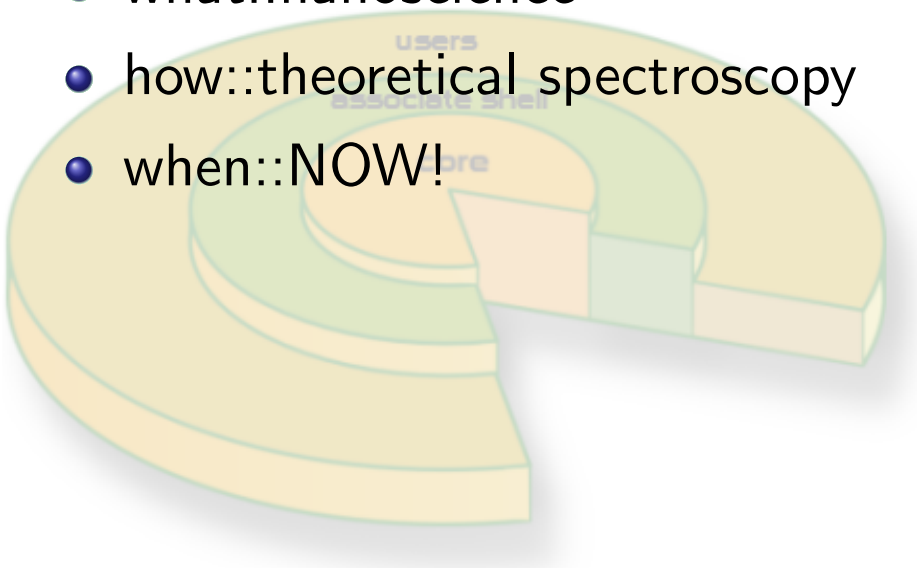
European Theoretical Spectroscopy Facility

ETSF

European Theoretical Spectroscopy Facility

A European Facility:

- what::nanoscience
- how::theoretical spectroscopy
- when::NOW!



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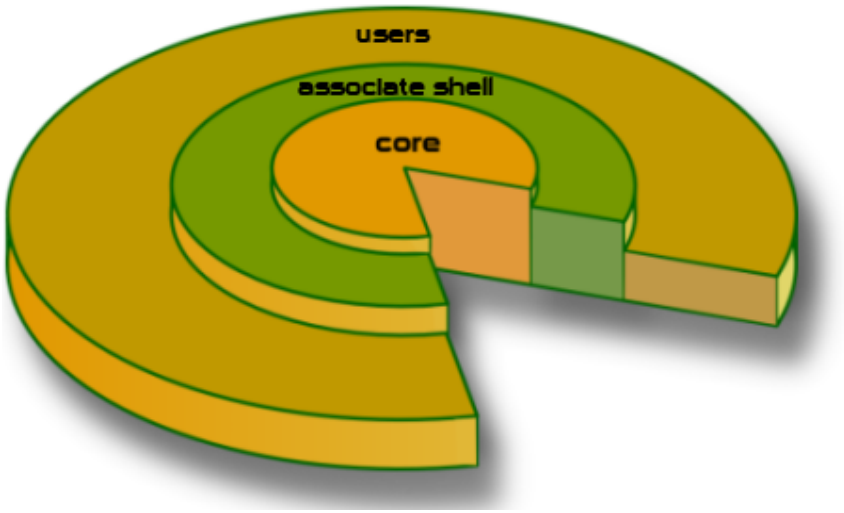

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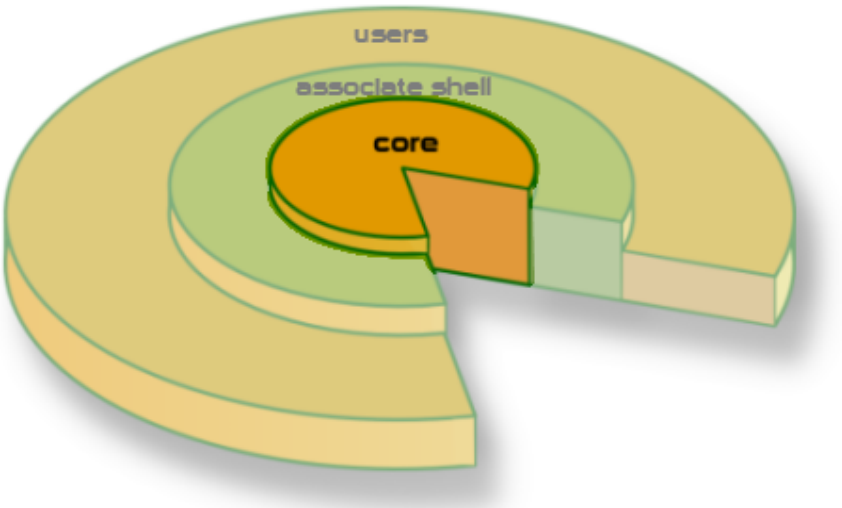

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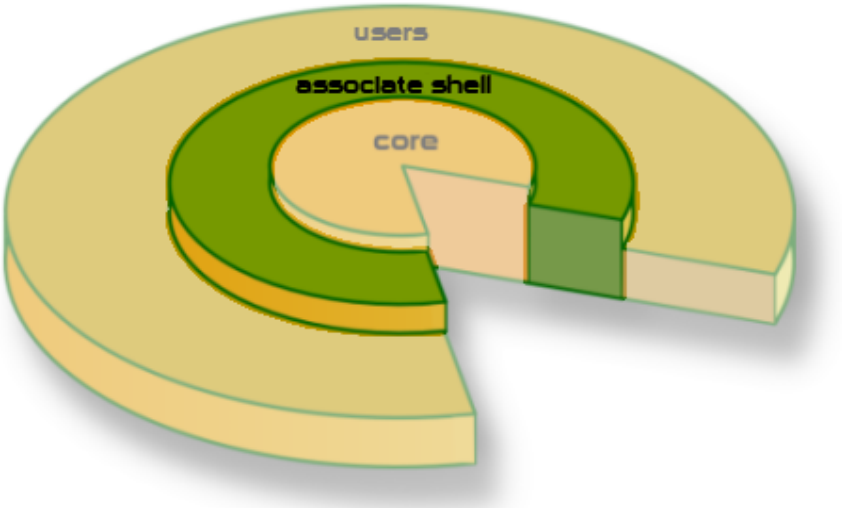
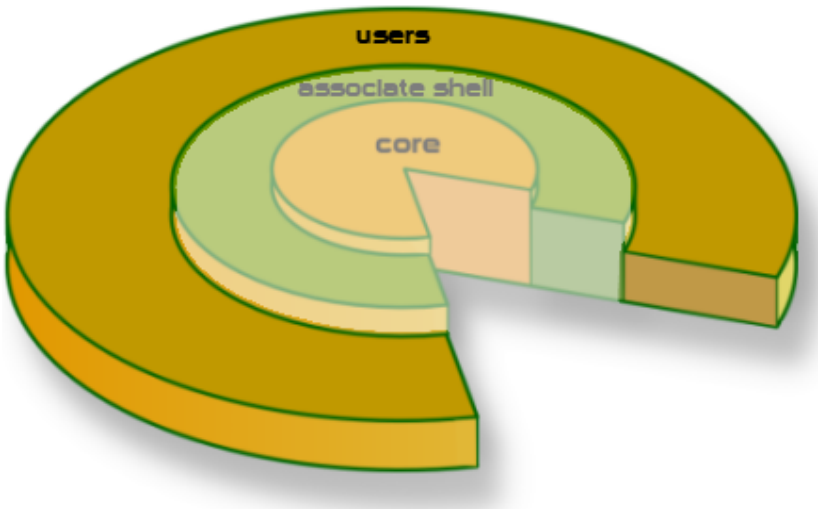


Groups working in the same domain: theoretical spectroscopy

A broad community of theoretical research groups working on related topics.
They develop theory and code, and provide services to users just like members of the Core.

European Theoretical Spectroscopy Facility



Users of the Facility will be a large and varied group of researchers from the public or private sector wishing to benefit from developments in the field of electronic excitations through the different services of the ETSF.

European Theoretical Spectroscopy Facility

- calls for proposal
- commission of customer-driven software development and applications
- project consultancy
- training events (hand-on, workshops)
- software downloads

European Theoretical Spectroscopy Facility

First call for user projects:

First trimester 2007!!

http://www.etsf.eu

T.Patman - atp500@york.ac.uk

Alternative formulation for Abs and ELS

$\mathbf{q} \longrightarrow 0$ case

$$\mathrm{ELS}(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}\left\{\varepsilon^{-1}_{00}(\mathbf{q},\omega)\right\} \;;\; \mathrm{Abs}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Im}\left\{\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)}\right\}$$

$$\mathrm{ELS}(\omega) = -v_0\ \mathrm{Im}\left\{\chi_{00}(\omega)\right\} \quad ; \quad \mathrm{Abs}(\omega) = -\mathrm{v}_0\ \mathrm{Im}\left\{\bar{\chi}_{00}(\omega)\right\}$$

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

$$\bar{\chi} = \chi^0 + \chi^0\,(\bar{v} + f_{xc})\,\bar{\chi}$$

$$\bar{v}_{\mathbf{G}} = \begin{cases} v_{\mathbf{G}} & \forall \mathbf{G} \neq 0 \\ 0 & \mathbf{G} = 0 \end{cases}$$

back

TDDFT: Refraction index of Si within Mapping Theory

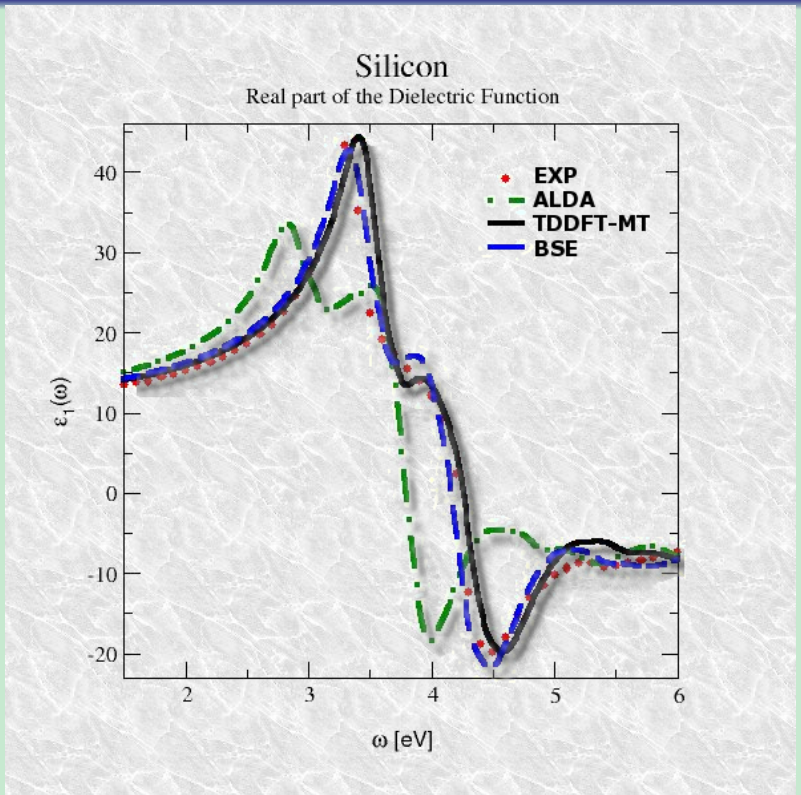
Refraction index of Silicon

ALDA vs BSE vs MT
vs Experiment
$\text{Abs} = \text{Im}\{\varepsilon_M\}$

$$\chi = \chi_0 + \chi_0 (v + f_{xc}) \chi$$

$$f_{xc} = \chi_0^{-1} GGWGG \chi_0^{-1}$$

▸ back



F.Sottile, unpublished.