Time Dependent Density Functional Theory

Introduction and Applications

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European Theoretical Spectroscopy Facility

ÉCOLE POLYTECHNIQUE ParisTech

Outline

Outline

1. TDDFT
   - Motivations
   - Linear Response Approach
2. Applications (ELS)
3. Analysis

Outline

Why Density Functional

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

$$\updownarrow$$

$$G(\mathbf{r}_1, \mathbf{r}_2)$$

$$\updownarrow$$

$$\rho(\mathbf{r})$$

Why Density Functional: an old strategy

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

$$\updownarrow$$

$$G(\mathbf{r}_1, \mathbf{r}_2)$$

$$\updownarrow$$

$$\rho(\mathbf{r})$$

Thomas-Fermi, Slater, Kohn

Density Functional ... Successfull ?

TABLE I: *Physical Review* articles with more than 1000 citations through June 2003. *PR, Physical Review; PRB, Physical Review B; PRD, Physical Review D; PRL, Physical Review Letters; RMP, Reviews of Modern Physics.*

Publication	# cites	Av. Age	Title	Author(s)
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S. Redner http://arxiv.org/abs/physics/0407137

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Time Dependent DFT ... Why ?

Large field of research concerned with
many-electron systems in time-dependent fields

Different Phenomena

- absorption spectra
- energy loss spectra
- X scattering
- high-harmonic generation
- photo-emission

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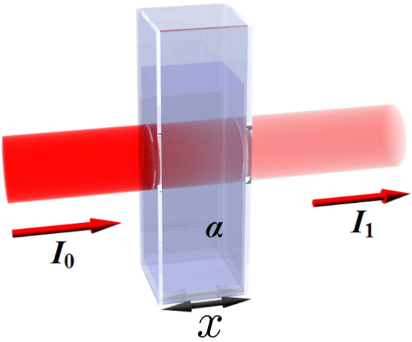

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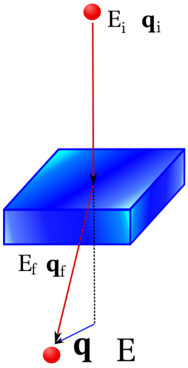

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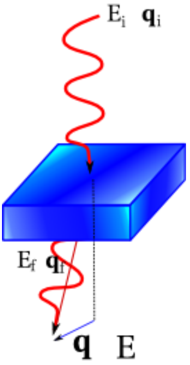

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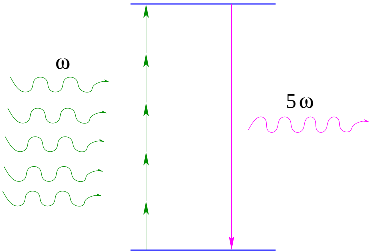

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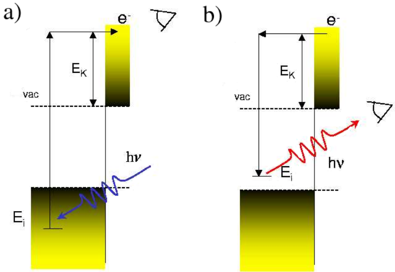
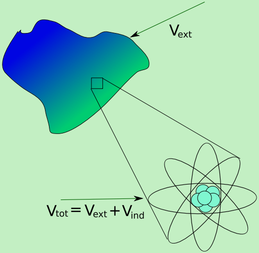


Outline

Linear Response Approach

System submitted to an external perturbation



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

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

Dielectric function ε

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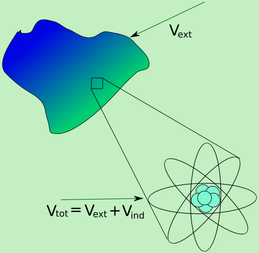

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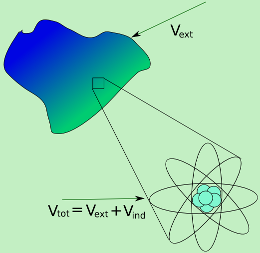

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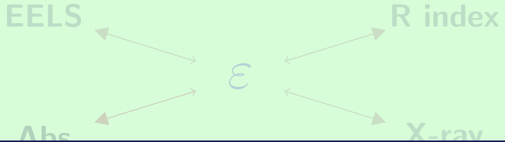

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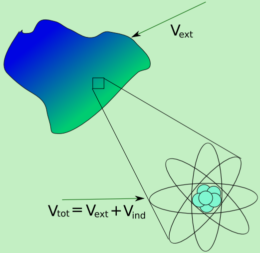

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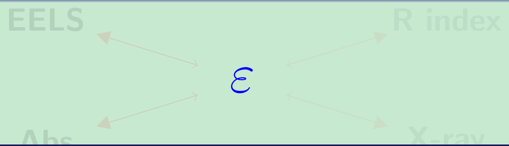

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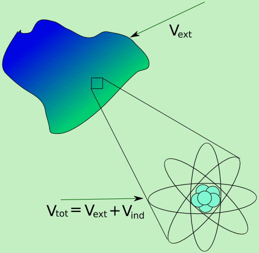

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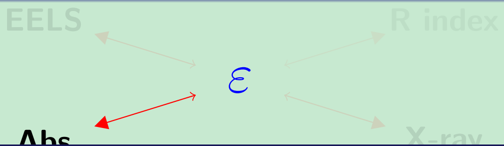

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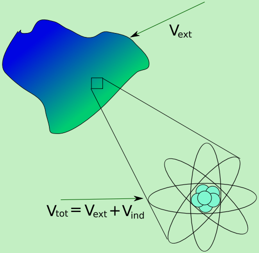

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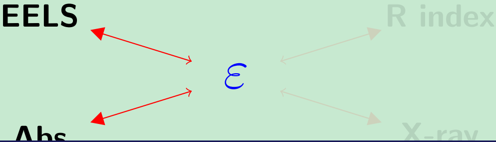

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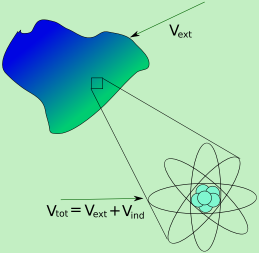

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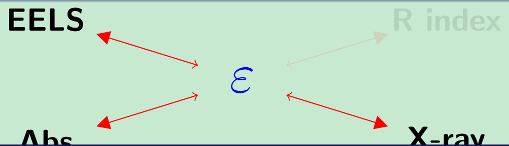

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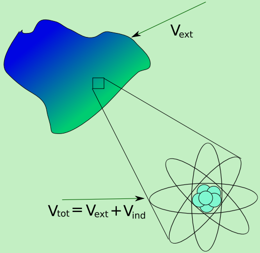

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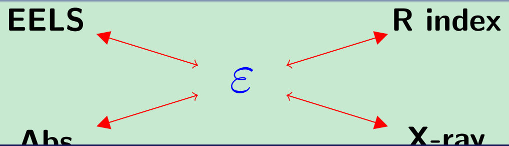

Linear Response Approach

Definition of polarizability

not polarizable $\Rightarrow$ $V_{tot} = V_{ext}$ $\Rightarrow$ $\varepsilon^{-1} = 1$

polarizable $\Rightarrow$ $V_{tot} \neq V_{ext}$ $\Rightarrow$ $\varepsilon^{-1} \neq 1$

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

χ is the polarizability of the system

Linear Response Approach

Definition of polarizability

$$\begin{array}{rcccl} \text{not polarizable} & \Rightarrow & V_{tot} = V_{ext} & \Rightarrow & \varepsilon^{-1} = 1 \\ \textit{polarizable} & \Rightarrow & V_{tot} \neq V_{ext} & \Rightarrow & \varepsilon^{-1} \neq 1 \\ & & & & \varepsilon^{-1} = 1 + v\chi \end{array}$$

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Linear Response Approach

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Linear Response Approach

Polarizability

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

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

Linear Response Approach

Polarizability

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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

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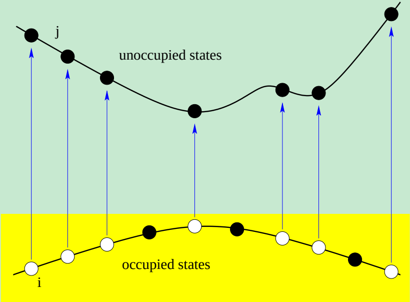

Linear Response Approach

Polarizability

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$$\Updownarrow$$

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

$$\chi \delta V_{ext} = \chi^0 \left(\delta V_{ext} + \delta V_H + \delta V_{xc}\right)$$

$$\chi = \chi^0 \left(1 + \frac{\delta V_H}{\delta V_{ext}} + \frac{\delta V_{xc}}{\delta V_{ext}}\right)$$

$$\frac{\delta V_H}{\delta V_{ext}} = \frac{\delta V_H}{\delta n} \frac{\delta n}{\delta V_{ext}} = v\chi$$

$$\frac{\delta V_{xc}}{\delta V_{ext}} = \frac{\delta V_{xc}}{\delta n} \frac{\delta n}{\delta V_{ext}} = f_{xc}\chi$$

with $\mathbf{f_{xc}}$ = **exchange-correlation kernel**

Linear Response Approach

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

with $\mathbf{f_{xc}}$ = **exchange-correlation kernel**

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Linear Response Approach

Polarizability χ in TDDFT

1. DFT ground-state calc. $\longrightarrow \quad \phi_i, \epsilon_i \qquad [V_{xc}]$
2. $\phi_i, \epsilon_i \quad \longrightarrow \quad \chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j)}$
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. $\chi = \chi^0 + \chi^0 \left(v + f_{xc}\right) \chi$

Linear Response Approach

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Theoretical Spectroscopy

$$\chi(\mathbf{r},\mathbf{r}',\omega) \rightarrow \chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) \rightarrow \varepsilon^{-1}_{00}(\mathbf{q},\omega)$$

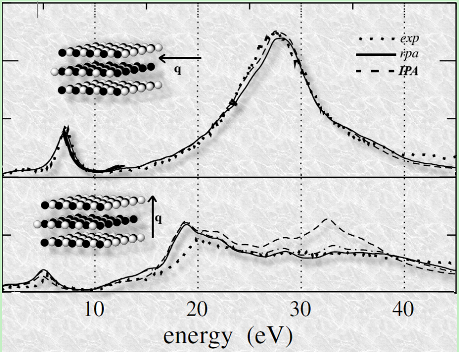
$$\text{Energy Loss Function} = -\text{Im}\left\{\varepsilon^{-1}_{00}(\mathbf{q},\omega)\right\}$$

$$\text{Absorption} = \text{Im}\left\{\frac{1}{\varepsilon^{-1}_{00}(\mathbf{q},\omega)}\right\}$$

Outline

EELS of Graphite

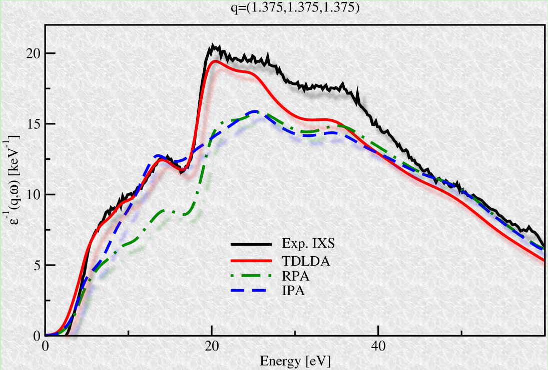
Some good results ... (graphite)



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

Inelastic X-ray Scattering

TD-LDA on IXS of Silicon



H-C. Weissker *et al.*, Physical Review Letters **97**, 237602 (2006)

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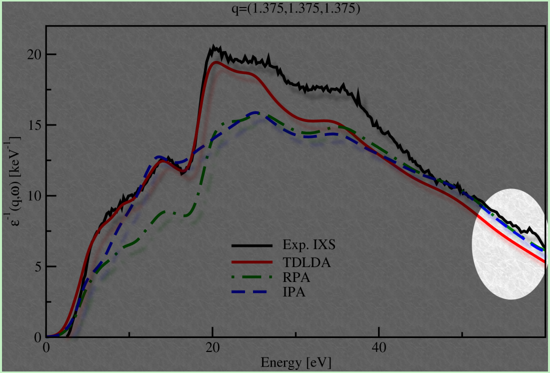
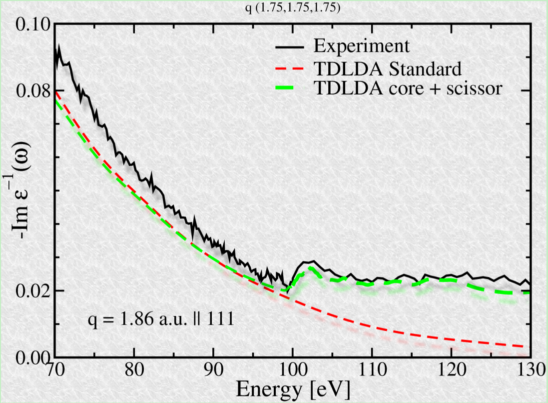


H-C. Weissker *et al.*, Physical Review Letters **97**, 237602 (2006)

Semi-core states

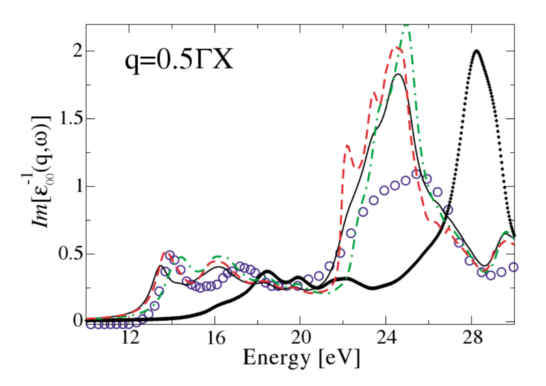
L-edge of Silicon



Luppi *et al.* Phys. Rev. B **78**, 245124 (2008)

EELS of LiF : many-body effects (beyond TDLDA)

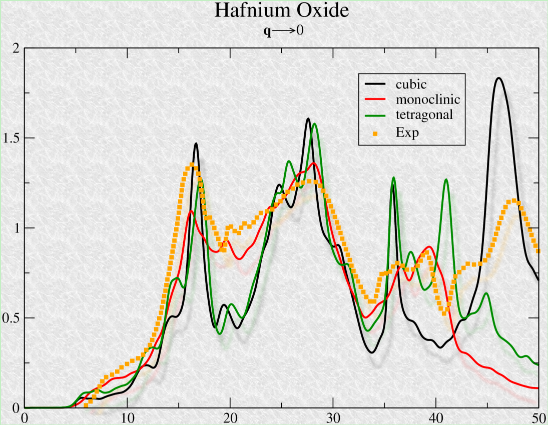
$\mathbf{q} = 0.5\Gamma X$



A.Marini *et al.*, PRL **91**, 256402 (2003).

Prediction

ELS of Hafnium Oxide



Zobelli and Sottile, work in progress.

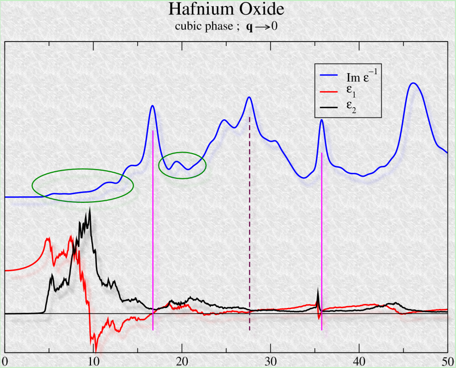
Outline

Why the numerical approach is important

Analysis

Analysis

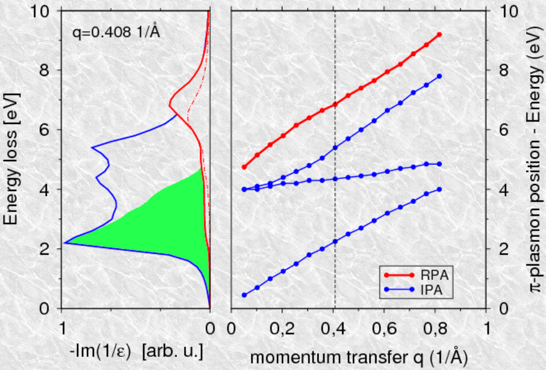
ELS of Hafnium Oxide



Zobelli and Sottile, work in progress

Analysis

ELS of Nanotubes via Graphene analysis



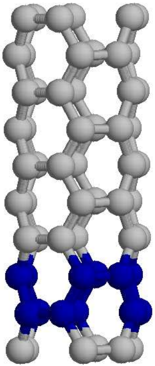
Kramberger *et al.*, Phys. Rev. Lett. **100**, 196803 (2008)

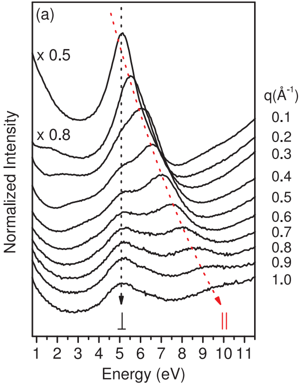
EELS of nanotubes: plasmon dispersion

VA-SWCNT

diameter: 2nm

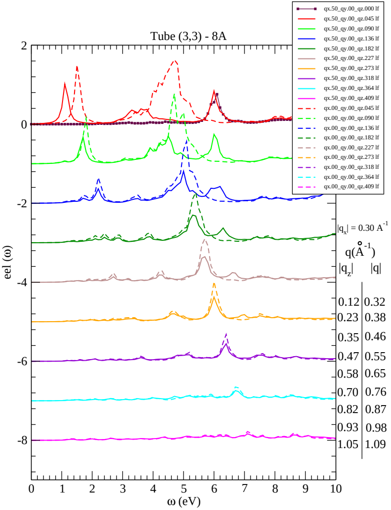
nearly isolated



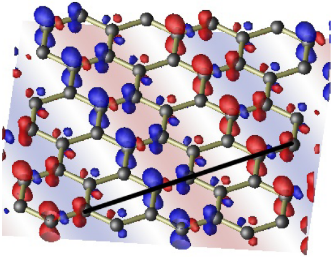


Kramberger *et al.*, Phys. Rev. Lett. **100**, 196803 (2008)

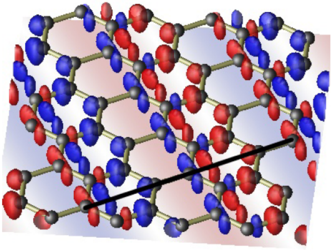
EELS of nanotubes: plasmon dispersion



Graphic tools: 'see' the plasmons or the excitons



E=9eV

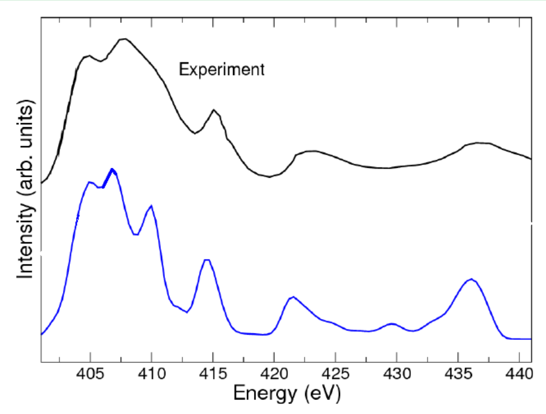


E=30eV

See Ralf Hambach's Poster.

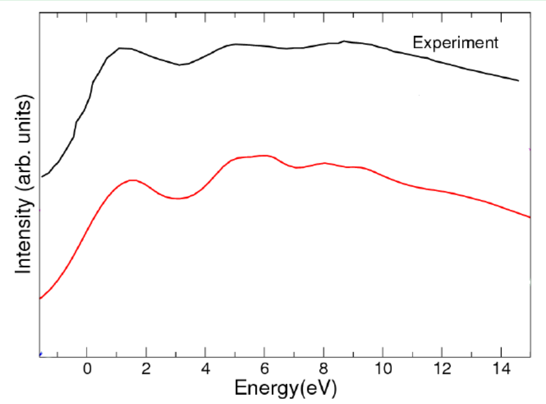
ELNES of BN

Nitrogen Edge



Courtesy of Sangeeta Sharma.

ELNES of Cu

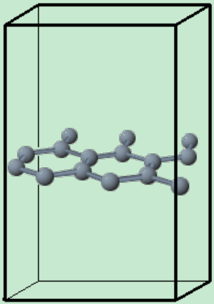


Courtesy of Sangeeta Sharma.

Numerical simulations

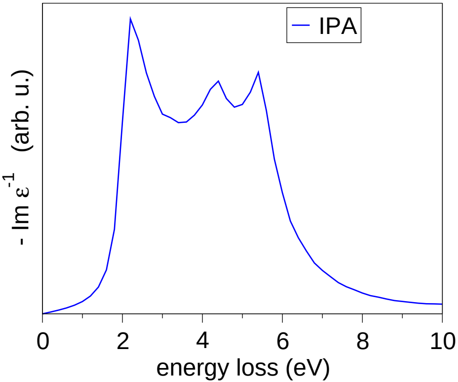
ab-initio calculations

- DFT ground-state calculations (LDA)
- Independant Particles polarizability: χ^0
- RPA Full polarisability: $\chi = \left[1 - \chi^0 v\right]^{-1} \chi^0$
- Dielectric function $\varepsilon^{-1} = 1 + v\chi$
- energy loss function $-\mathrm{Im}\{\varepsilon^{-1}(\mathbf{q}, \omega)\}$

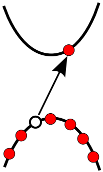


Independent particle picture

energy loss in graphene
(in-plane, $q = 0.41\text{Å}$)

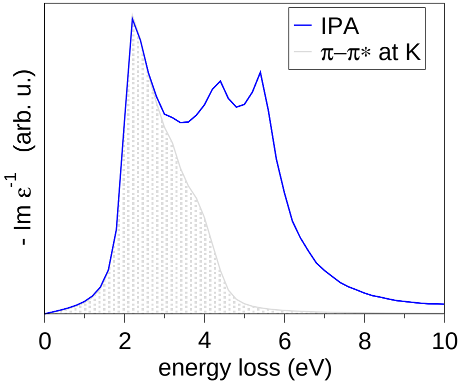


$\Longrightarrow$ given by χ^0:
interpretation in terms of
band-transitions

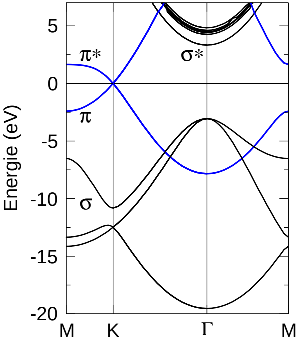


Independent particle picture

energy loss in graphene
(in-plane, $q = 0.41$Å)

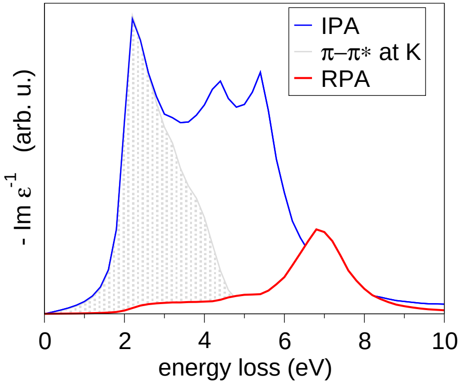


bandstructure



RPA: random phase approx.

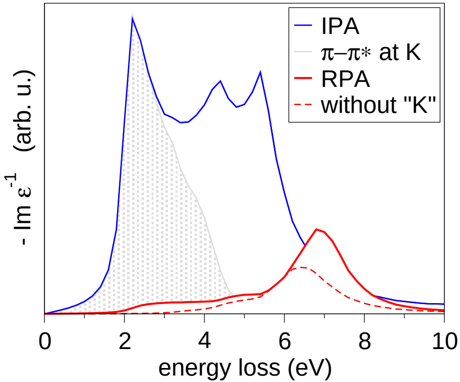
energy loss in graphene
(in-plane, $q = 0.41\text{Å}$)



- given by χ:
  no interpretation by band-transitions
- contributions from K
- mixing of transitions

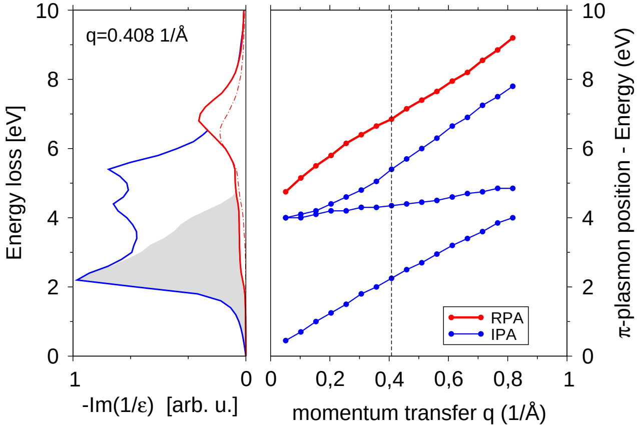
RPA: random phase approx.

energy loss in graphene
(in-plane, $q = 0.41$Å)

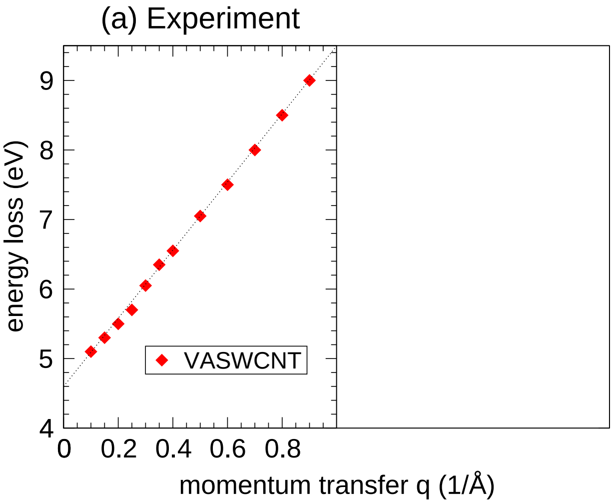


- given by χ:
  no interpretation by band-transitions
- contributions from K
- mixing of transitions

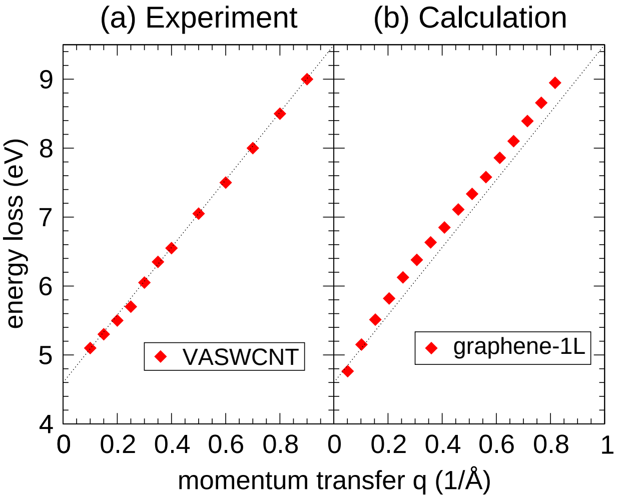
Plasmon dispersion



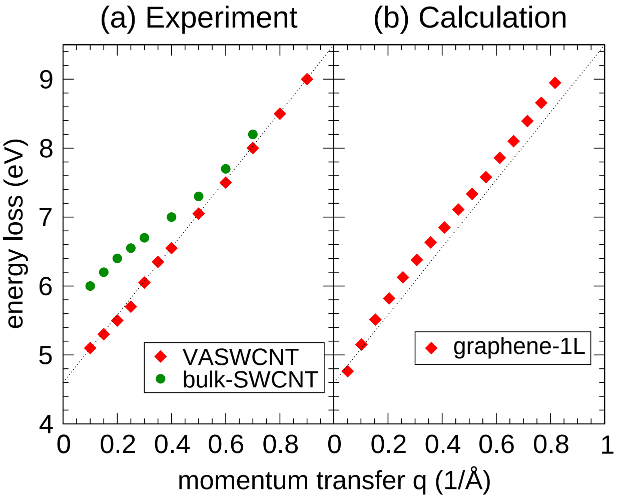
SWCNT vs. Graphene

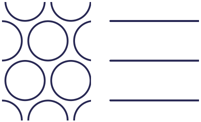


SWCNT vs. Graphene



SWCNT vs. Graphene





SWCNT vs. Graphene