Overview of RPA from the condensed matter perspective

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ÉCOLE POLYTECHNIQUE

cea COMMISSARIAT A L'ENERGIE ATOMIQUE

Outline

1. History

2. Look at the reponse

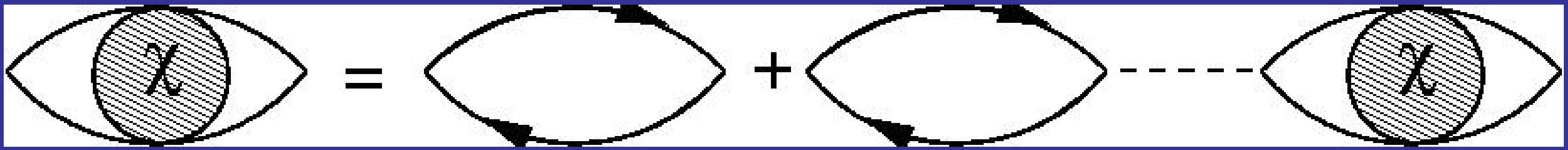
3. Look at a spectral function

4. Look at the total energy

1. History and Definition

Bohm and Pines 1952: response of an electron gas to an effective single particle potential

Equivalence *(Ehrenreich and Cohen 1959)* to the linearized time-dependent Hartree Approximation *(Lindhard 1954)*



RPA ~ bubble approximation *(Hubbard 1957)*

No exchange contribution

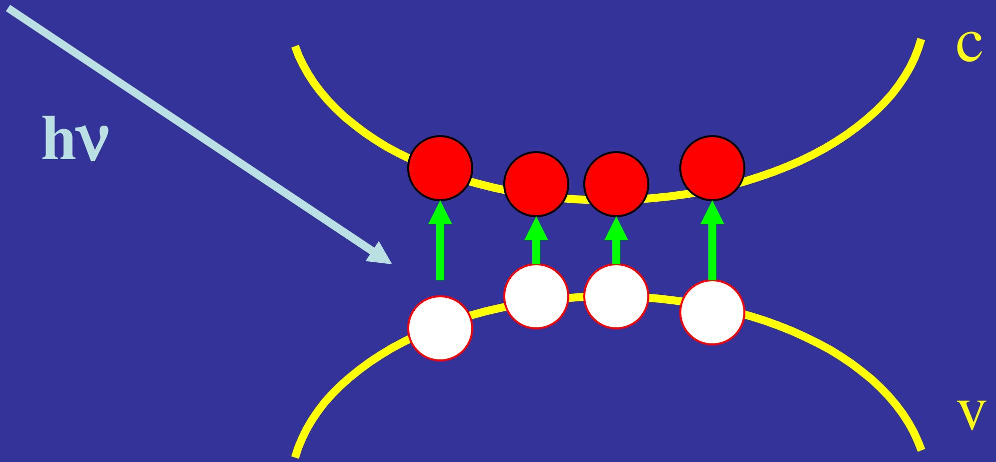
2. Look at the response

a. Connection to experiment

b. Long range and short range

c. Failures

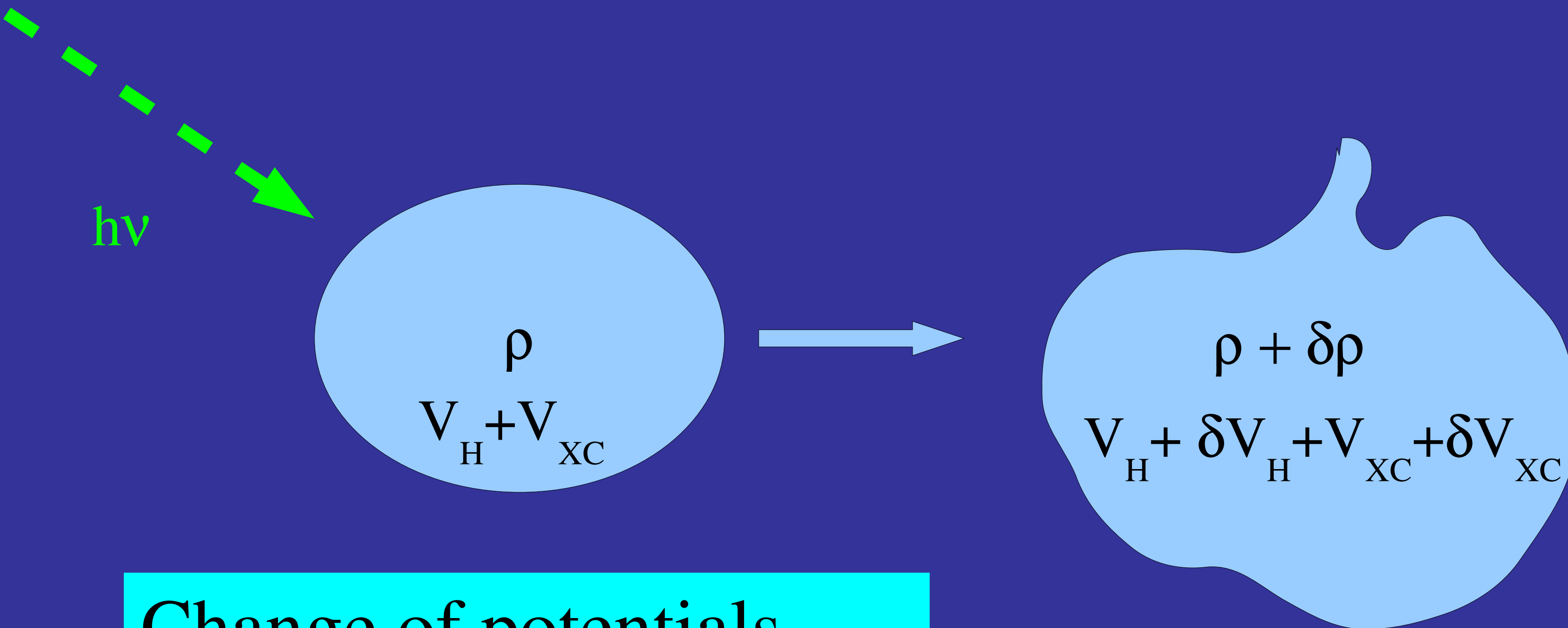
Independent electrons and transitions



$$\mathrm{Im}\,[\chi_0] \sim -\sum_{vc} |\langle v|D|c\rangle|^2\, \delta(E_c - E_v - \omega)$$

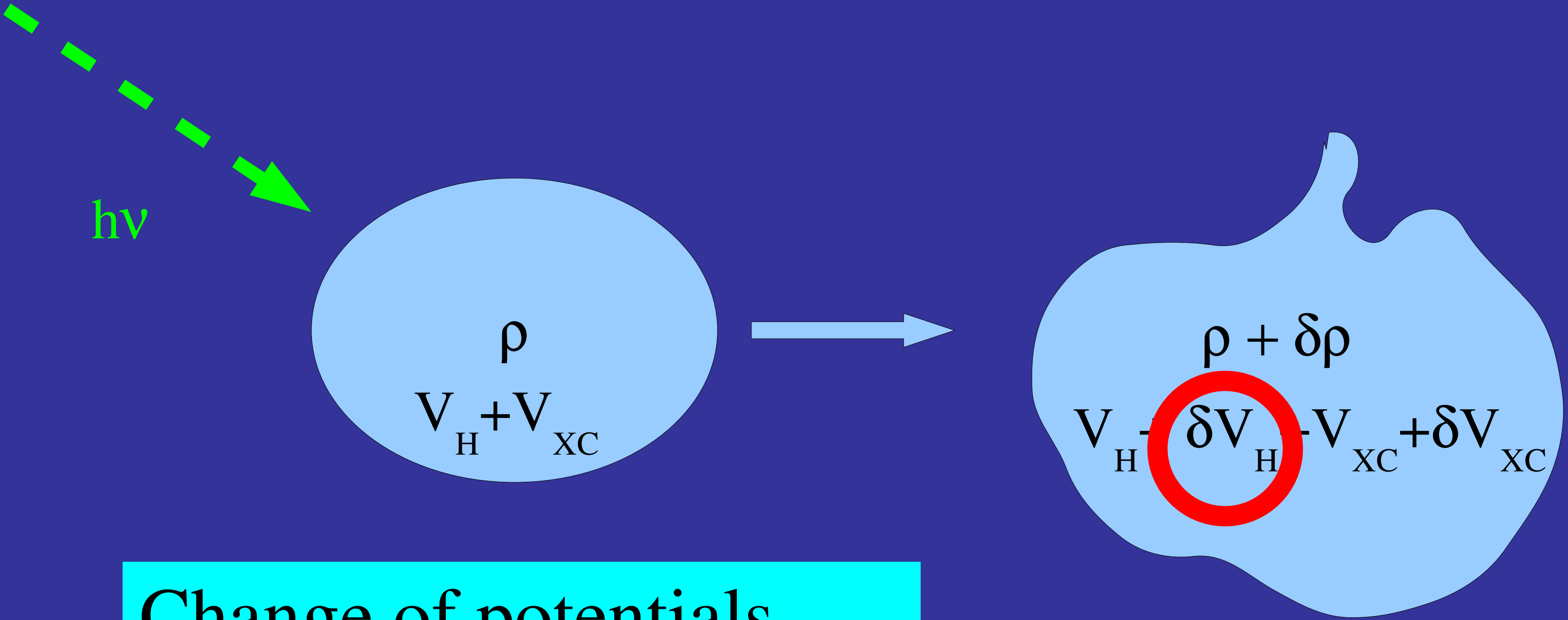
Partial DOS → EELS~XAS

Excitation ?



Change of potentials

Excitation ?



Change of potentials

Induced Hartree: long-range and local field effects

RPA

RPA:

$\varepsilon = 1 - v\chi_0$ $\qquad V_{ext} = \varepsilon\, V_{tot}$

$\varepsilon^{-1} = (1 - v\chi_0)^{-1} = 1 + v\chi = 1 + v\chi_0 (1 - v\chi_0)^{-1}$

$\chi = \chi_0 + \chi_0 v \chi$ $\qquad \bar{\chi} = \chi_0 + \chi_0 \bar{v}\, \bar{\chi}$

$\delta V_H / \delta \rho$

$V_{ind} = v\chi\, V_{ext}$

$\delta V_H / \delta \rho$ (micro)

$V_{ind} = v\chi\, (V_{ext} + V_{ind}^{0})$

Loss: $-\mathrm{Im}(\chi)$ $\qquad$ Abs: $\mathrm{Im}(1/\varepsilon^{-1}) = v\mathrm{Im}(\bar{\chi})$

$\delta\ V_H/\delta\ \rho$

TDDFT-RPA:Û $\chi = \chi_0 + \chi_0 [\, v \,] \chi$

$v\,(q+G) \sim 1/|q+G|^2$
$G=0 \rightarrow$ plasmon
$G \neq 0 \rightarrow$ crystal local field effects

RPA:

$\varepsilon = 1 - v\chi_0$ $V_{ext} = \varepsilon V_{tot}$

$\varepsilon^{-1} = (1 - v\chi_0)^{-1} = 1 + v\chi = 1 + v\chi_0 (1 - v\chi_0)^{-1}$

$\chi = \chi_0 + \chi_0 v \chi$ $\bar{\chi} = \chi_0 + \chi_0 \bar{v} \bar{\chi}$

$\delta V_H / \delta \rho$

$\delta V_H / \delta \rho$ (micro)

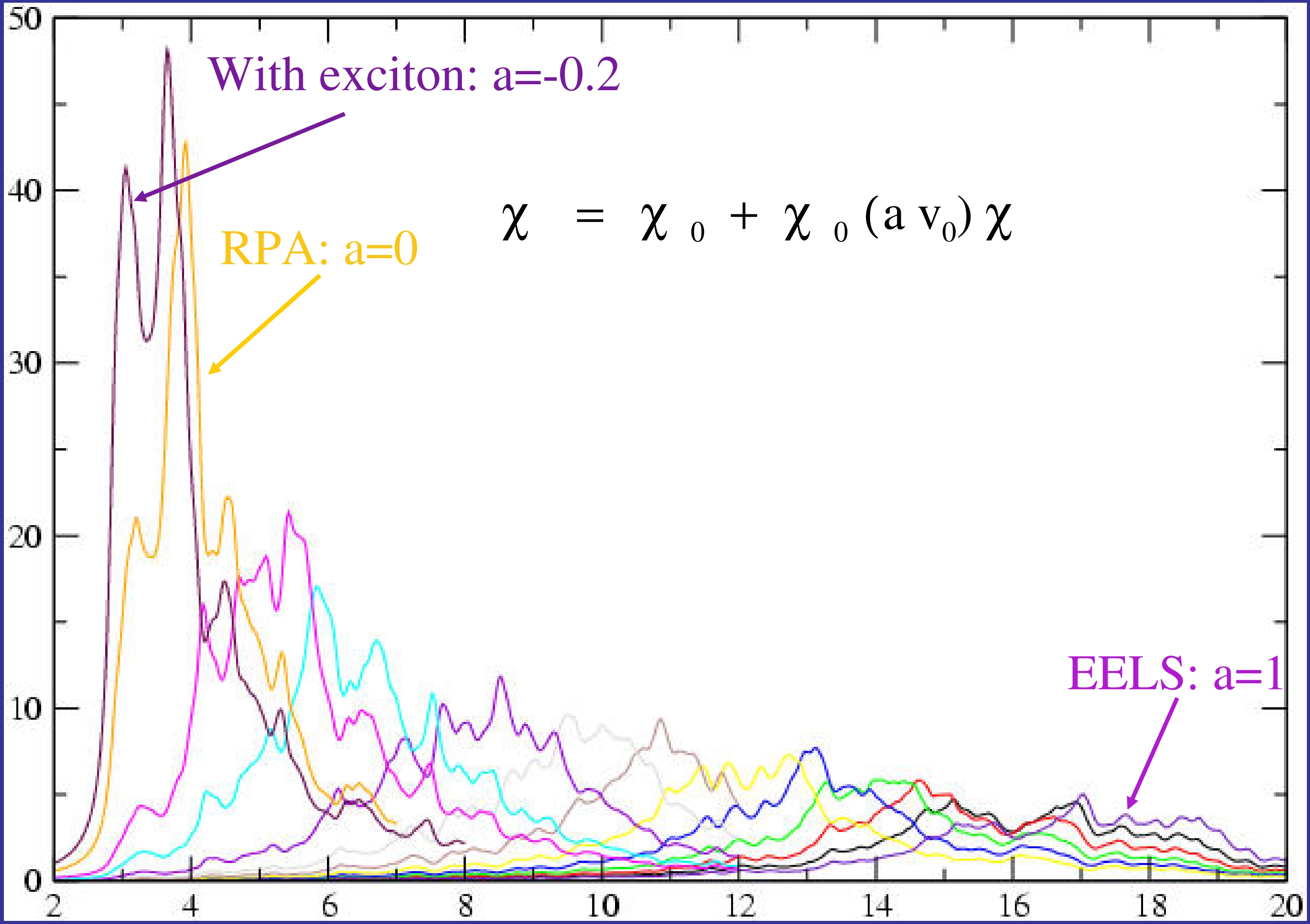
$V_{ind} = v\chi V_{ext}$

$V_{ind} = v\chi (V_{ext} + V_{ind}^{0})$

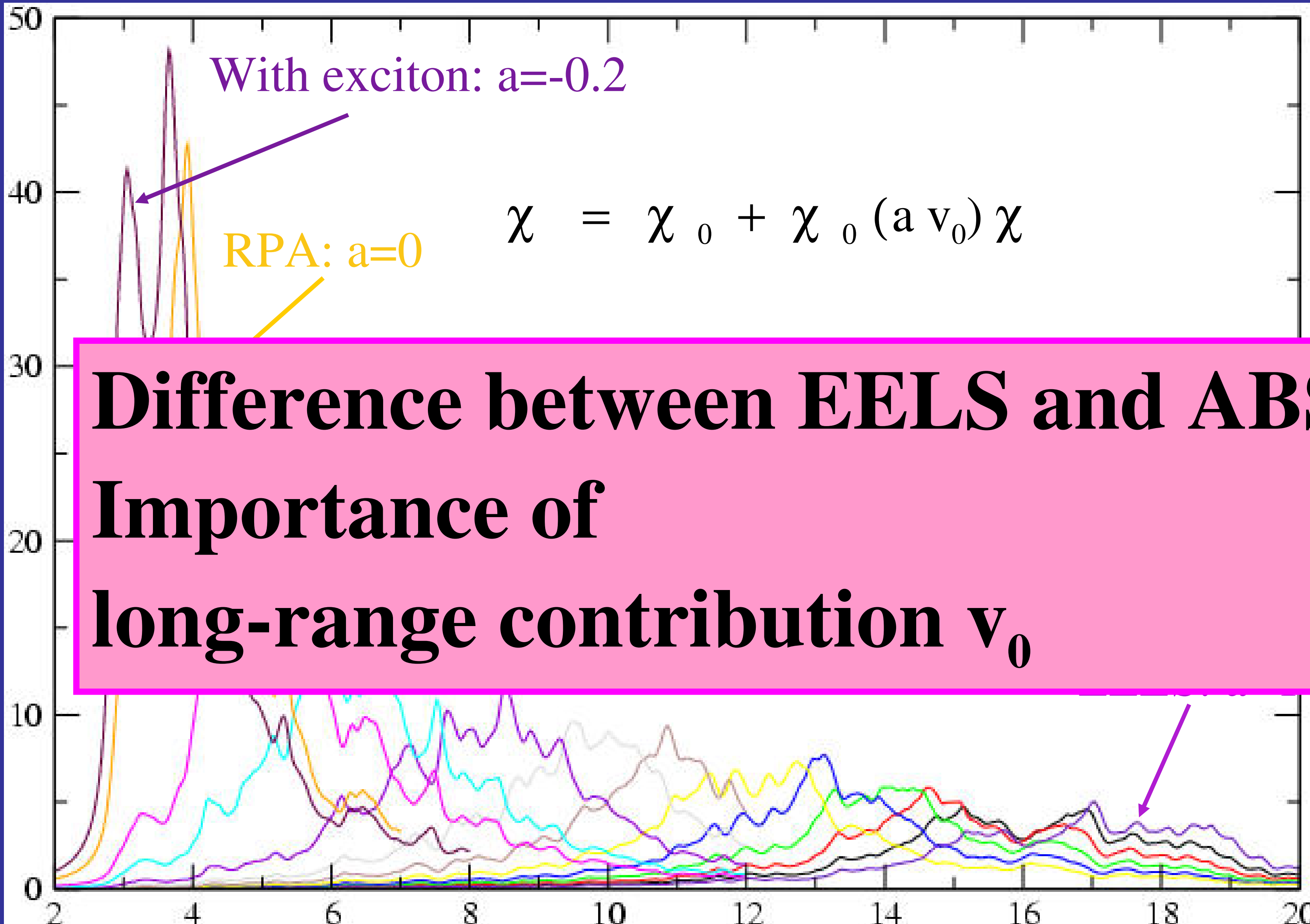
Loss: $-\mathrm{Im}(\chi)$

$1/q^2$

Abs: $\mathrm{Im}(1/\varepsilon^{-1}) = v\mathrm{Im}(\bar{\chi})$

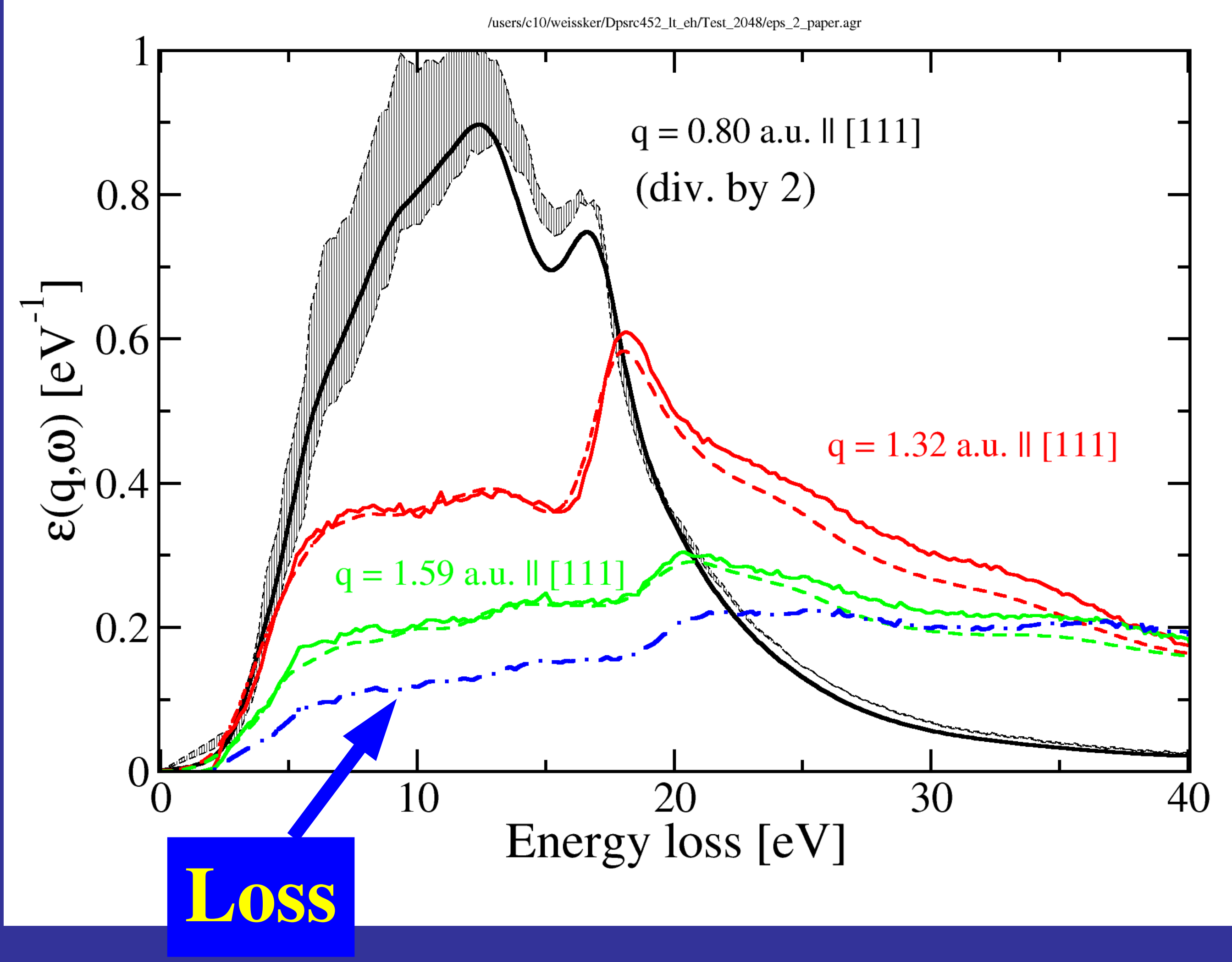


Sottile et al, Int. J. Quant. Chem. (2002)

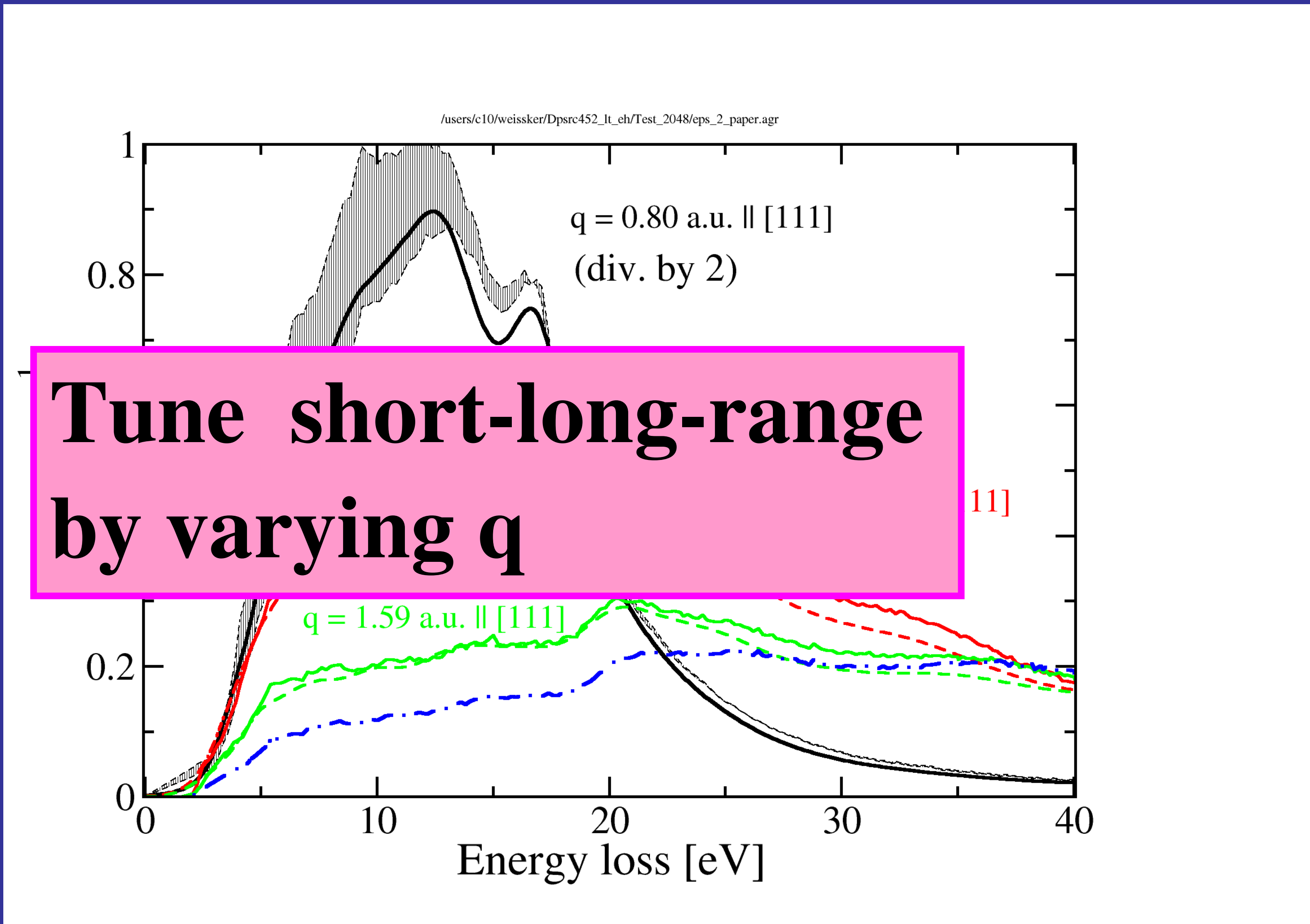


Difference between EELS and ABS: Importance of long-range contribution v_0

Sottile et al, Int. J. Quant. Chem. (2002)



H. Weissker et al., Collaboration LSI – ESRF (ID16)



Tune short-long-range by varying q

H. Weissker et al., Collaboration LSI – ESRF (ID16)

RPA including crystal local field effects: $\bar{v}$

$\varepsilon = 1 - v\chi_0$ $\qquad V_{ext} = \varepsilon\, V_{tot}$

$\varepsilon^{-1} = (1 - v\chi_0)^{-1} = 1 + v\chi = 1 + v\chi_0 (1 - v\chi_0)^{-1}$

$\chi = \chi_0 + \chi_0 v \chi$ $\qquad \bar{\chi} = \chi_0 + \chi_0 \bar{v}\, \bar{\chi}$

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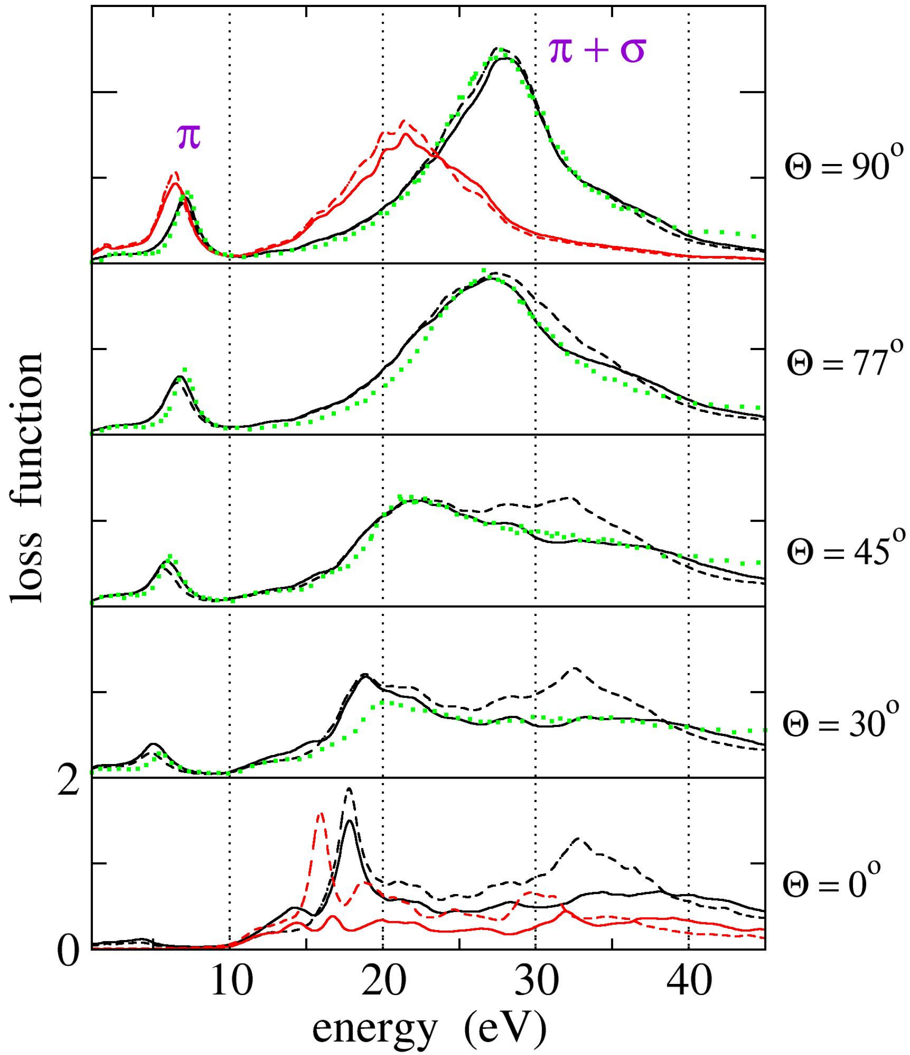
loss function versus momentum orientation



graphite

graphene (double spacing)

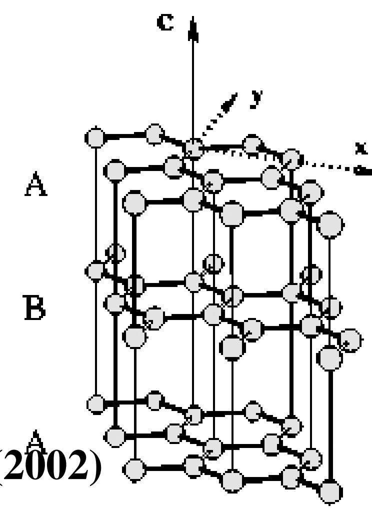
LFE ———

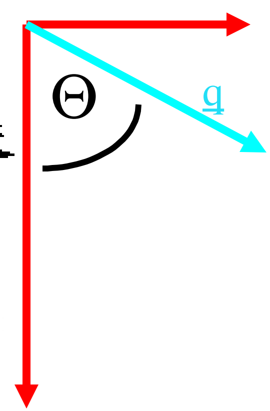
no LFE - - - - -

experiment ••••••••

IFW Dresden

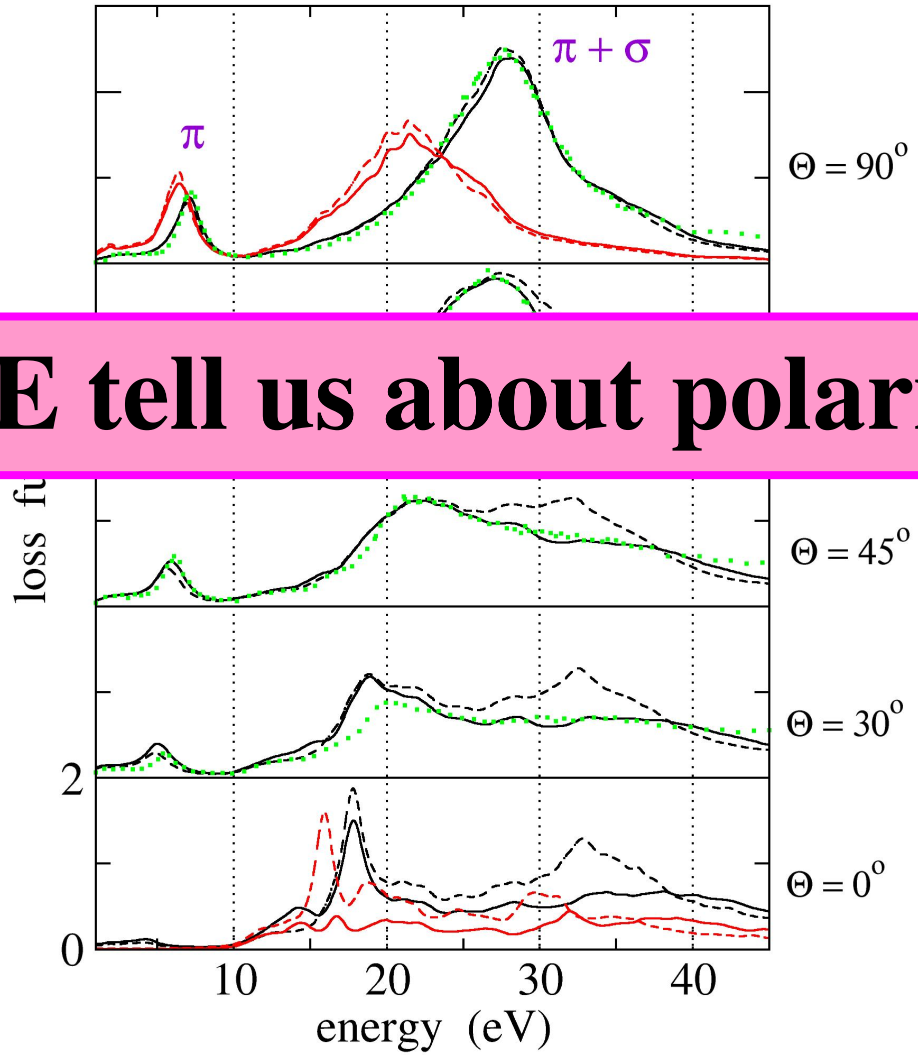
Pichler, Liu, Knupfer, Fink





Marinopoulos, Reining, Olevano et al. **PRL <u>89</u> , 076402 (2002)**

loss function versus momentum orientation



graphite

graphene (double spacing)

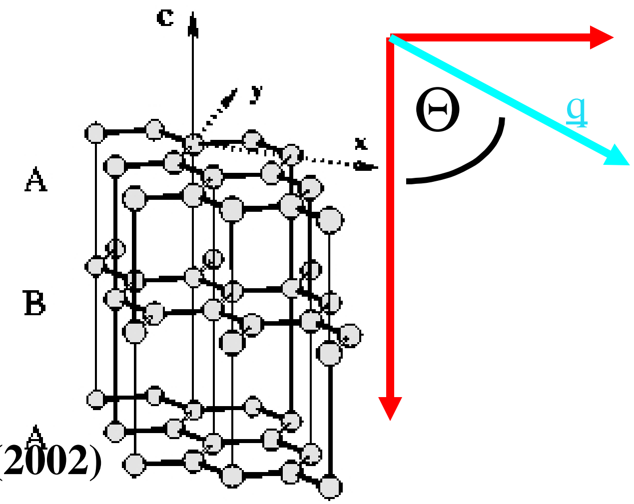
LFE ———

no LFE - - - - -

LFE tell us about polarizable objects

IFW Dresden

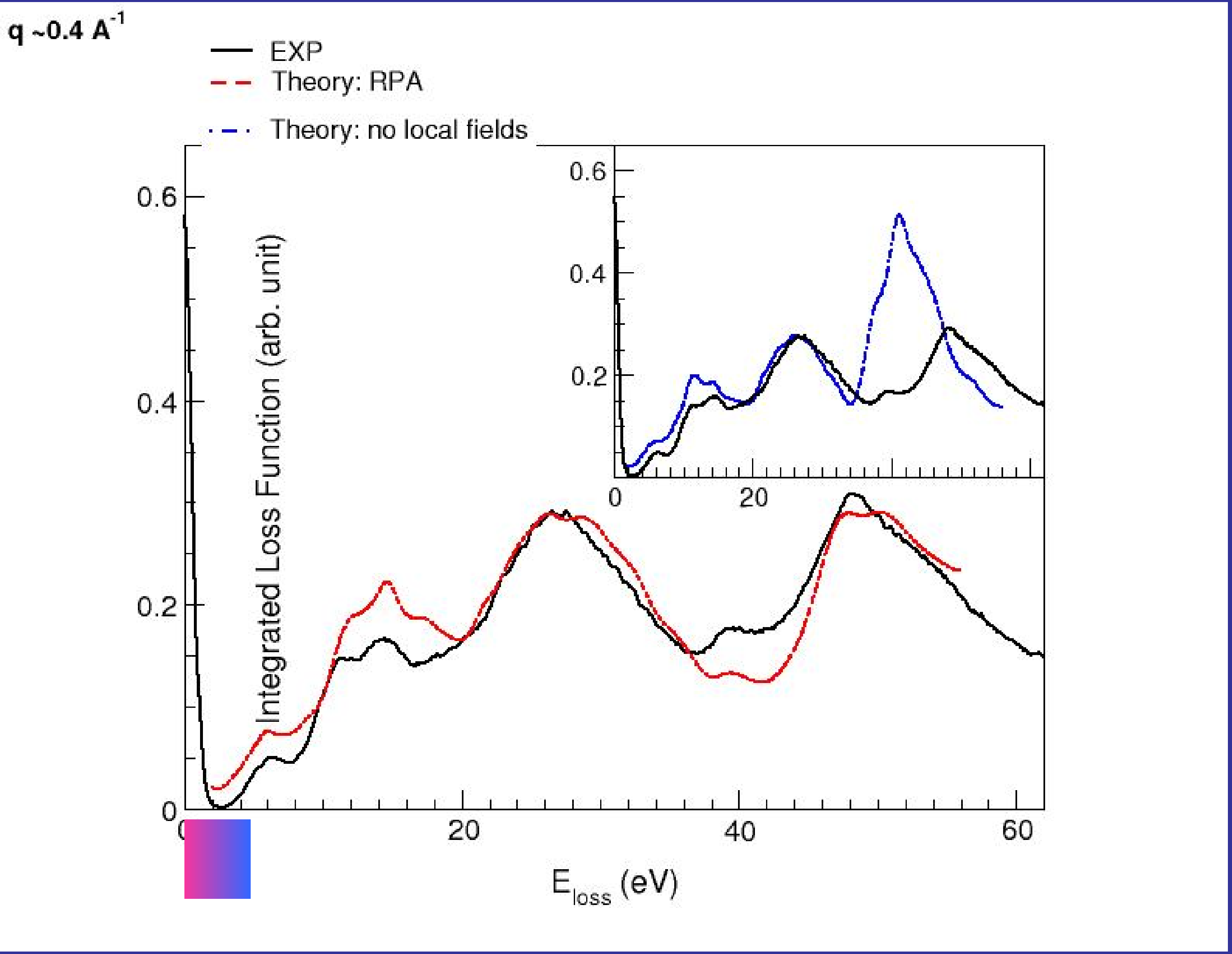
Pichler, Liu, Knupfer, Fink

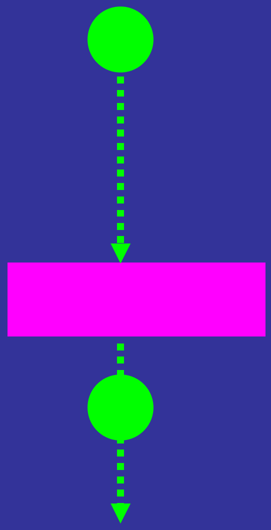


Marinopoulos, Reining, Olevano et al. **PRL** **89**, **076402 (2002)**

Rutile TiO_2

Titanium Dioxide

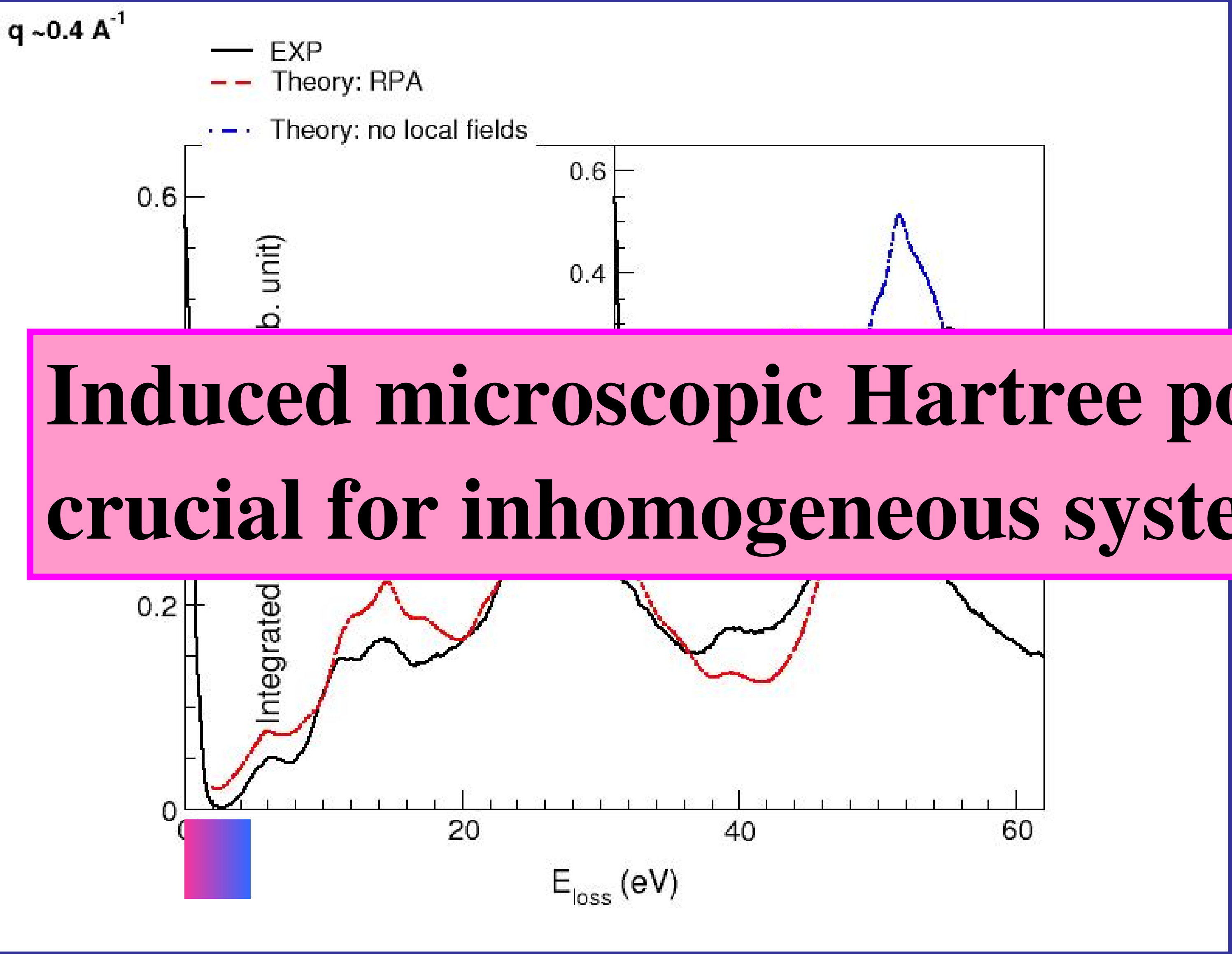




Vast, Reining, Olevano, Schattschneider, Jouffrey, PRL 88, 037601 (2002)

Rutile TiO_2

Titanium Dioxide



Induced microscopic Hartree potential crucial for inhomogeneous system

Vast, Reining, Olevano, Schattschneider, Jouffrey, PRL 88, 037601 (2002)

$\delta V_H/\delta \rho$

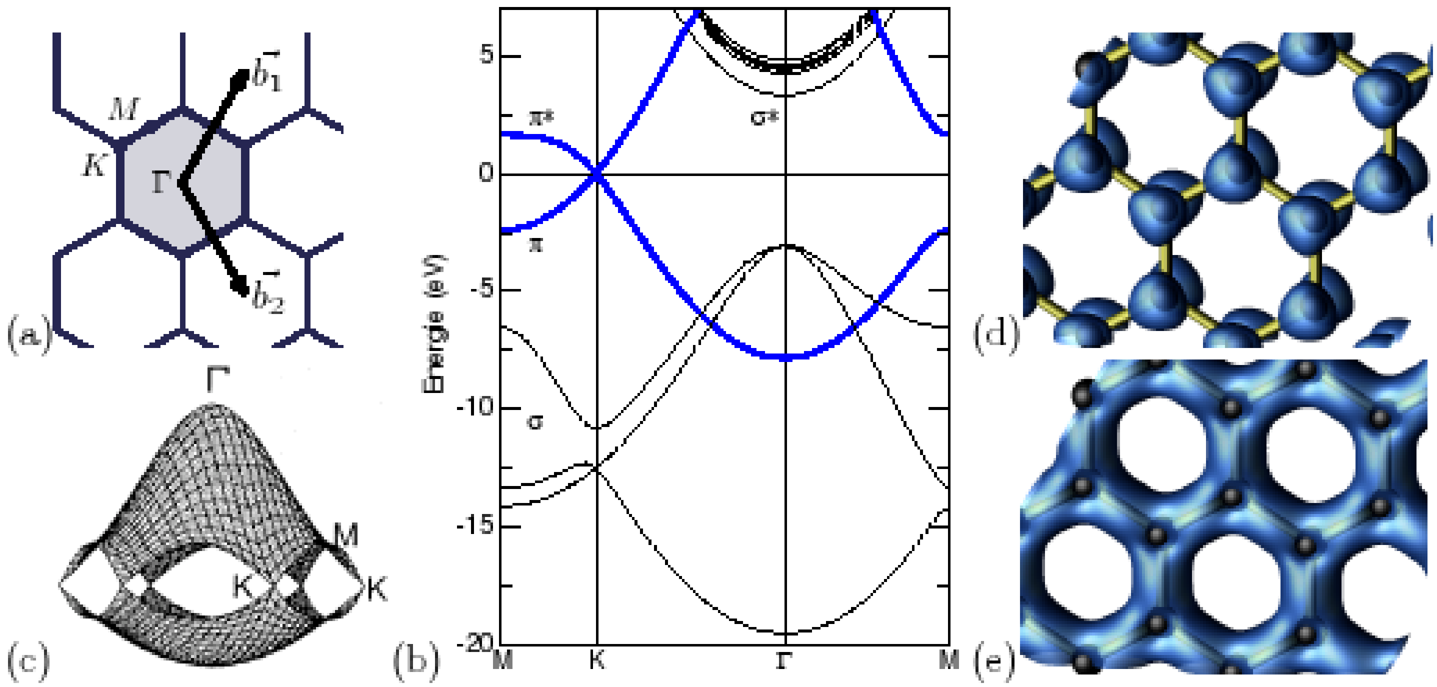
RPA: $\chi = \chi_0 + \chi_0 [v] \chi$

$v(q+G) \sim 1/|q+G|^2$

$G=0 \rightarrow$ plasmon

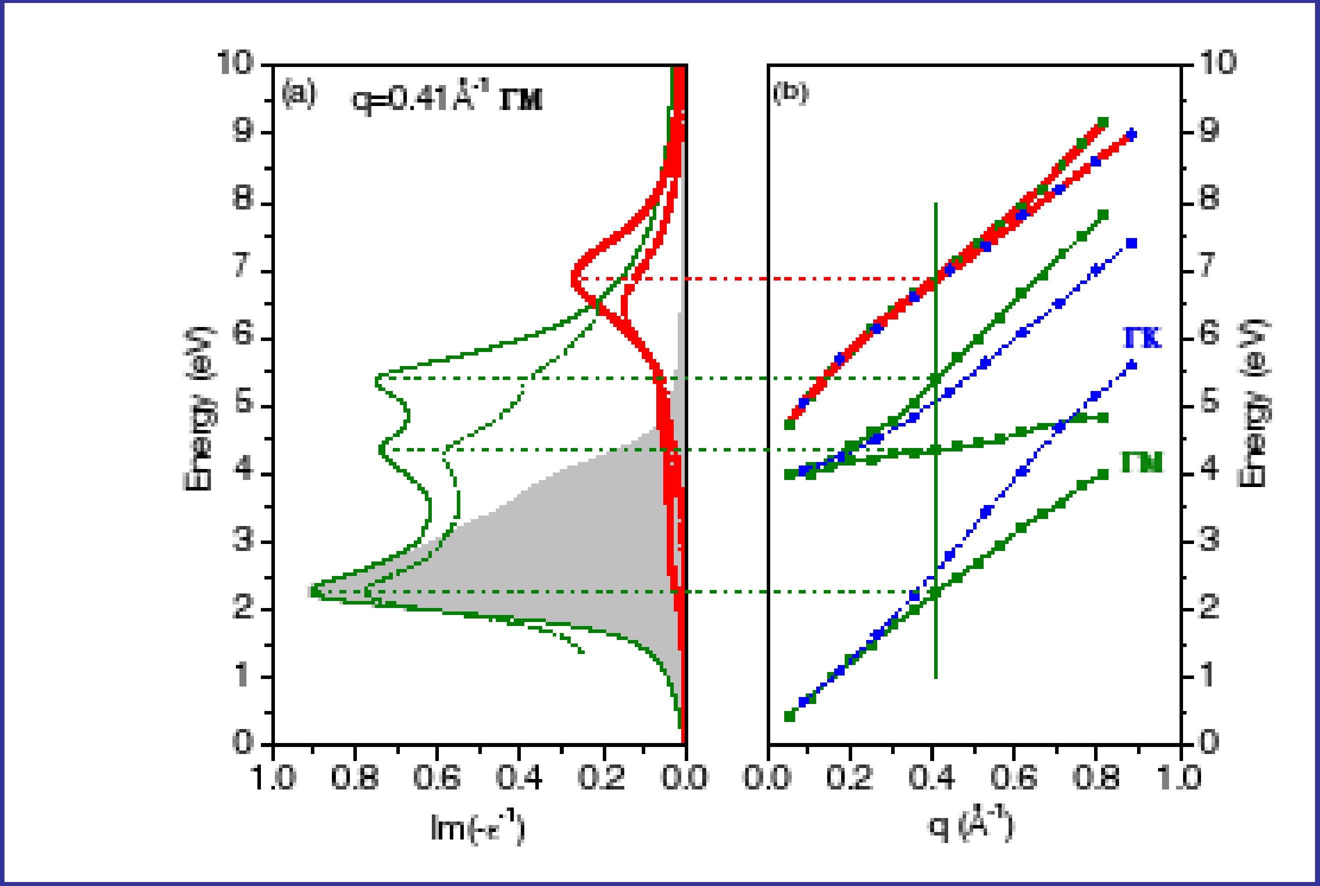
$G \neq 0 \rightarrow$ crystal local field effects

Graphene, π plasmon



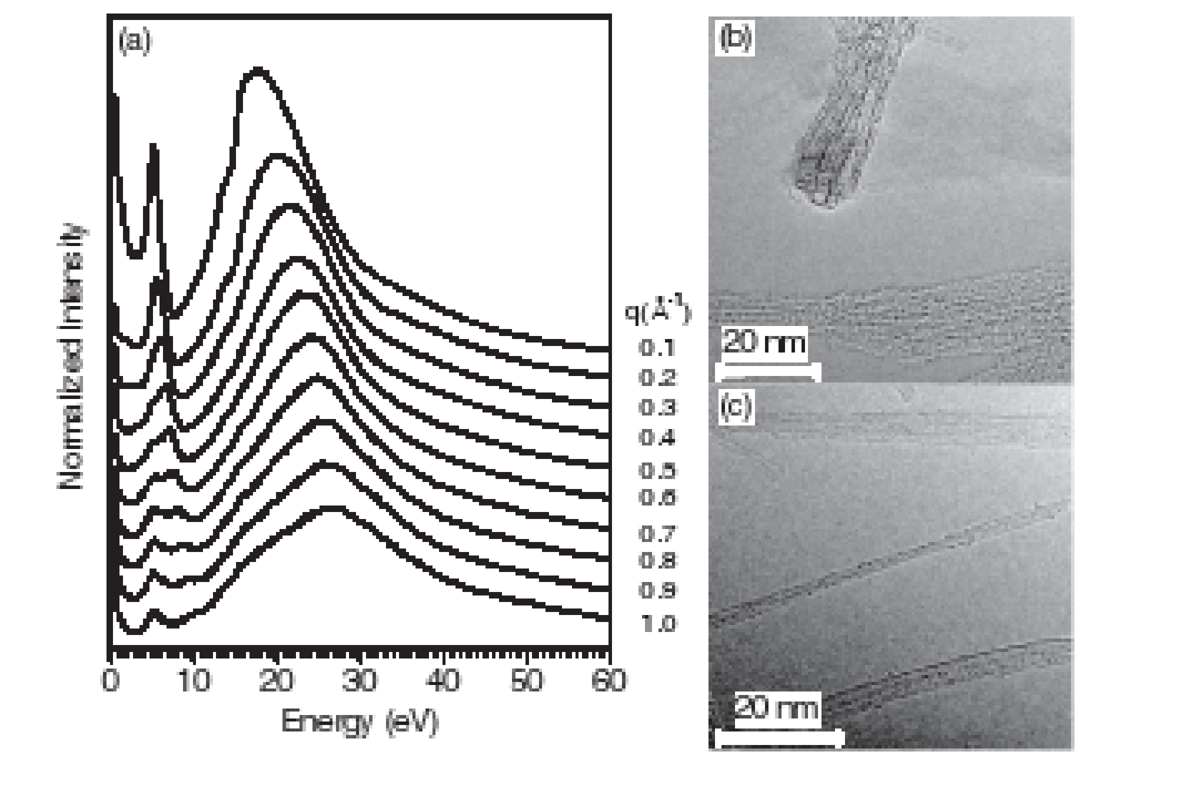
R. Hambach, Diplomarbeit

Graphene, π plasmon



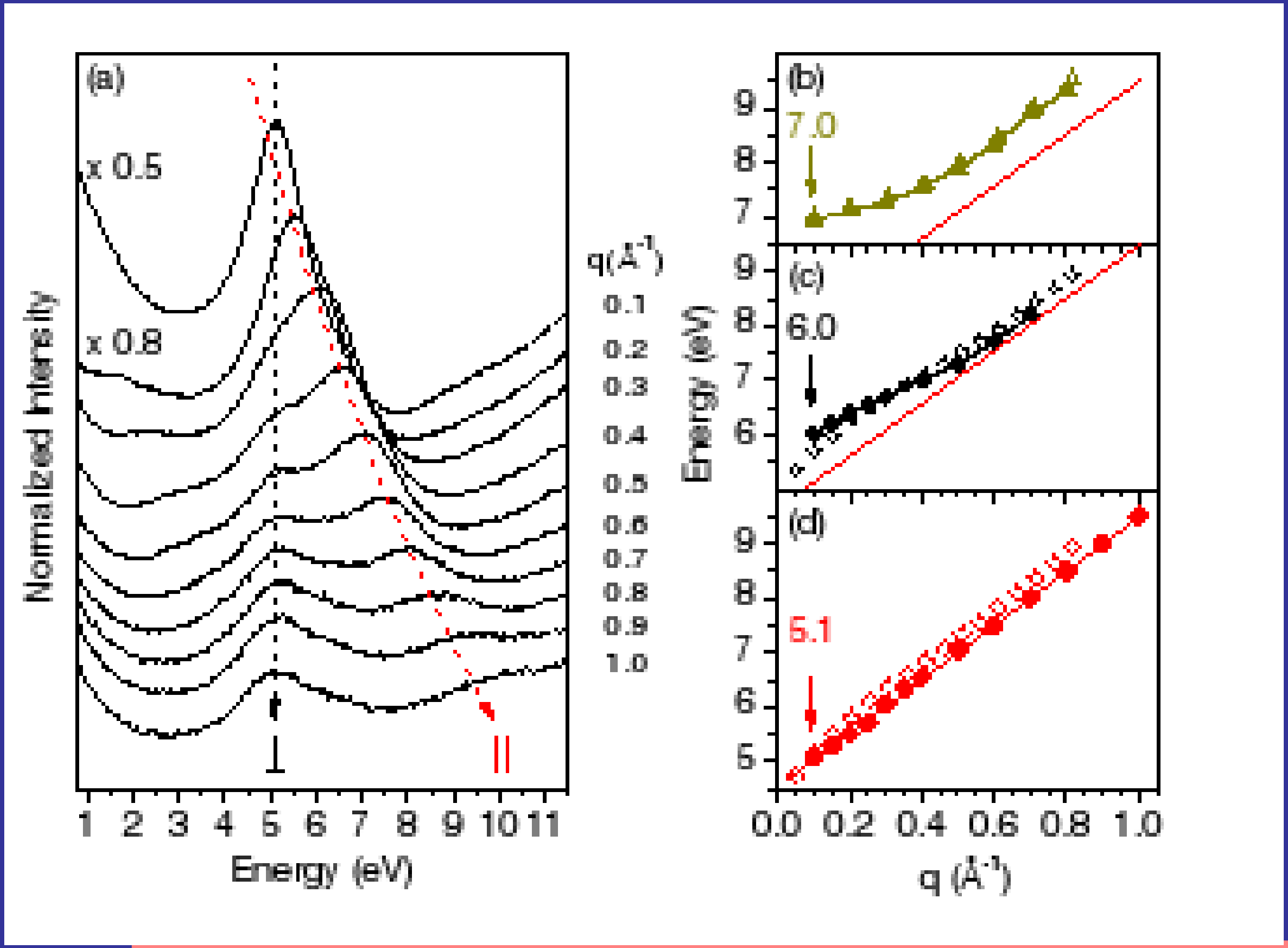
C. Kramberger et al., PRL 100, 196803 (2008)

Isolated carbon nanotube, π plasmon



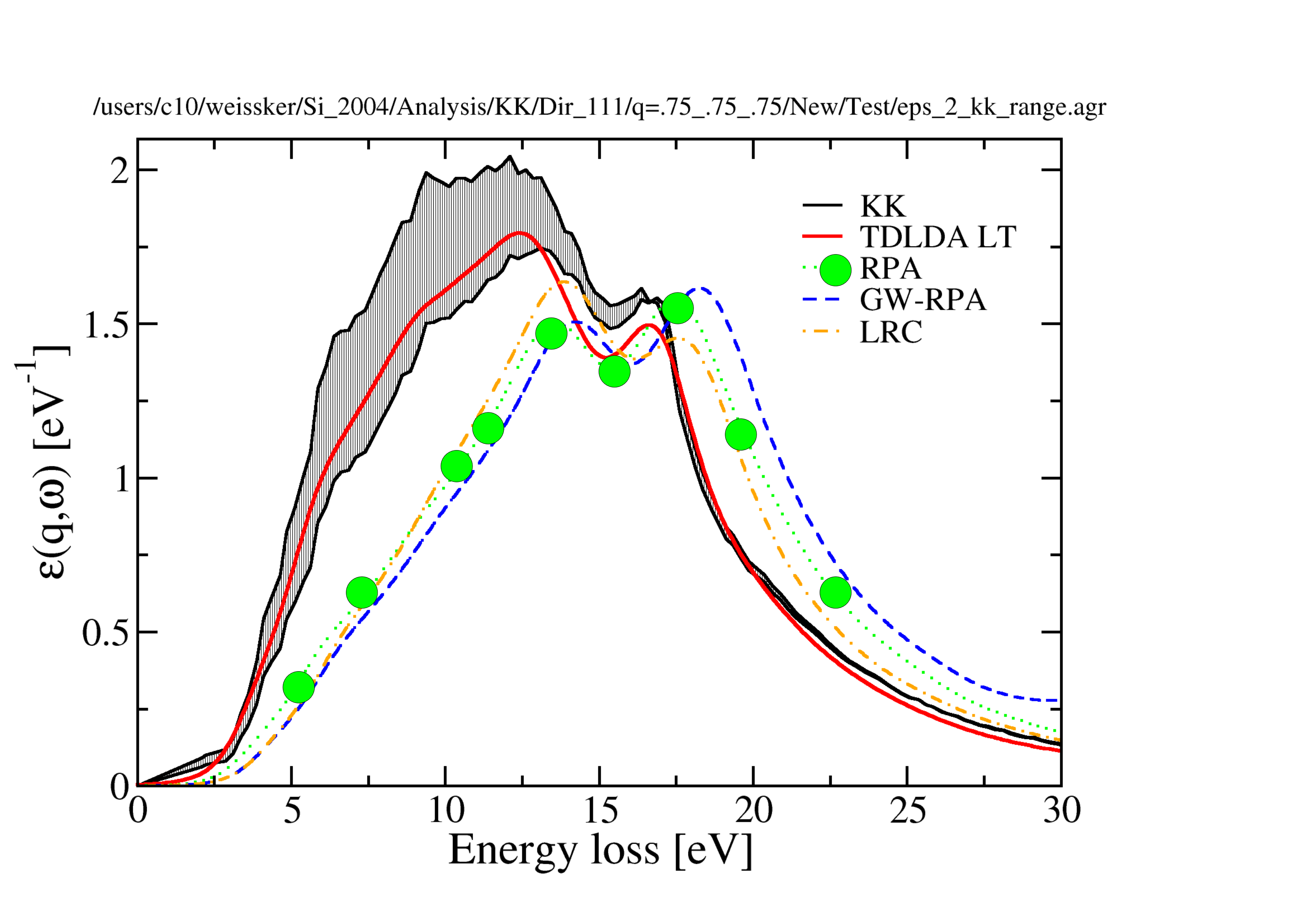
C. Kramberger et al., PRL 100, 196803 (2008)

Nanotubes and graphene, π plasmon dispersion

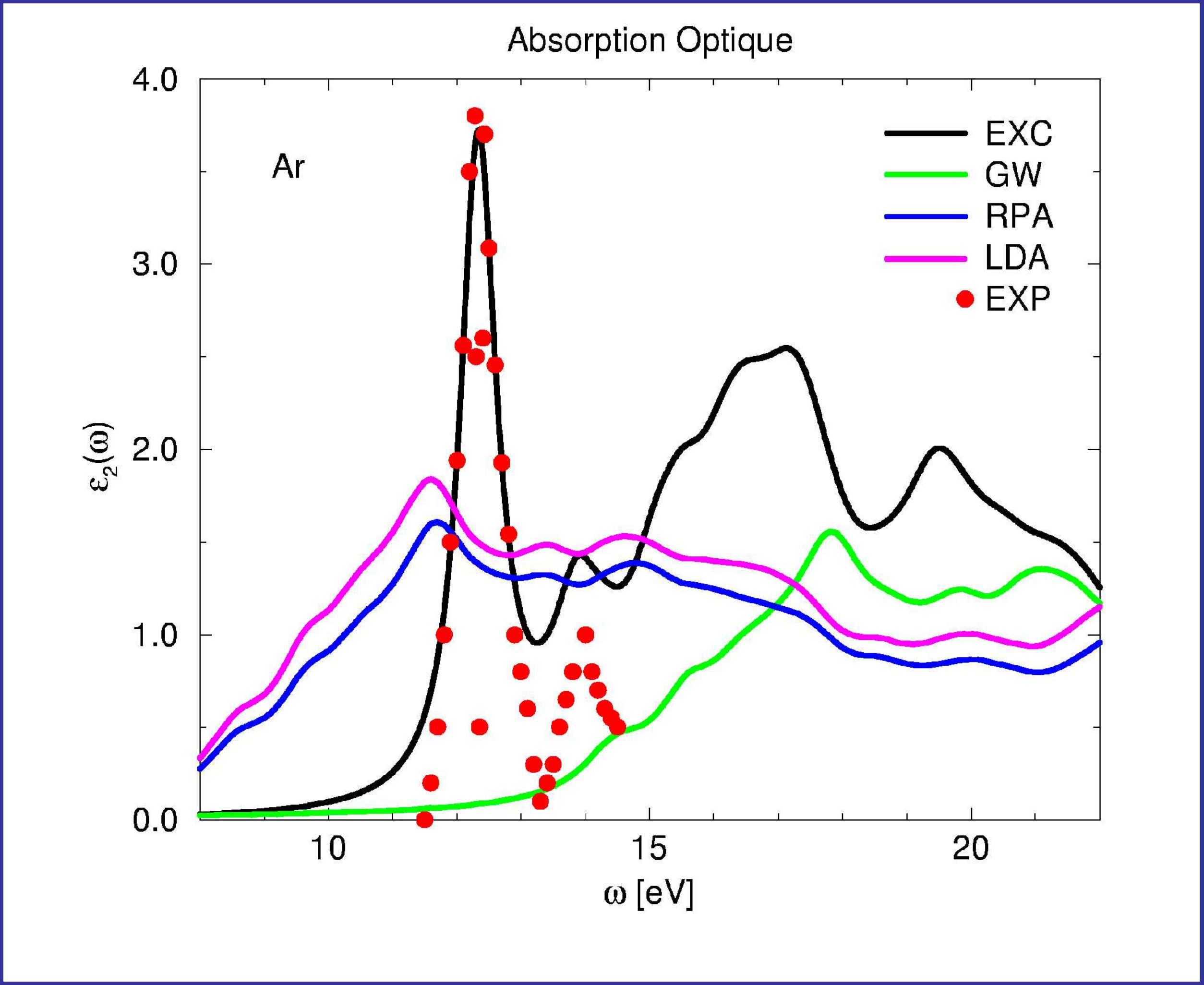


C. Kramberger et al., PRL 100, 196803 (2008)

More quantitatively?



H. Weissker et al., Phys. Rev. Lett. **97**, 237602 (2006)
Collaboration LSI – ESRF (ID16)



...or even qualitatively?

3. Look at a spectral function

a. Appearance of the (RPA) response function

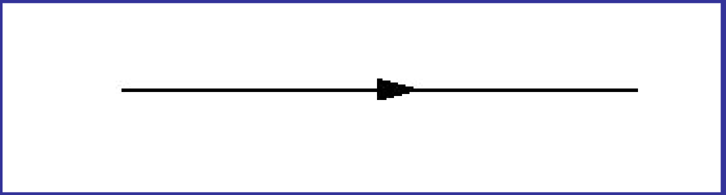
b. Effects of the (RPA) response function

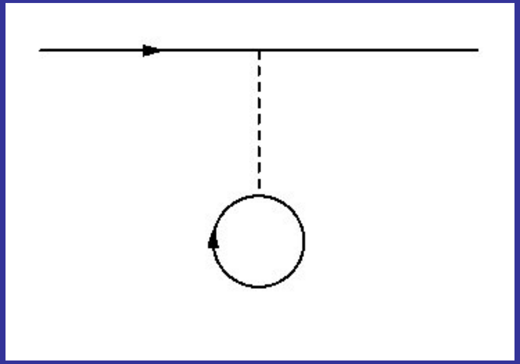
c. Failures

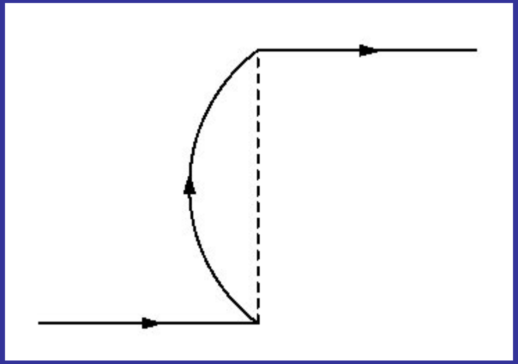
G=.....

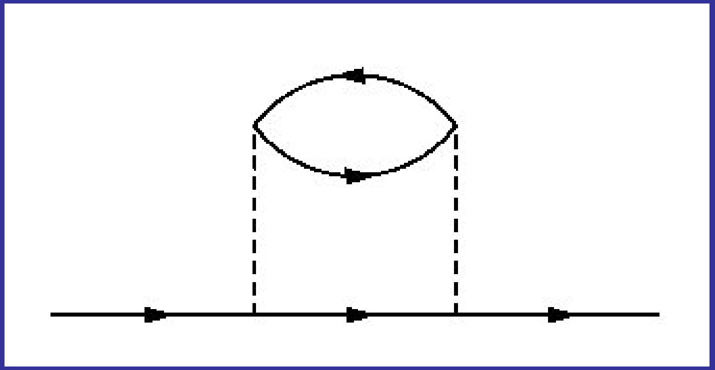
$$G(1,2) = -i \langle T[\psi(1)\psi^{\dagger}(2)] \rangle$$

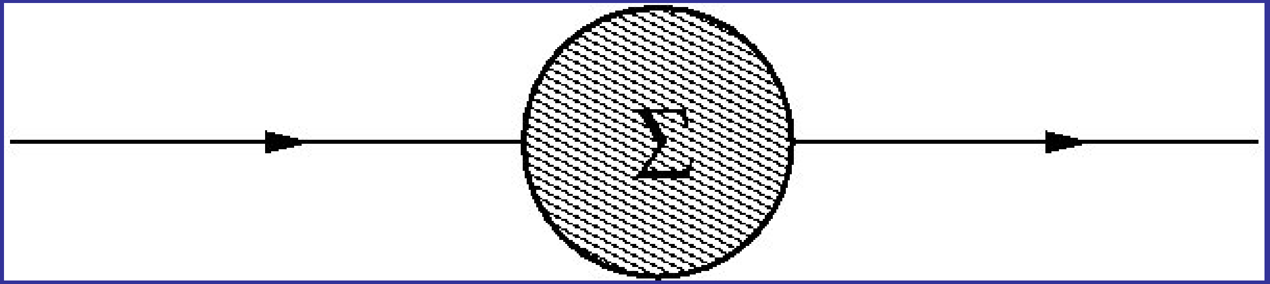
$$1=(r_1,\sigma_1,t_1)$$





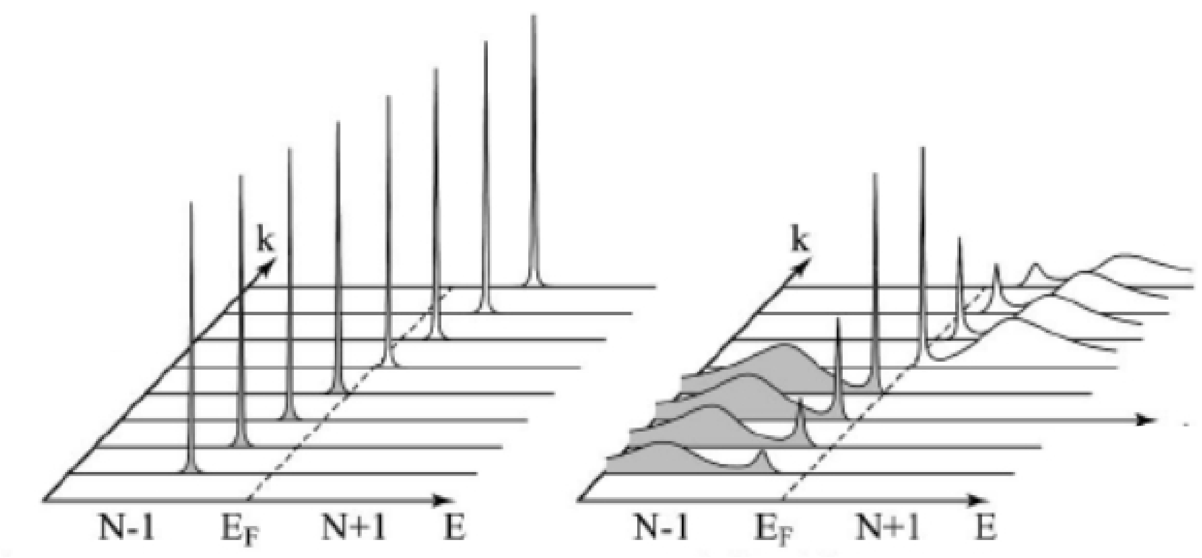






Dyson equation: $G=G_0 + G_0\,\Sigma\, G$

$A(\omega) \sim \mathrm{Im}[G(\omega)]$



From Damascelli et al., RMP 75, 473 (2003)

$V_H(12) = -i\delta(12)G(33^+)v_c(31)$

$\Sigma_x(12) = iG(12^+)v_c(21)$

$$\Sigma_{xc}(1,2) = \Sigma_x + iG(1\bar{3})\Xi(\bar{3},\bar{5};2,\bar{6})L(\bar{6}\bar{2};\bar{5}\bar{2})v_c(\bar{2},1) \qquad (1)$$

$$\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}') := -i\delta(\bar{3}\bar{3}')\delta(\bar{2}',\bar{2})v_c(\bar{3}\bar{2}) + \frac{\delta\Sigma_{xc}(\bar{3},\bar{3}')}{\delta G(\bar{2}',\bar{2})} \qquad (2)$$

Interaction = variation of “potential”

$$L(1,2,1',2') = L_0(1,2,1',2') + L_0(1,\bar{3}',1',\bar{3})\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}')L(\bar{2}',2,\bar{2},2') \qquad (3)$$

What does the system do (create e-h pairs....)

$$L_0(1,2,1',2') = G(1,2')G(2,1') \qquad (4)$$

$V_H(12) = -i\delta(12)G(33^+)v_c(31)$

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$$L_0(1,2,1',2') = G(1,2')G(2,1') \tag{4}$$

System does nothing: HF

Only classical part of Ξ: $L \rightarrow i\chi$, $\Sigma_{xc} \rightarrow iG(v_c + v_c\,\chi\,v_c) = iGW$

$V_H(12) = -i\delta(12)G(33^+)v_c(31)$ $\Sigma_x(12) = iG(12^+)v_c(21)$

$$\Sigma_{xc}(1,2) = \Sigma_x + iG(1\bar{3})\Xi(\bar{3},\bar{5};2,\bar{6})L(\bar{6}\bar{2};\bar{5}\bar{2})v_c(\bar{2},1) \qquad (1)$$

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Interaction = variation of “potential”

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What does the system do (create e-h pairs....)

$$L_0(1,2,1',2') = G(1,2$$

W consistently in RPA

System does nothing: HF

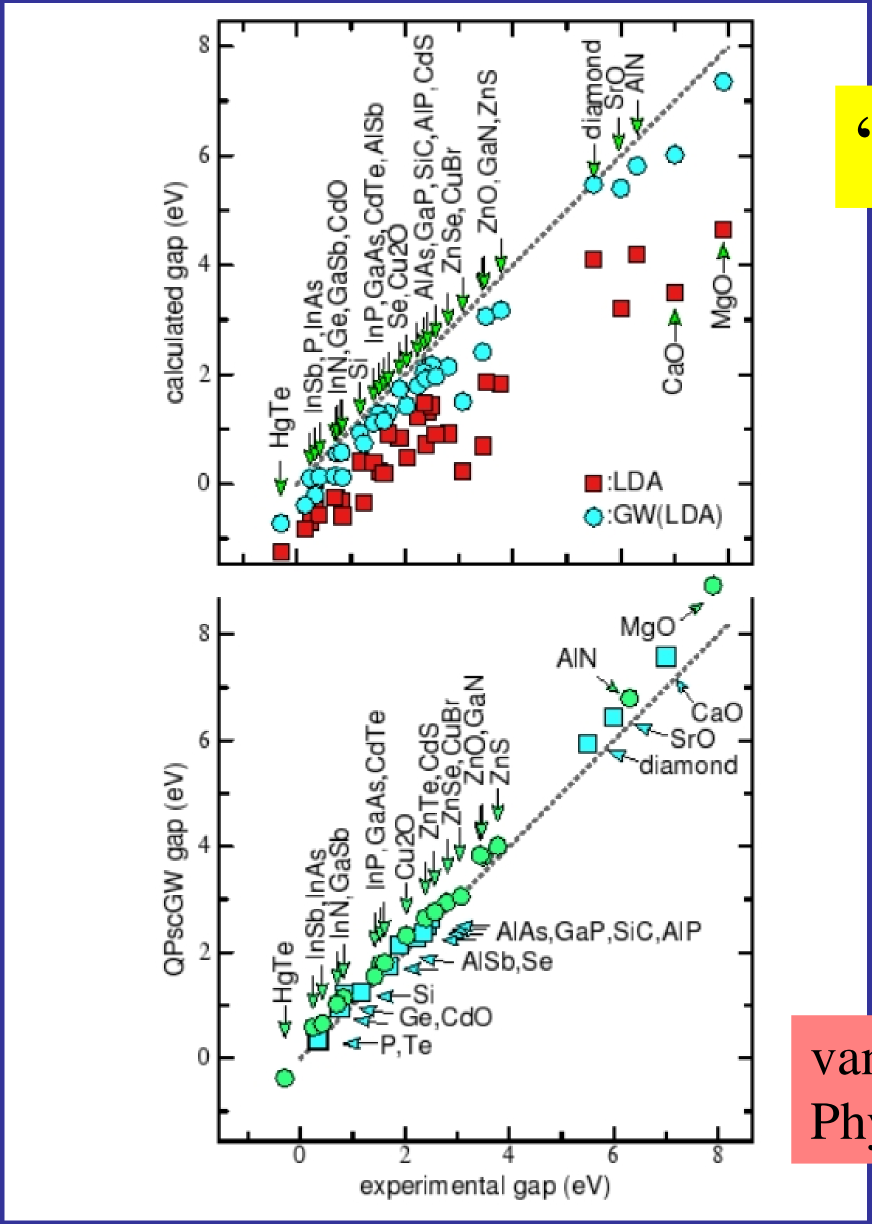
Only classical part of Ξ: $L \rightarrow i\chi$, $\Sigma_{xc} \rightarrow iG(v_c + v_c\,\chi\,v_c) = iGW$

RPA screening in GW?

→ self-consistent screening of Fock exchange

localization

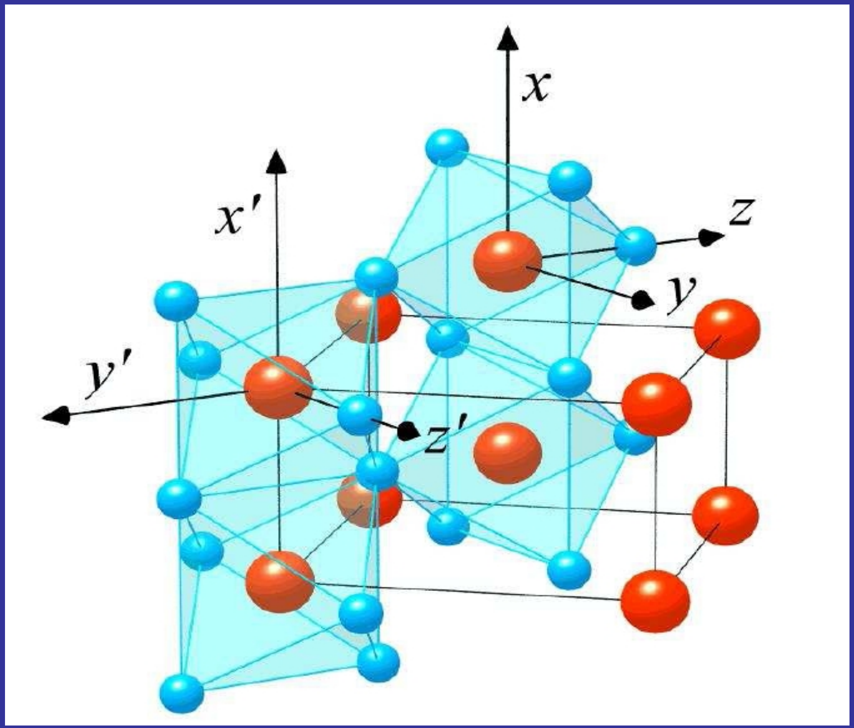
Improve QP energies and wavefunctions



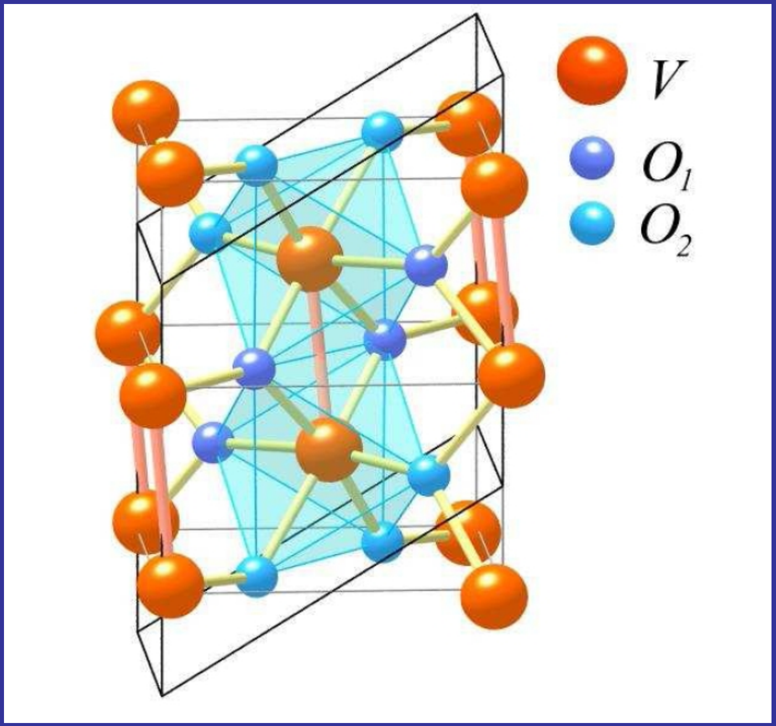
"RPA form" (bubble)

van Schilfgaarde, Kotani, Faleev,
Phys. Rev. Lett. 96, 226402 (2006)

Even qualitatively important - VO_2

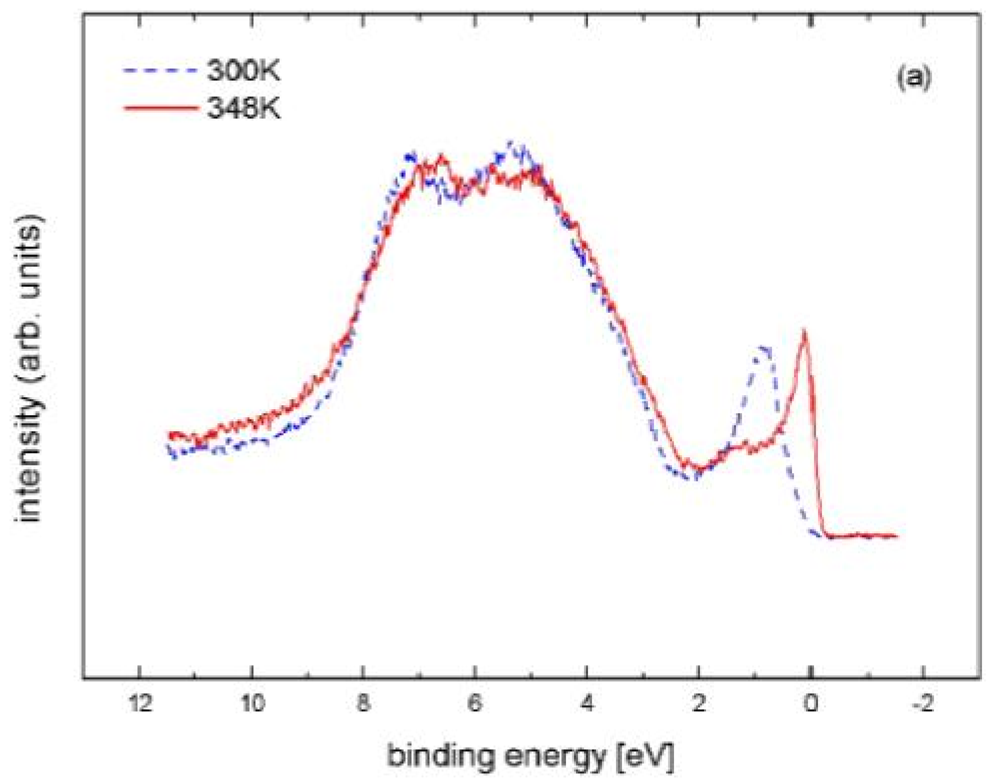


rutile

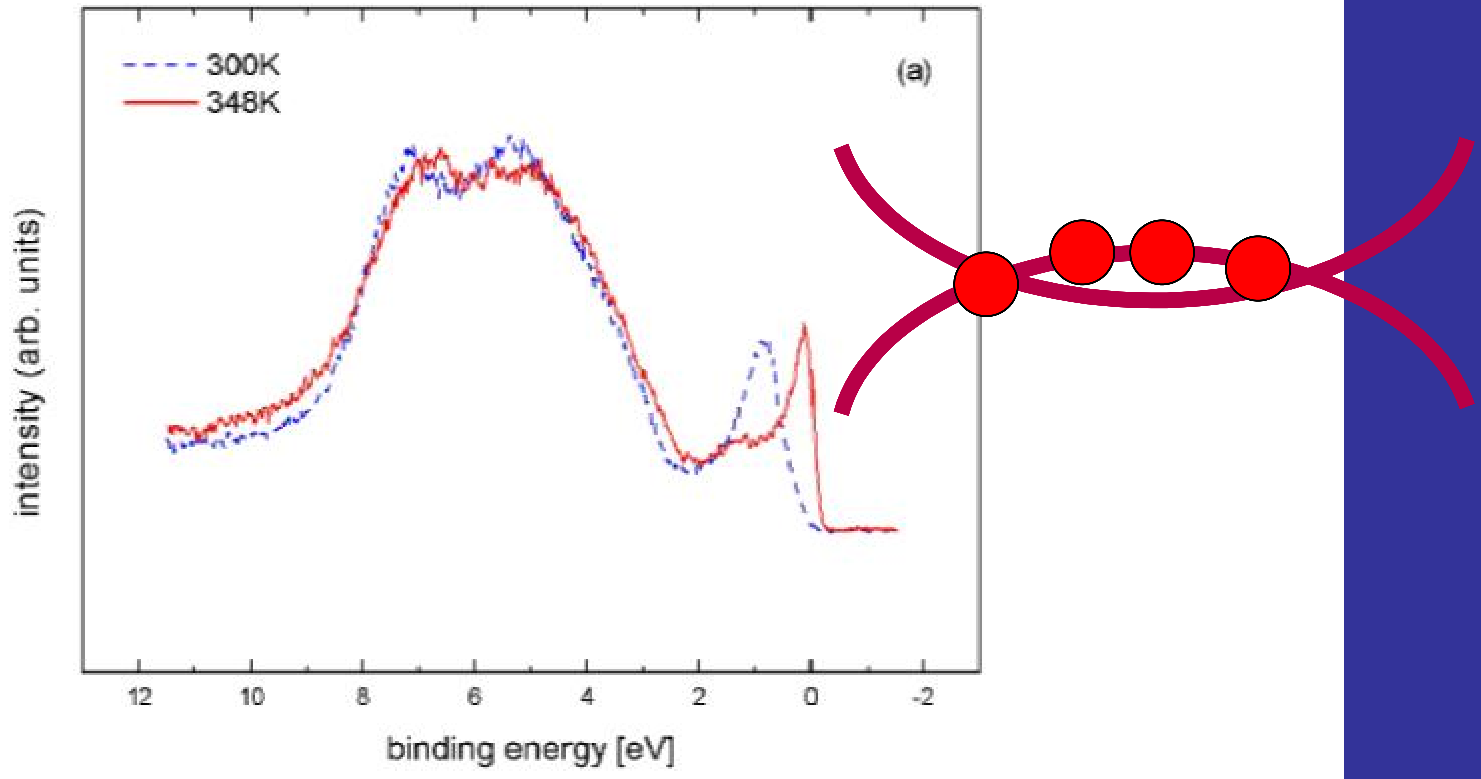


monoclinic

Matteo Gatti et al.



T. C. Koethe et al., Phys. Rev. Lett. 97, 116402 (2006).



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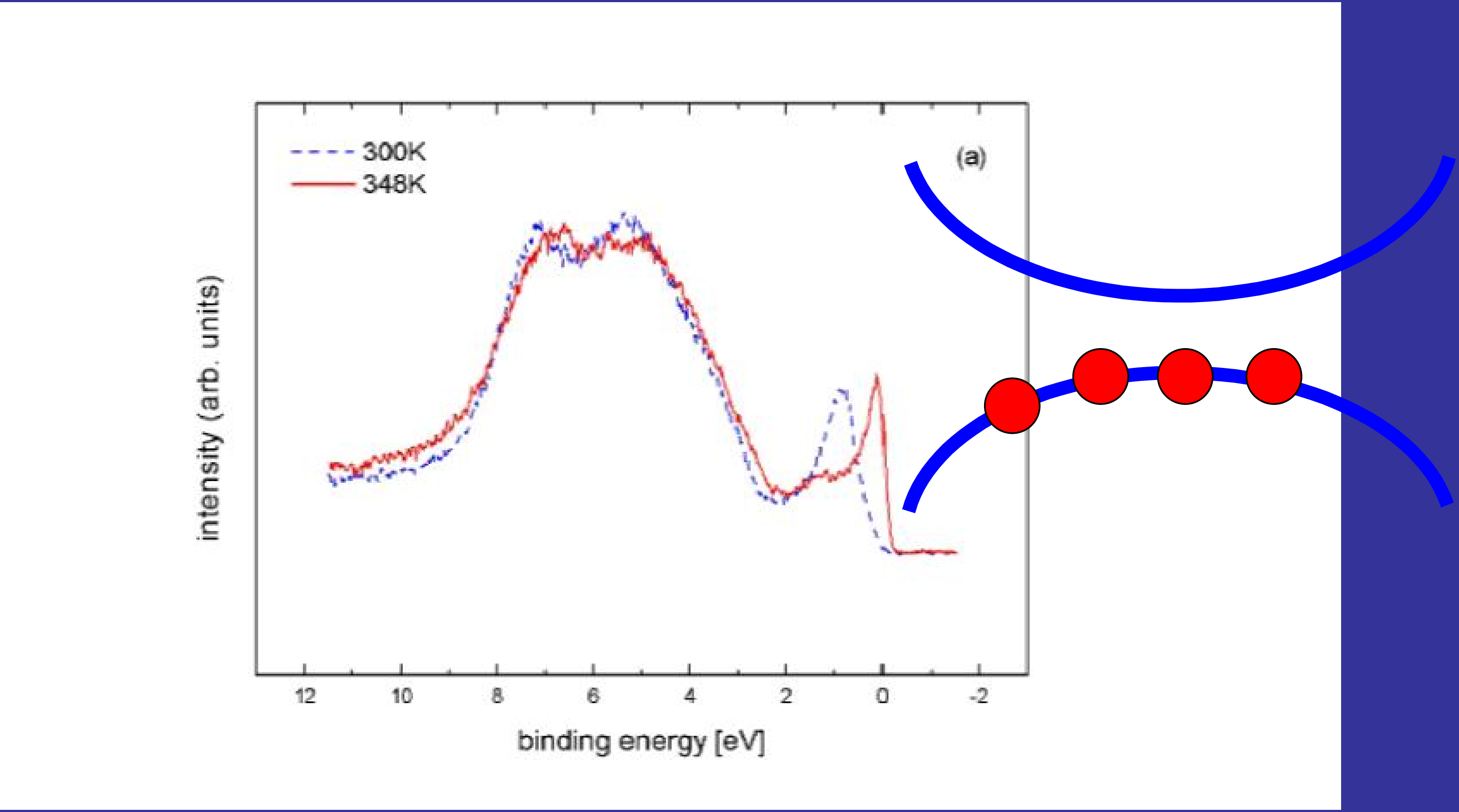
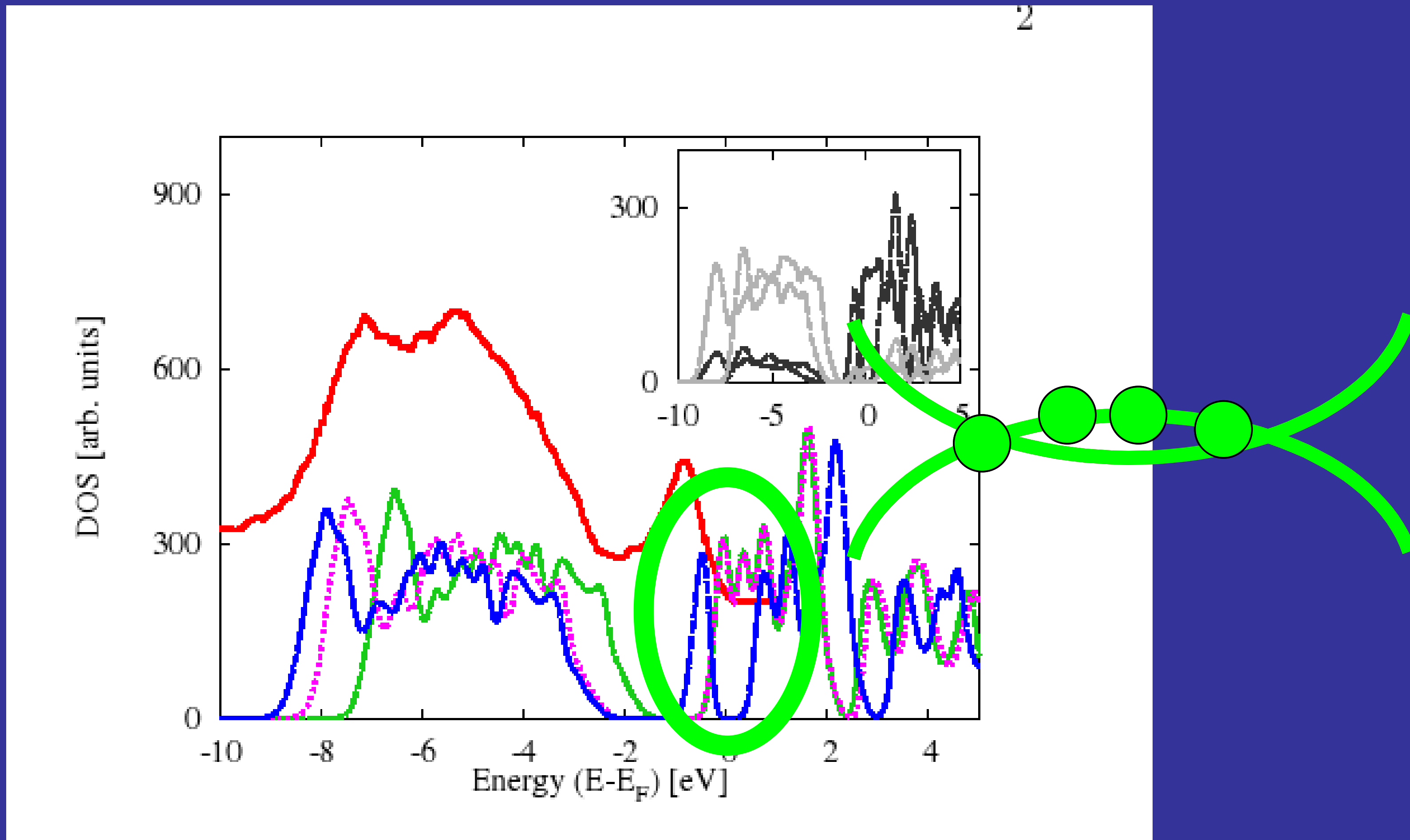


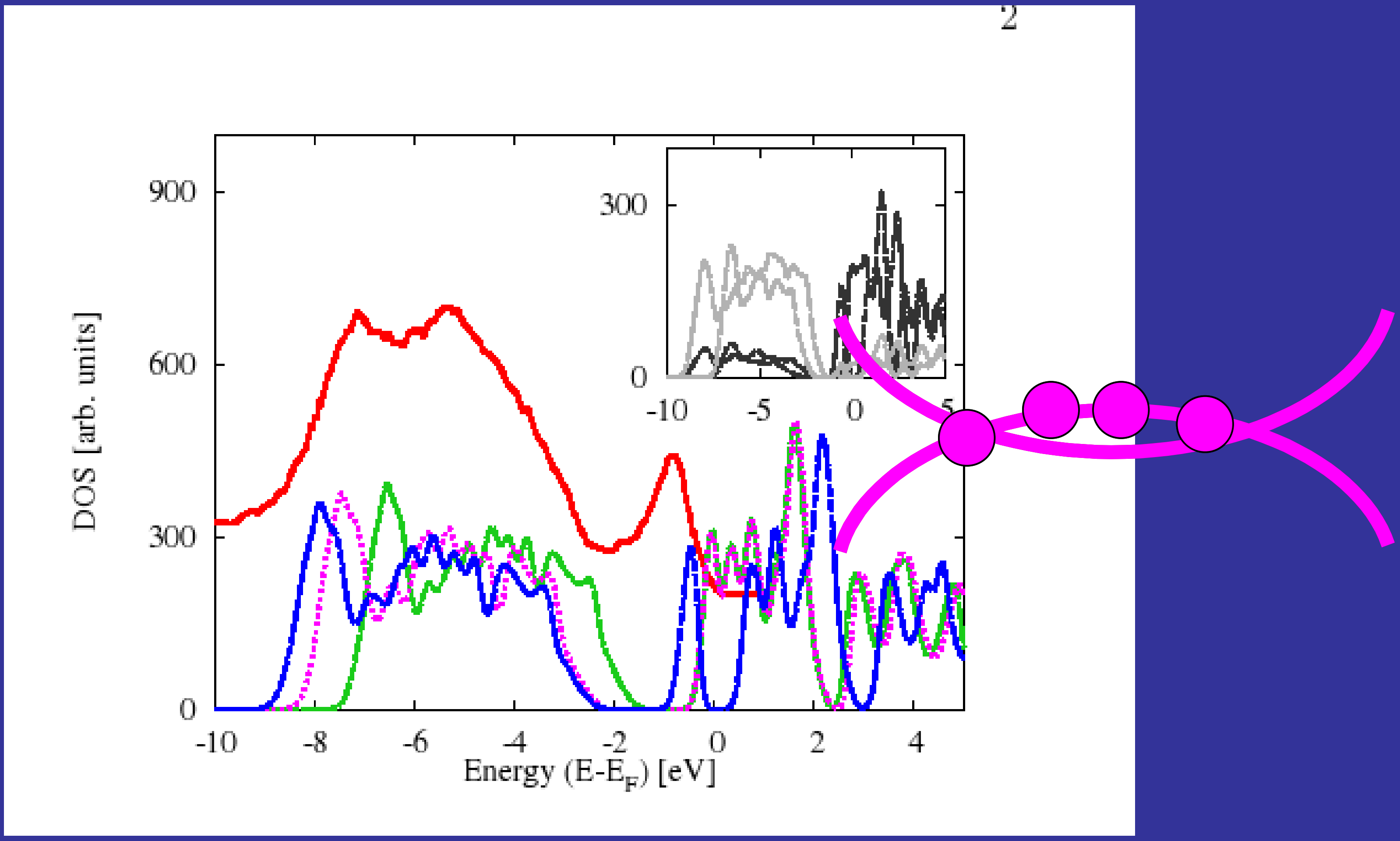
T. C. Koethe et al., Phys. Rev. Lett. 97, 116402 (2006).

LDA insulator → metal ....



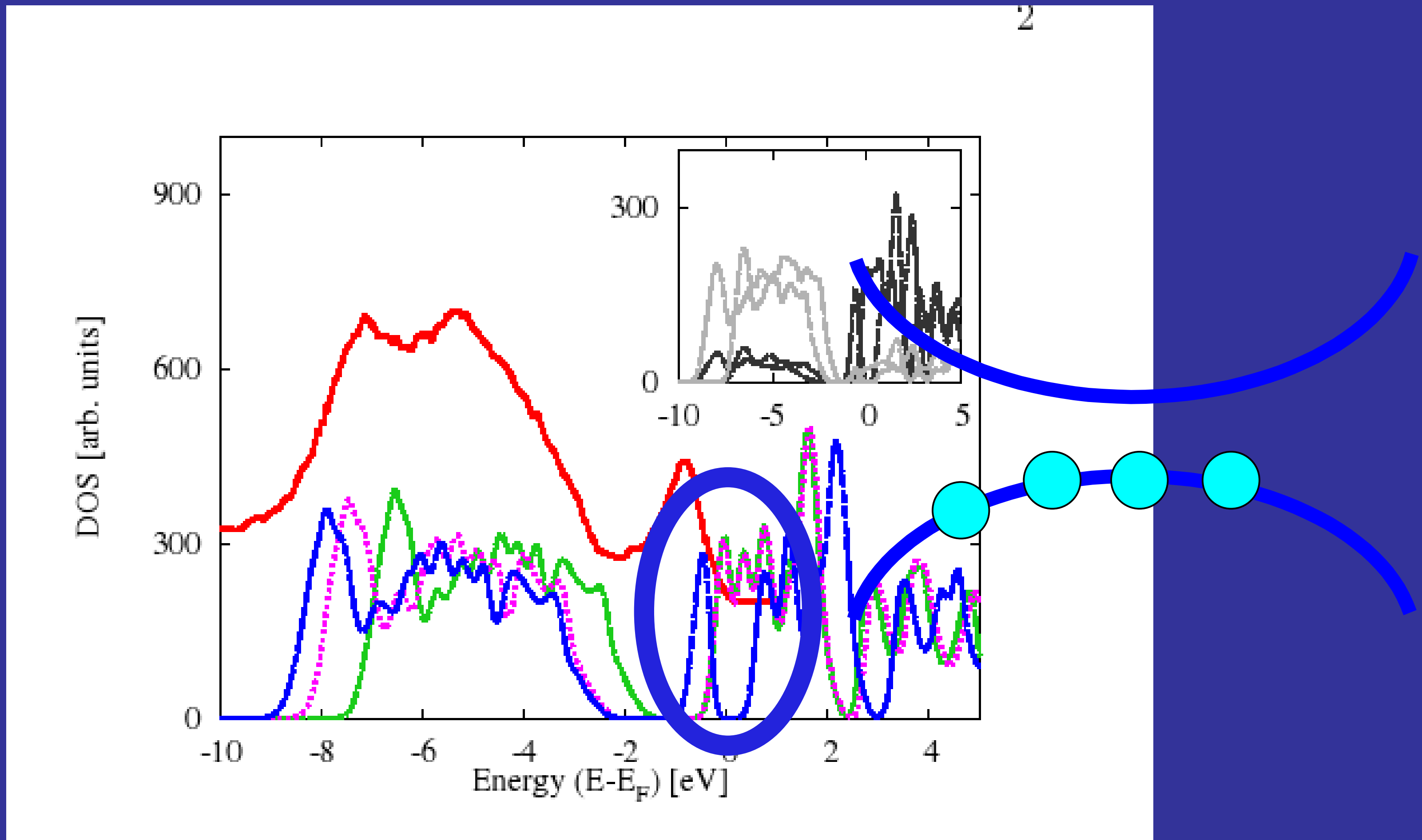
M. Gatti, F. Bruneval, V. Olevano and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007)

G_0W_0 insulator → metal !!!!!



M. Gatti, F. Bruneval, V. Olevano and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007)

sc GW insulator = insulator !!!



M. Gatti, F. Bruneval, V. Olevano and L. Reining,
Phys. Rev. Lett. **99**, 266402 (2007)

Away from the LDA starting point!

→ S. V. Faleev, M. van Schilfgaarde, and T. Kotani, PRL 93, 126406 (2004).

→ Bruneval, Vast, and Reining, Phys. Rev. B 74, 045102 (2006).*COHSEX*

→ T. Miyake et al., Phys. Rev. B 74, 245231 (2006).*LDA+U*

→ F. Fuchs, et al., Phys. Rev. B 76, 115109 (2007). *Hybrids*

→ Hong Jiang et al., , Phys. Rev. Lett. 102, 126403 (2009). *LDA+U*

→ P. Rinke et al., New J. Phys. 7, 126 (2005). *KS-EXX*

→ ....

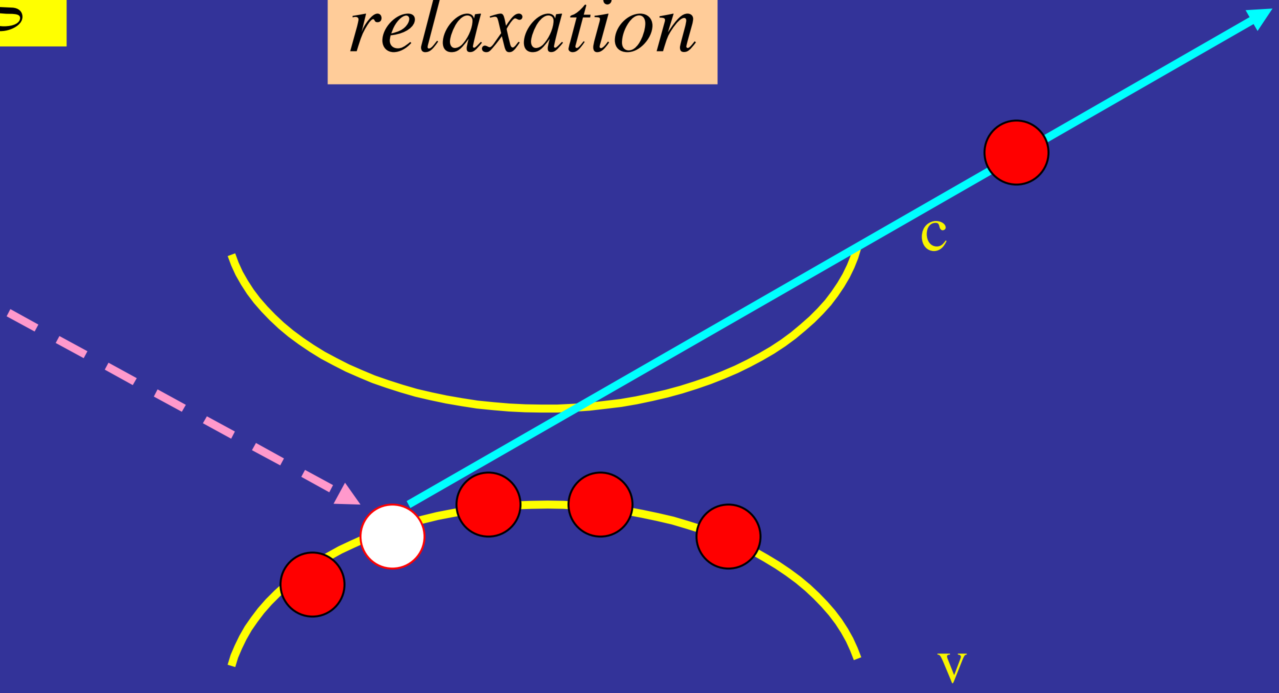
RPA: flexible screening

→ Fock exchange

localization

→ Screening

relaxation



...of practical importance: example photovoltaics

Quasiparticle energies within sc-GW for CIS

$CuInS_2$

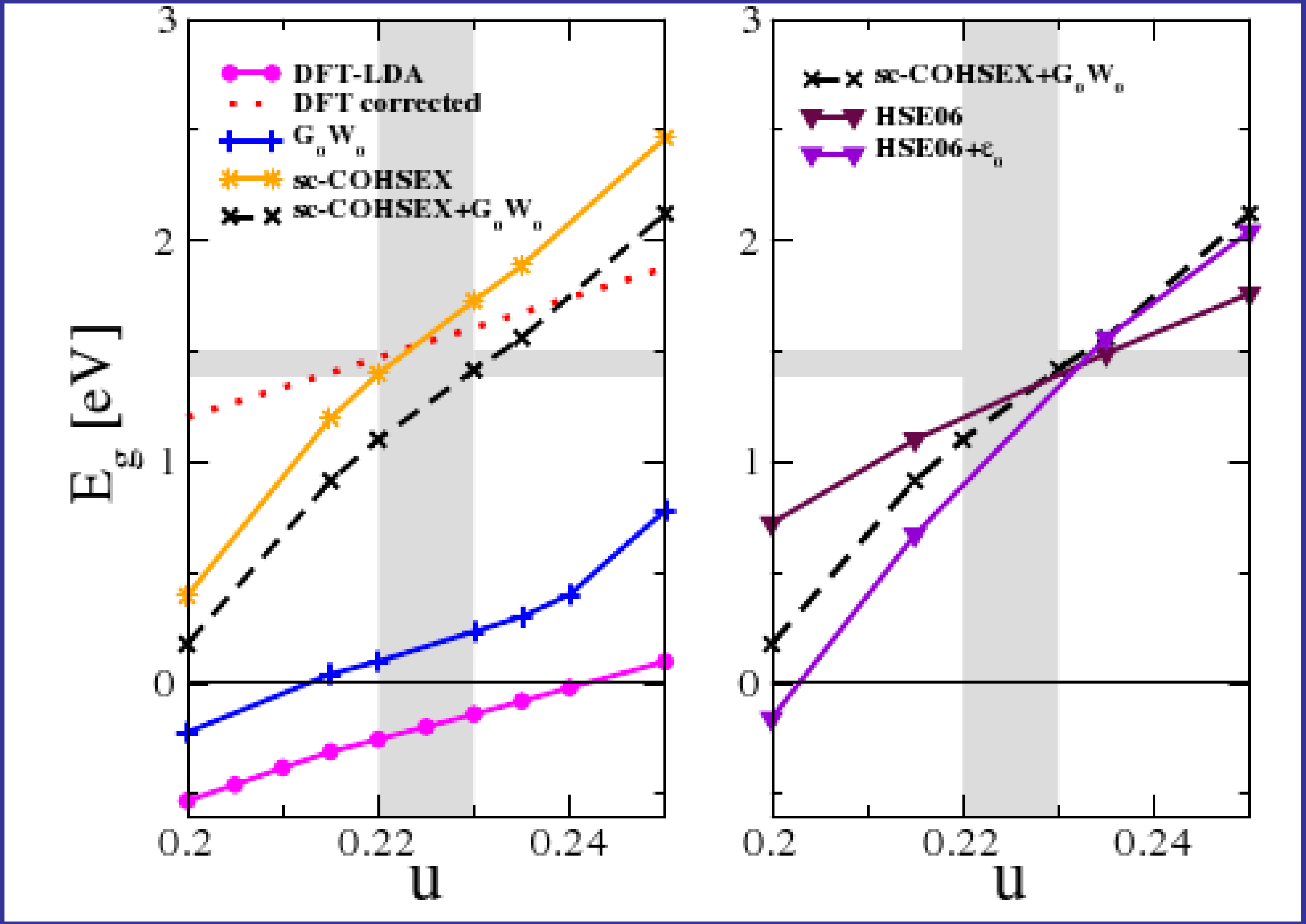
	DFT-LDA	G_0W_0	sc-GW	exp.
E_g	-0.11	0.28	1.48	1.54
In-(S,Se)	6.5	6.9	7.0	6.9
(Se,S) s band	12.4	13.0	13.6	12.0
In 4 d band	14.6	16.4	18.2	18.2

$CuInSe_2$

	DFT-LDA	G_0W_0	sc-GW	exp.
E_g	-0.29	0.25	1.14	1.05 (+0.2)
In-(S,Se)	5.8	6.15	6.64	6.5
(Se,S) s band	12.6	12.9	13.6	13.0
In 4 d band	14.7	16.2	17.8	18.0

J. Vidal et al., PRL in press (2010)

Bandgaps in function of structure (Cu-S)



Hybrids ~ approximate GW with almost fixed screening

RPA: dynamical screening

→ Fock exchange

→ Screening

→ Screening (dynamical)

W(ω) leads to imaginary part

$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_i \frac{f^i(\mathbf{r})f^{i*}(\mathbf{r}')}{\omega - \varepsilon_i} \tag{1}$$

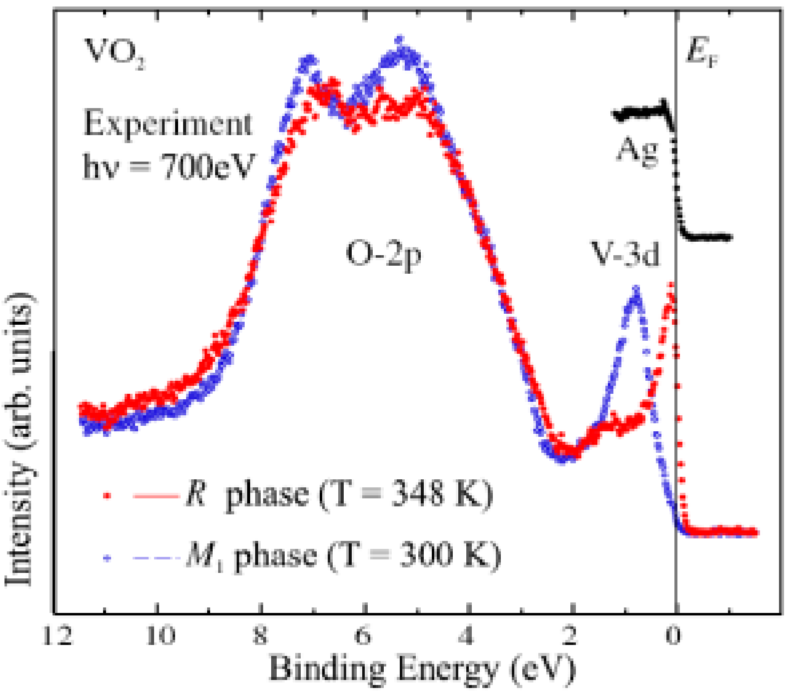
$$W(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{|\mathbf{r}-\mathbf{r}'|} + \sum_s \frac{2\omega_s V^s(\mathbf{r})V^s(\mathbf{r}')}{\omega^2 - \omega_s^2}, \tag{2}$$

$$\langle k|\Sigma_c|k\rangle = \sum_{i,s\neq 0} \frac{|V_{ki}^s|^2}{\omega - \omega_s sgn(\mu - \varepsilon_i) - \varepsilon_i} \tag{3}$$

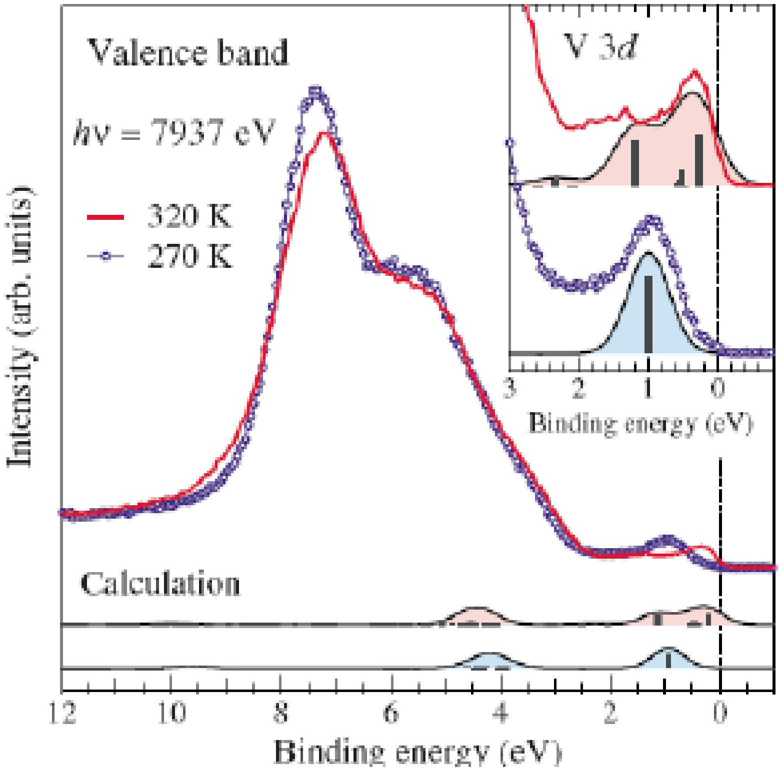
$$A_k(\omega) = \frac{1}{\pi}|ImG_{kk}(\omega)| = \frac{1}{\pi}\frac{|Im\Sigma_{kk}(\omega)|}{(\omega - \varepsilon_k - Re\Sigma_{kk}(\omega))^2 + (Im\Sigma_{kk}(\omega))^2} \tag{4}$$

Broadening (lifetime), satellites

Photoemission spectra

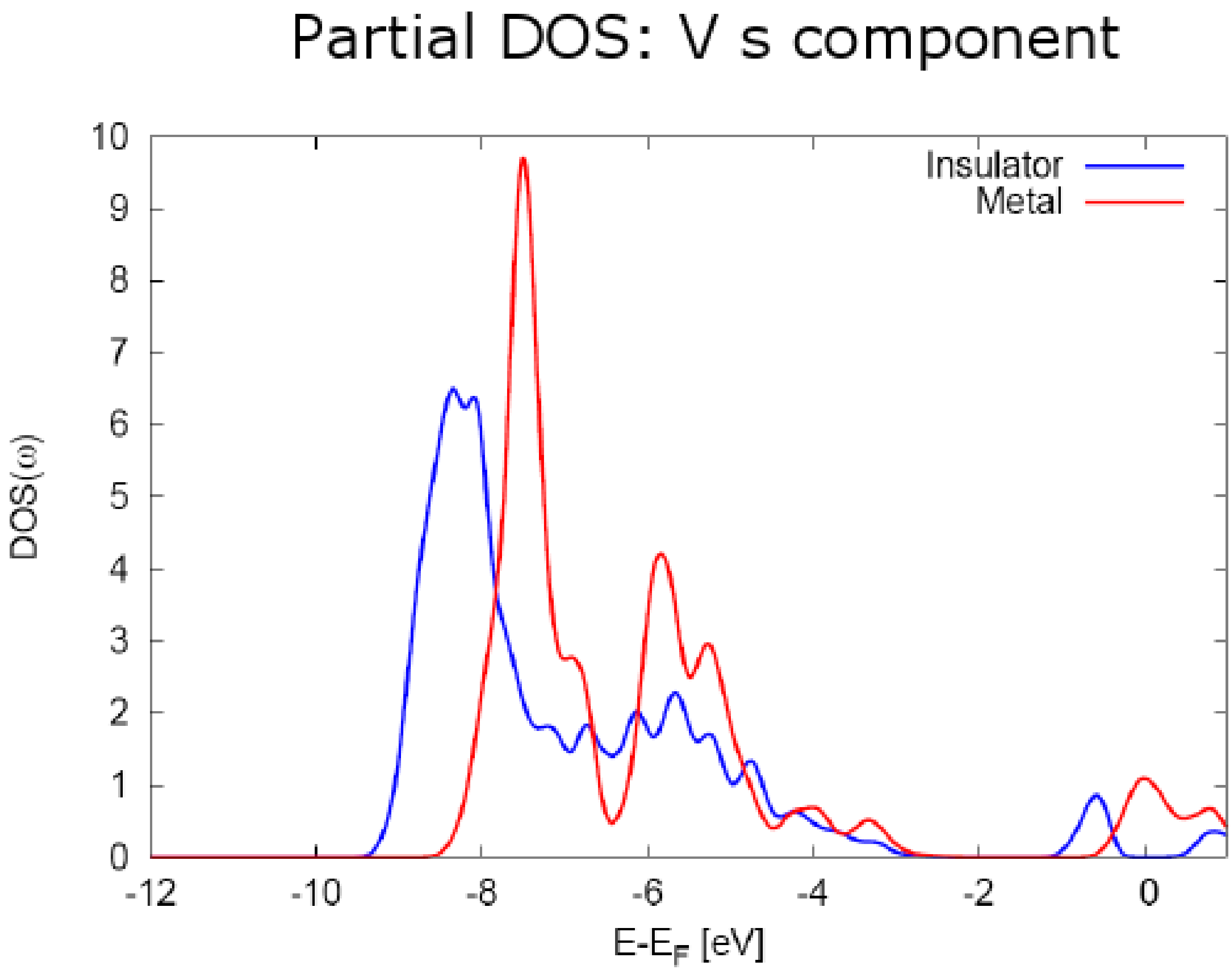


From: Koethe *et al*. PRL 97 (2006)

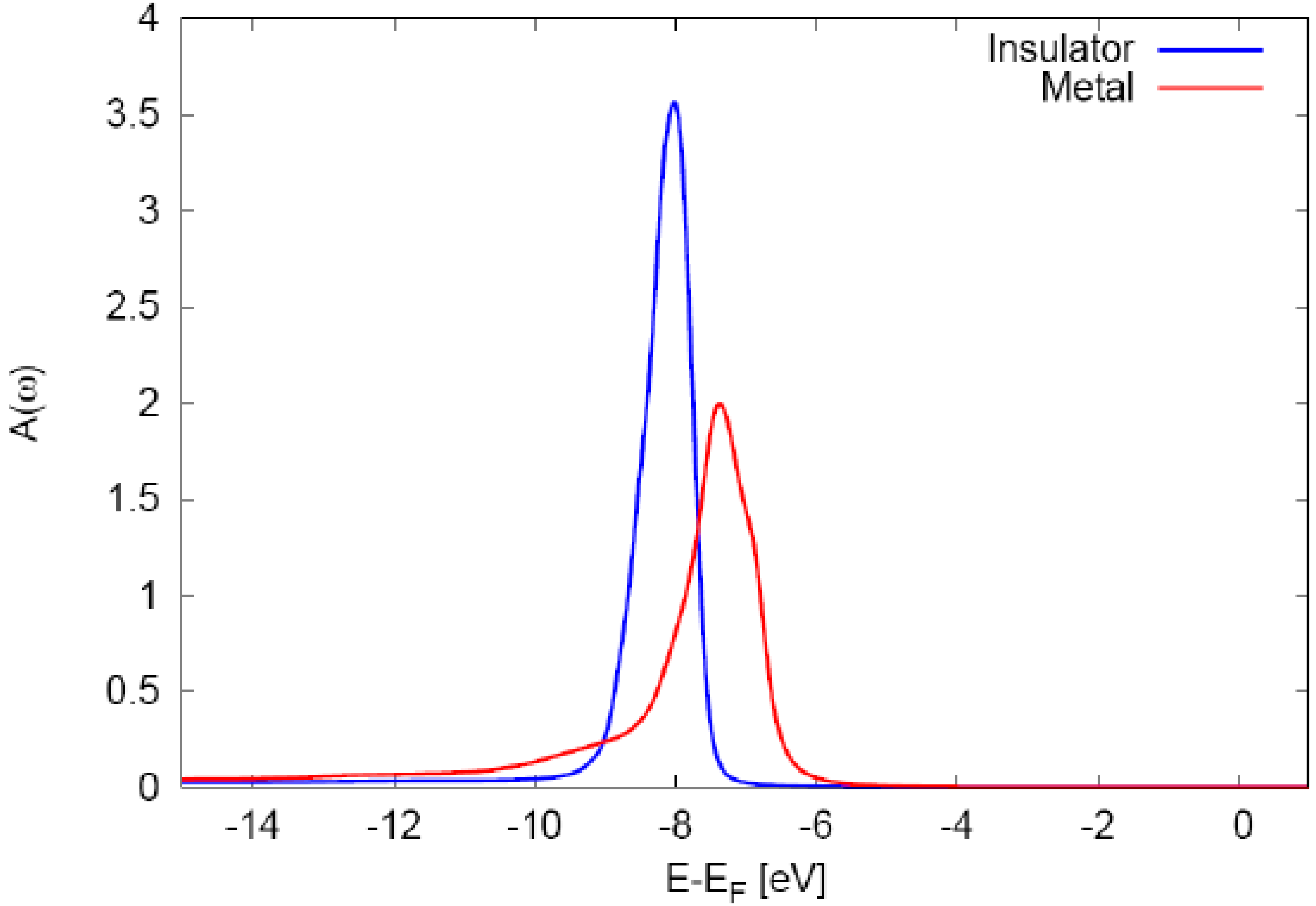


From: Eguchi *et al*. PRB 78 (2008)

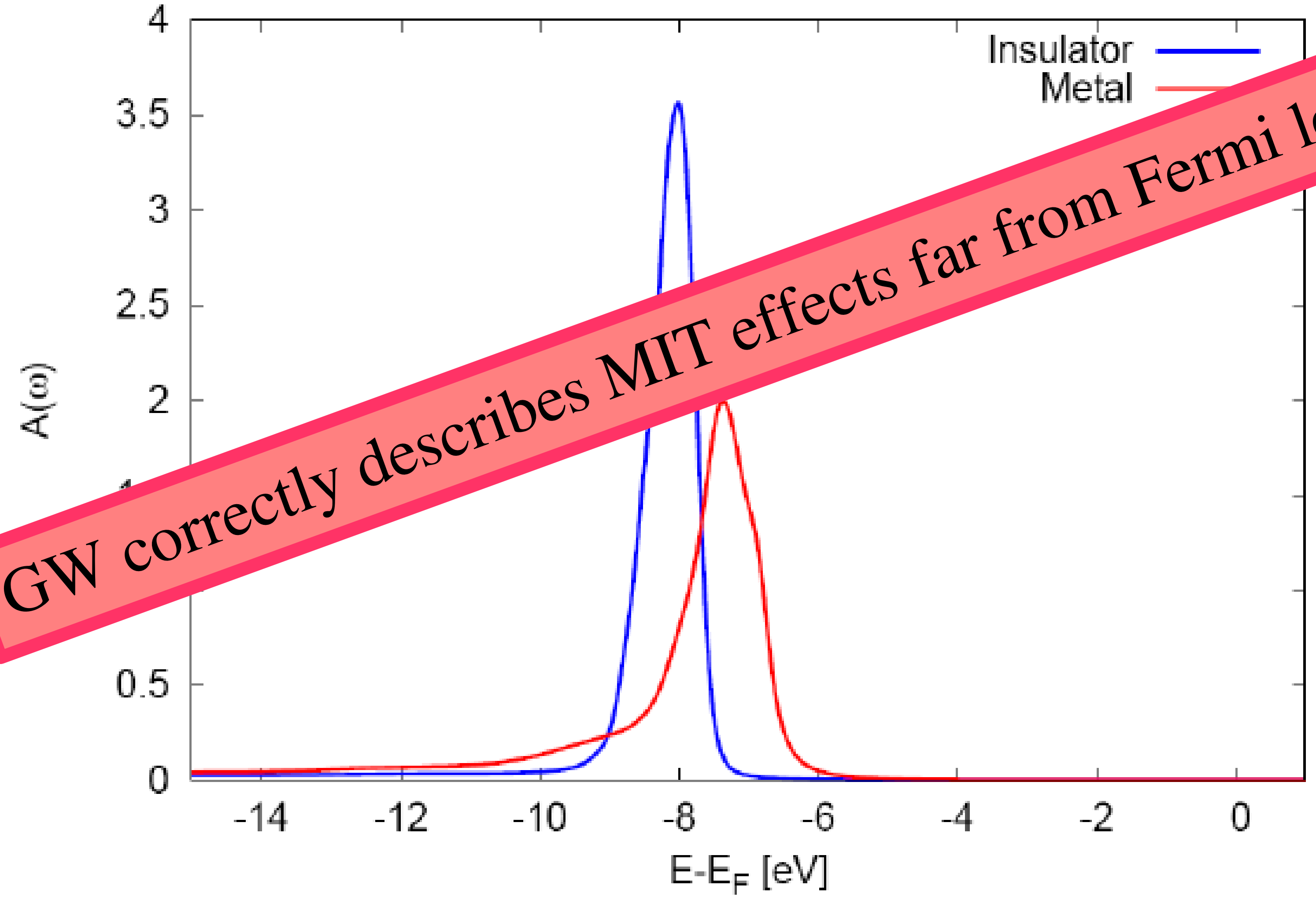
Identification of the peak: partial DOS



GW spectral function



GW spectral function



GW correctly describes MIT effects far from Fermi level

VOLUME 89, NUMBER 9 PHYSICAL REVIEW LETTERS 26 AUGUST 2002

Role of Surface Plasmons in the Decay of Image-Potential States on Silver Surfaces

A. García-Lekue,[1] J. M. Pitarke,[1,2] E. V. Chulkov,[2,3] A. Liebsch,[4] and P. M. Echenique[2,3]

PHYSICAL REVIEW B **76**, 195116 (2007)

Many-pole model of inelastic losses in x-ray absorption spectra

J. J. Kas,[1] A. P. Sorini,[1] M. P. Prange,[1] L. W. Cambell,[2] J. A. Soininen,[3] and J. J. Rehr[1]

VOLUME 87, NUMBER 24 PHYSICAL REVIEW LETTERS 10 DECEMBER 2001

Anomalous Quasiparticle Lifetime in Graphite: Band Structure Effects

Catalin D. Spataru,[1,2] Miguel A. Cazalilla,[3] Angel Rubio,[4,5] Lorin X. Benedict,[6]

W(ω) leads to structured imaginary part

$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_i \frac{f^i(\mathbf{r})f^{i*}(\mathbf{r}')}{\omega - \varepsilon_i} \tag{1}$$

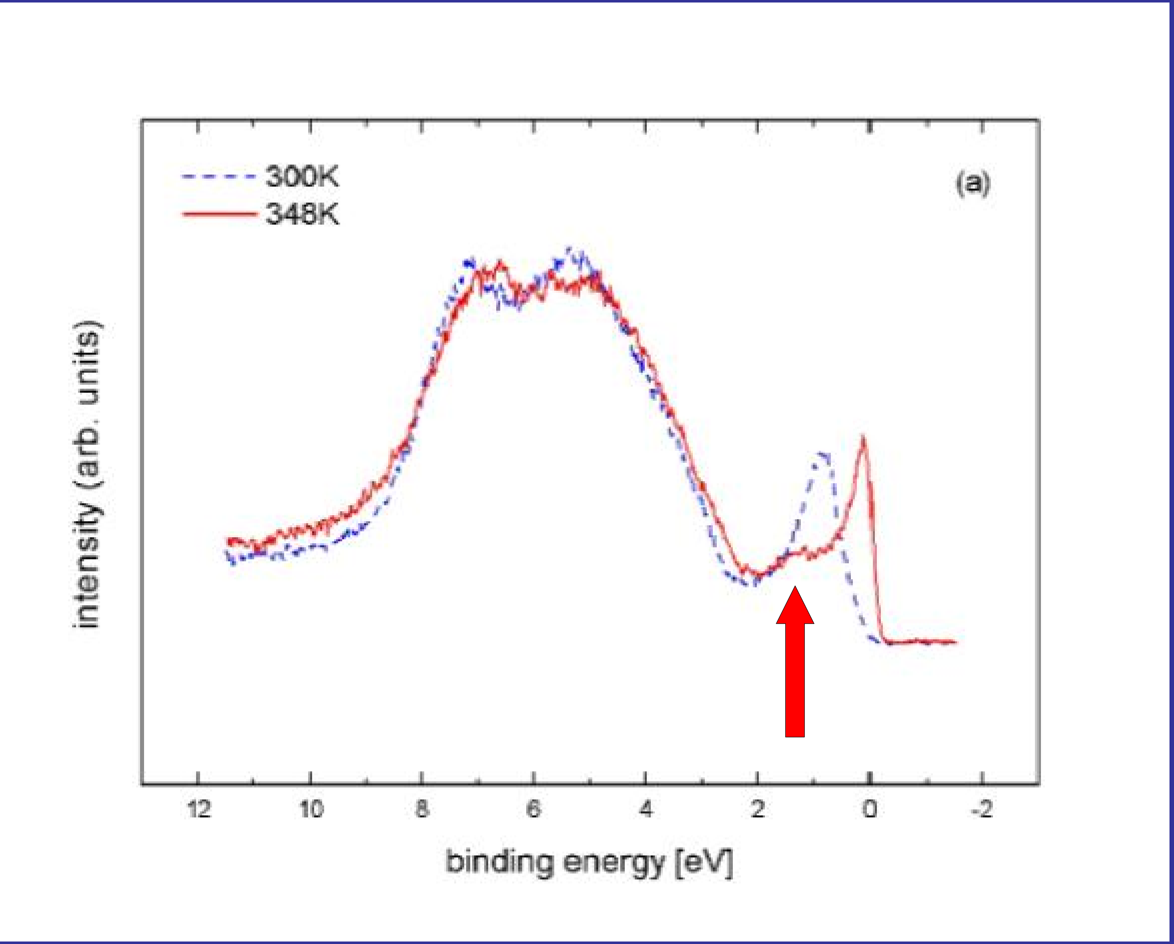
$$W(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{|\mathbf{r}-\mathbf{r}'|} + \sum_s \frac{2\omega_s V^s(\mathbf{r})V^s(\mathbf{r}')}{\omega^2 - \omega_s^2}, \tag{2}$$

$$\langle k|\Sigma_c|k\rangle = \sum_{i,s\neq 0} \frac{|V_{ki}^s|^2}{\omega - \omega_s sgn(\mu - \varepsilon_i) - \varepsilon_i} \tag{3}$$

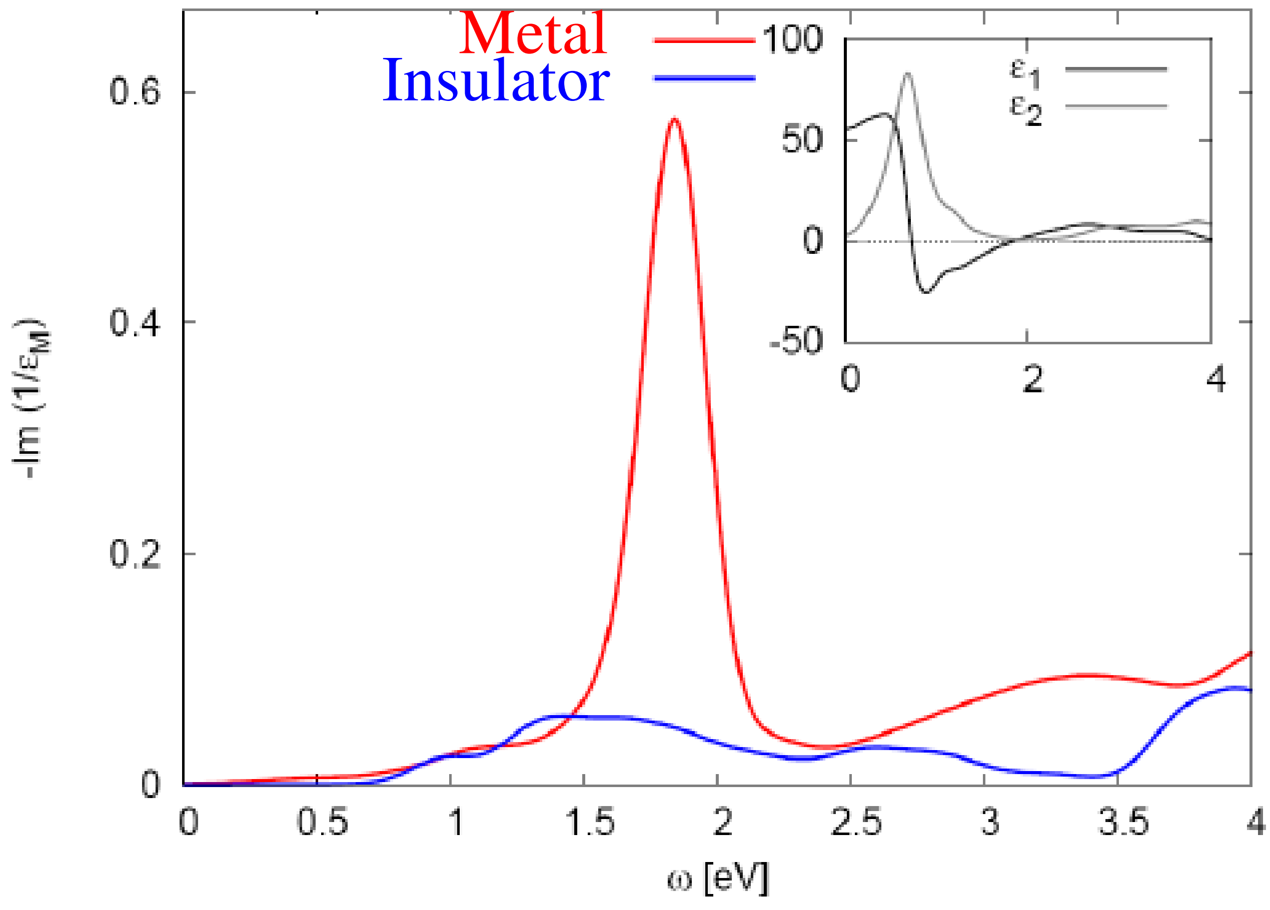
$$A_k(\omega) = \frac{1}{\pi}|ImG_{kk}(\omega)| = \frac{1}{\pi}\frac{|Im\Sigma_{kk}(\omega)|}{(\omega - \varepsilon_k - Re\Sigma_{kk}(\omega))^2 + (Im\Sigma_{kk}(\omega))^2} \tag{4}$$

Broadening (lifetime), satellites

VO_2

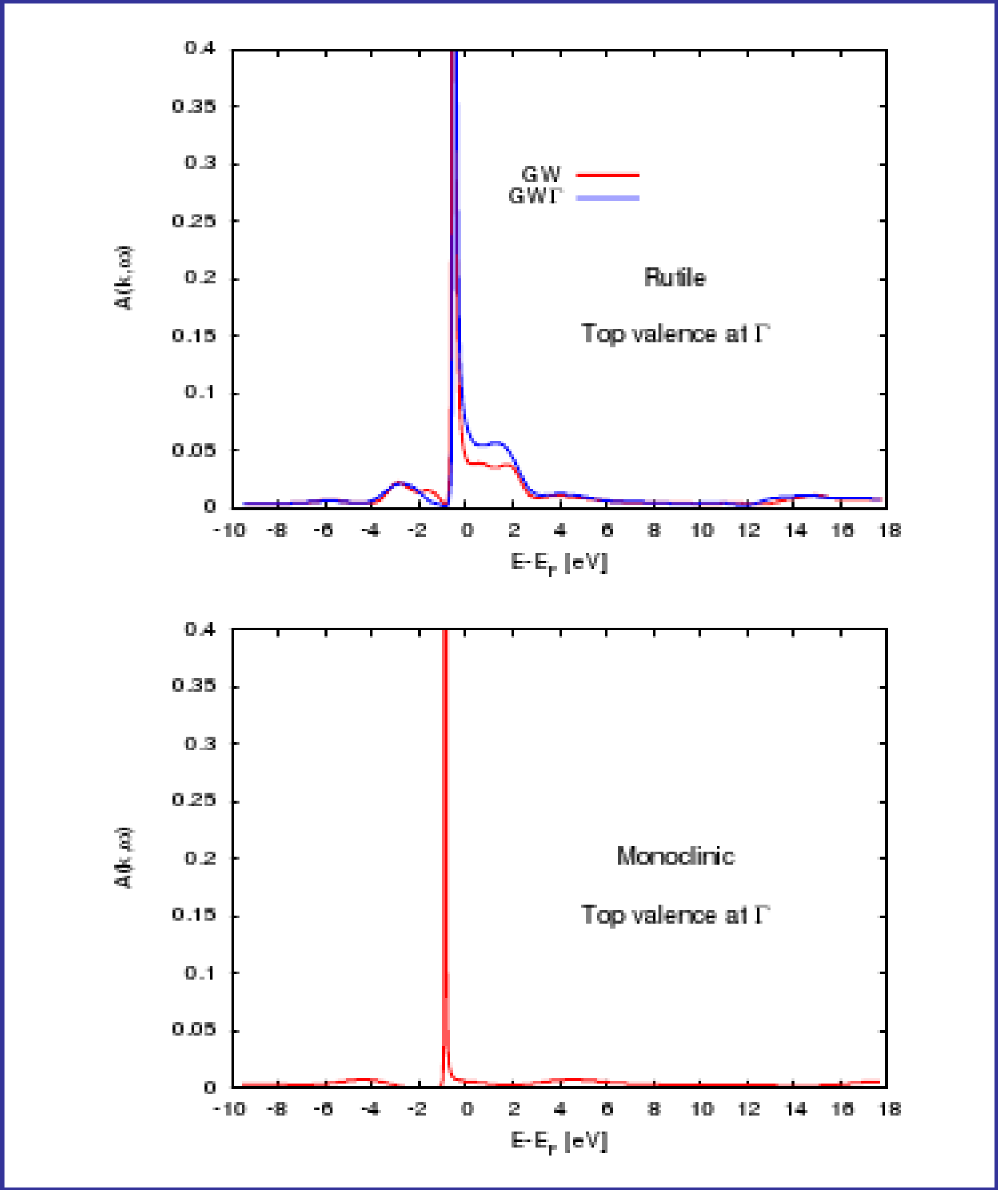


T. C. Koethe et al., Phys. Rev. Lett. 97, 116402 (2006).

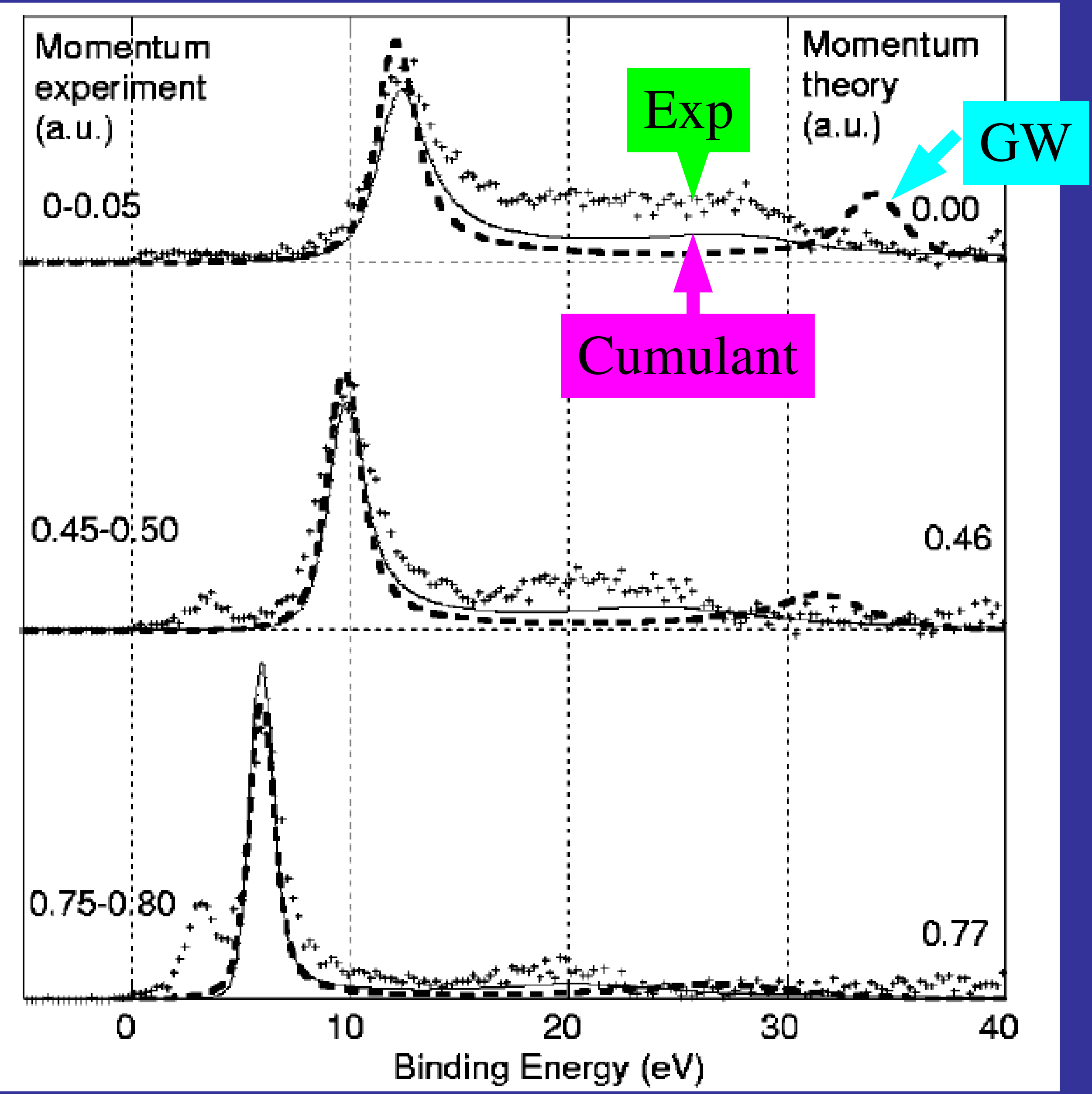


(small finite q)

see also Exp.: Abe *et al.* Jpn. J. Appl. Phys (1997)


GW
GWΓ
Rutile
Top valence at Γ
A(k, ω)
E-E$_F$ [eV]
Monoclinic
Top valence at Γ
A(k, ω)
E-E$_F$ [eV]

Silicon



Kheifets, Sashin, Vos, Weigold, Aryasetiawan, PRB 68, 233205 (2003)

Satellites qualitative.

But coupling to excitations overall important

→ renormalizes energies

→ explains lifetimes

→ gives rise to van der Waals

e.g. Garcia Gonzalez + Godby, PRL 88, 056406 (2002)

→ distorts bands

e.g. Trevisanutto et al., PRL 101, 226405 (2008);
Park et al., PRL 102, 076803 (2009)

→ can be generalized (e.g. phonons)

e.g. A. Marini, PRL 101,106405 (2008)

e.g. Eiguren + Ambrosch Draxl, PRL 101, 036402 (2008)

Is there anything **BAD** about the RPA W in GW?

→ Fock exchange

→ Screening

→ Screening (dynamical)

→ Widely valid and efficient

→ Room for speedup

$$\Sigma_{xc}(1,2) = \Sigma_x + iG(1\bar{3})\Xi(\bar{3},\bar{5};2,\bar{6})L(\bar{6}\bar{2};\bar{5}\bar{2})v_c(\bar{2},1) \quad (1)$$

$$\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}') := -i\delta(\bar{3}\bar{3}')\delta(\bar{2}',\bar{2})v_c(\bar{3}\bar{2}) + \frac{\delta\Sigma_{xc}(\bar{3},\bar{3}')}{\delta G(\bar{2}',\bar{2})} \quad (2)$$

Interaction = variation of "potential"

$$L(1,2,1',2') = L_0(1,2,1',2') + L_0(1,\bar{3}',1',\bar{3})\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}')L(\bar{2}',2,\bar{2},2') \quad (3)$$

What does the system do (create e-h pairs....)

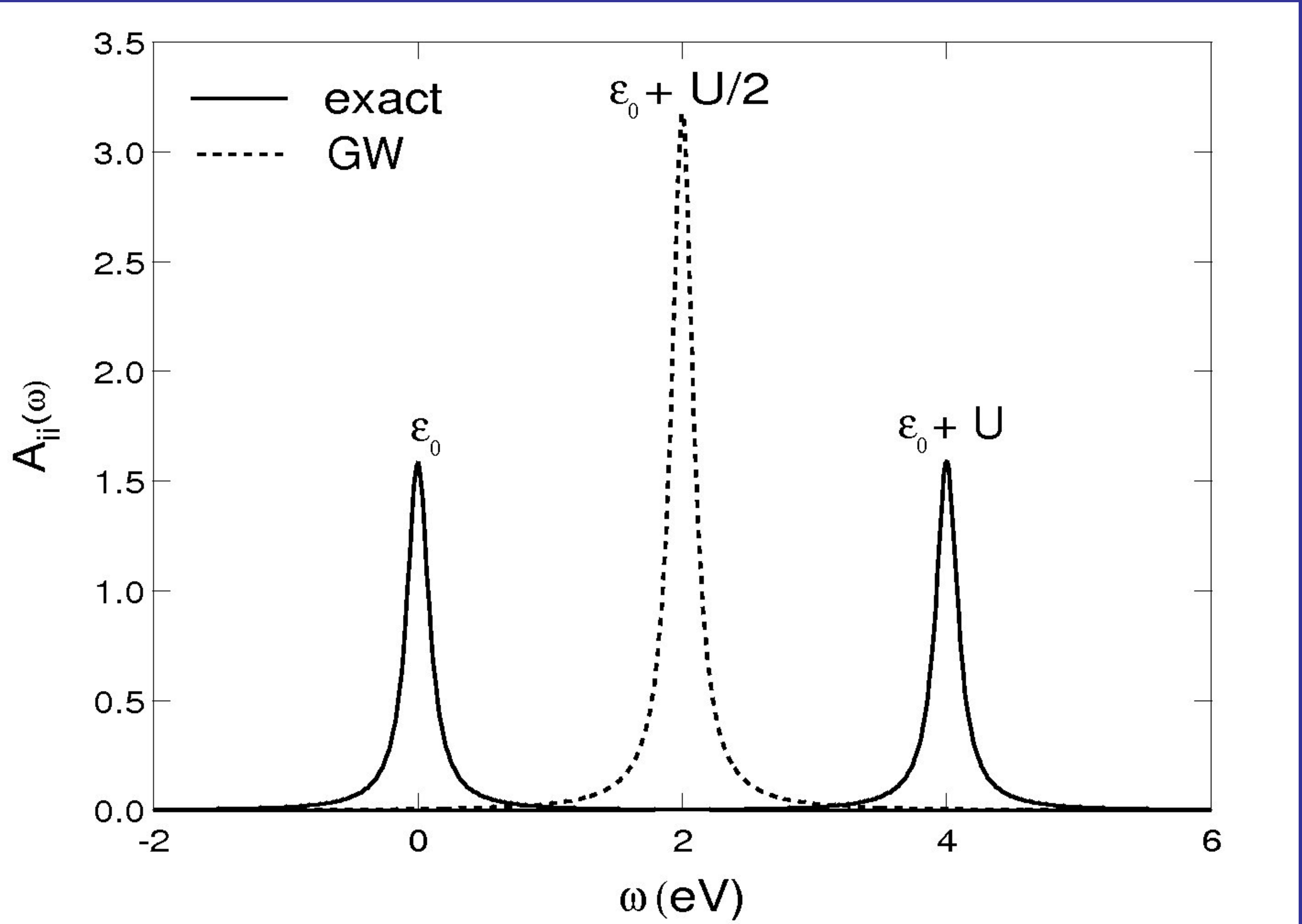
$$L_0(1,2,1',2') = G(1,2')G(2,1') \quad (4)$$

System does nothing: HF

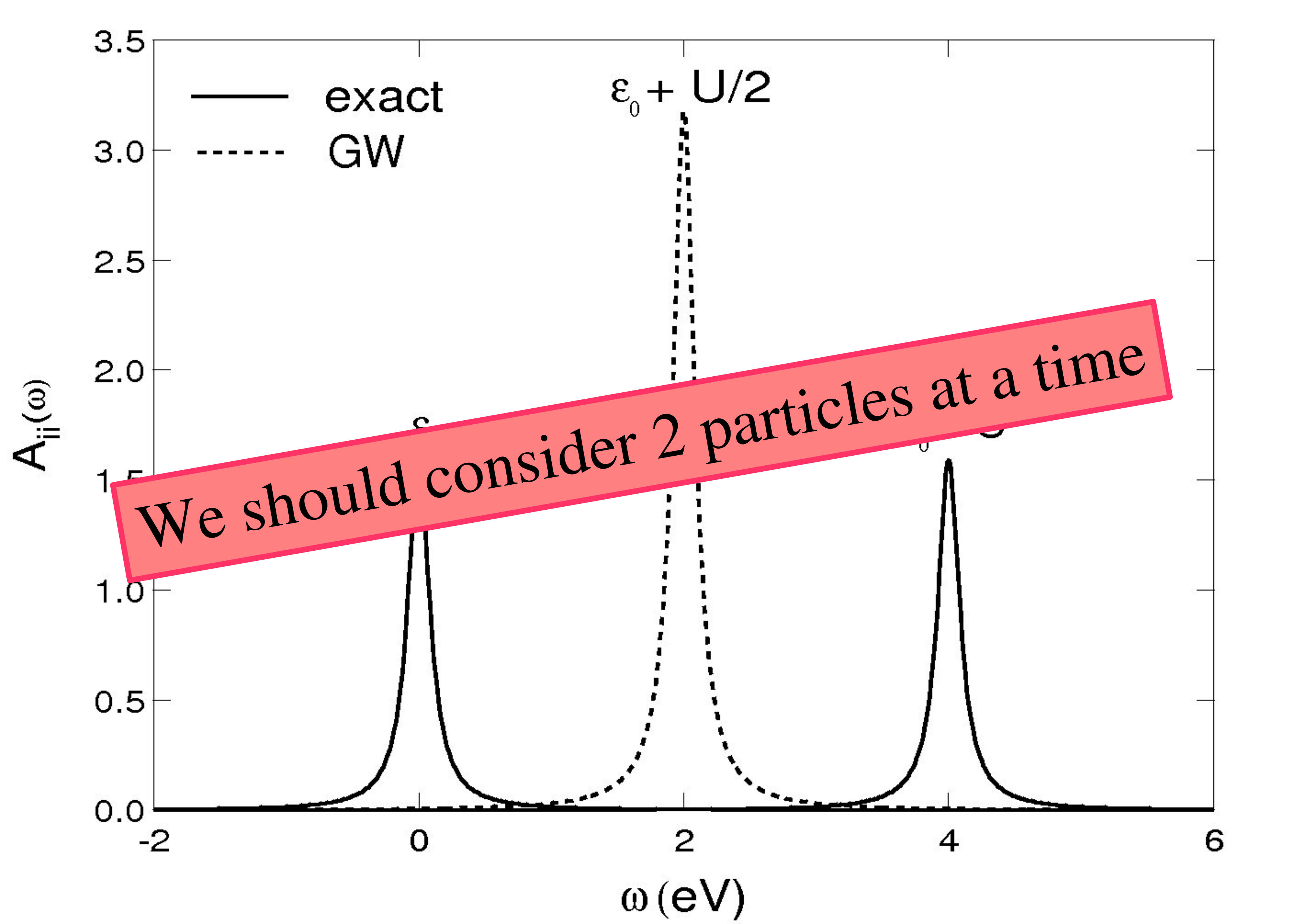
Only classical part of Ξ: $L \rightarrow i\chi$, $\Sigma_{xc} \rightarrow iGW$

Additional particle interacts in a classical way

2 site 1 electron Hubbard model; P. Romaniello et al. JPC 2009



2 site 1 electron Hubbard model; P. Romaniello et al. JPC 2009



$$\Sigma_{xc}(1,2) = \Sigma_x + iG(1\bar{3})\Xi(\bar{3},\bar{5};2,\bar{6})L(\bar{6}\bar{2};\bar{5}\bar{2})v_c(\bar{2},1) \tag{1}$$

$$\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}') := -i\delta(\bar{3}\bar{3}')\delta(\bar{2}',\bar{2})v_c(\bar{3}\bar{2}) + \frac{\delta\Sigma_{xc}(\bar{3},\bar{3}')}{\delta G(\bar{2}',\bar{2})} \tag{2}$$

Interaction = variation of “potential”

$$L(1,2,1',2') = L_0(1,2,1',2') + L_0(1,\bar{3}',1',\bar{3})\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}')L(\bar{2}',2,\bar{2},2') \tag{3}$$

What does the system do (create e-h pairs….)

$$L_0(1,2,1',2') = G(1,2')G(2,1') \tag{4}$$

System does nothing: HF

Only classical part of Ξ: L→iχ, Σ_{xc}→ iGW

Better Ξ: e.g. T-matrix approach

We are used to solve 2-particle equations: BSE

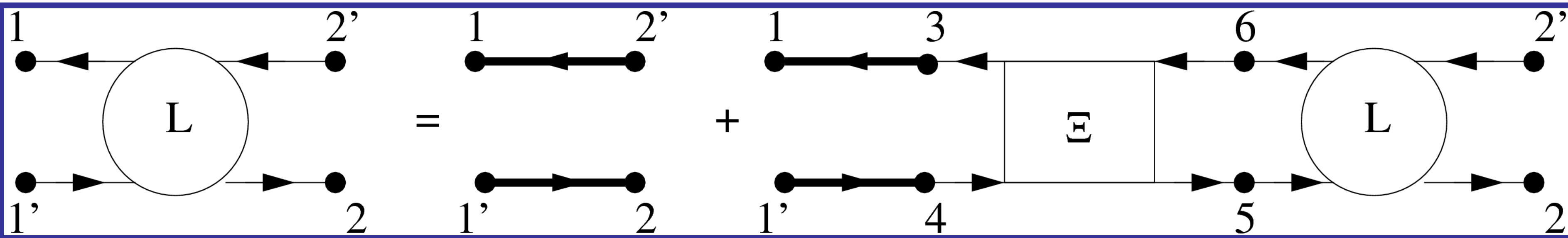
$$\Sigma_{xc}(1,2) = \Sigma_x + iG(1\bar{3})\Xi(\bar{3},\bar{5};2,\bar{6})L(\bar{6}\bar{2};\bar{5}\bar{2})v_c(1,\bar{2}) \quad (1)$$

$$\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}') := -i\delta(\bar{3}\bar{3}')\delta(\bar{2}',\bar{2})v_c(\bar{3}\bar{2}) + \frac{\delta\Sigma_{xc}(\bar{3},\bar{3}')}{\delta G(\bar{2}',\bar{2})} \quad (2)$$

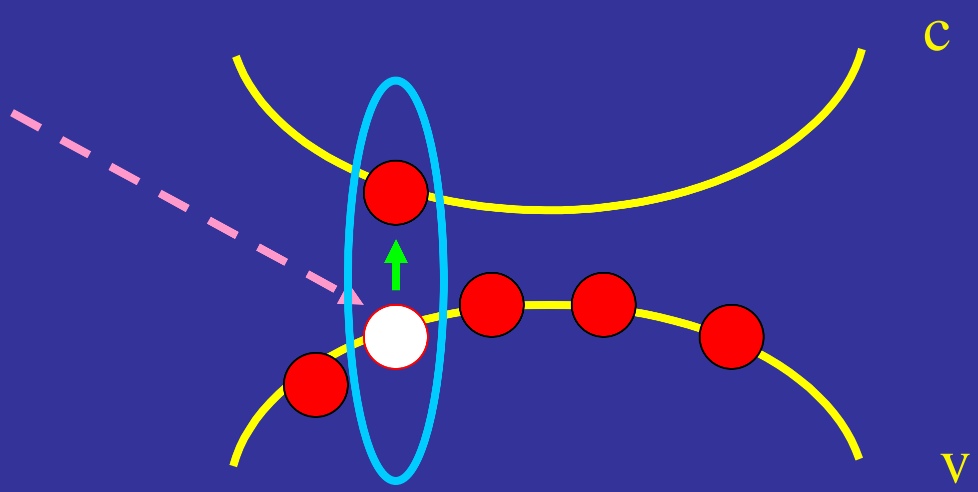
$$L(1,2,1',2') = L_0(1,2,1',2') + L_0(1,\bar{3}',1',\bar{3})\Xi(\bar{3},\bar{2},\bar{3}',\bar{2}')L(\bar{2}',2,\bar{2},2') \quad (3)$$

Dyson-like equation: BSE

$$L_0(1,2,1',2') = G(1,2')G(2,1') \quad (4)$$



Absorption ?



Electron-hole interaction

Excitonic effects

Bethe-Salpeter Equation

Like in GW:

→ Fock exchange — *Makes the electron-hole attraction*

→ Screening — *Calculated consistently*

→ Screening (dynamical) — *Makes more excitations*

→ Widely valid and efficient — *Many people*

→ Room for speedup — *Wannier functions, propagation, mixed TDDFT,...*

4. Look at the total energy

Adiabatic connection fluctuation dissipation theorem (ACFDT)

$$E_X^{EXX}[n] = -2 \times \frac{1}{2}\sum_{nm}^{occ} \int d^3\mathbf{r}\, d^3\mathbf{r}' \,\frac{c_{nm}(\mathbf{r})\, c_{mn}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$c_{nm}(\mathbf{r}) = \phi_n^*(\mathbf{r})\,\phi_m(\mathbf{r}).$$

$$E_C[n] = -\int_0^\infty \frac{du}{2\pi} \int_0^1 d\lambda \int d^3\mathbf{r}\, d^3\mathbf{r}' \,\frac{1}{|\mathbf{r}-\mathbf{r}'|} \times [\chi_\lambda(\mathbf{r},\mathbf{r}';iu) - \chi_0(\mathbf{r},\mathbf{r}';iu)]$$

........in DFT framework

Total energy in GW framework

$$\Phi_{GW} = \frac{1}{2}Tr\left[GV_H\right] + \frac{1}{2}Tr\left[G\Sigma_x\right] - Tr\left[\frac{1}{4}(v_cGG)^2 + \frac{1}{6}(v_cGG)^3 + \ldots\right]$$
$$= \frac{1}{2}Tr\left[GV_H\right] + \frac{1}{2}Tr\left[G\Sigma_x\right] + \frac{1}{2}Tr\left[v_cGG + ln(1 - v_cGG)\right].$$

$$\Omega_{Klein}[G_s] = \Phi[G_s] - Tr(G_0^{-1}G_s - 1) - Tr\ln(-G_s^{-1})$$

$$E^{GWA,s} = \Omega_{Klein}[G_s] + \mu N =$$

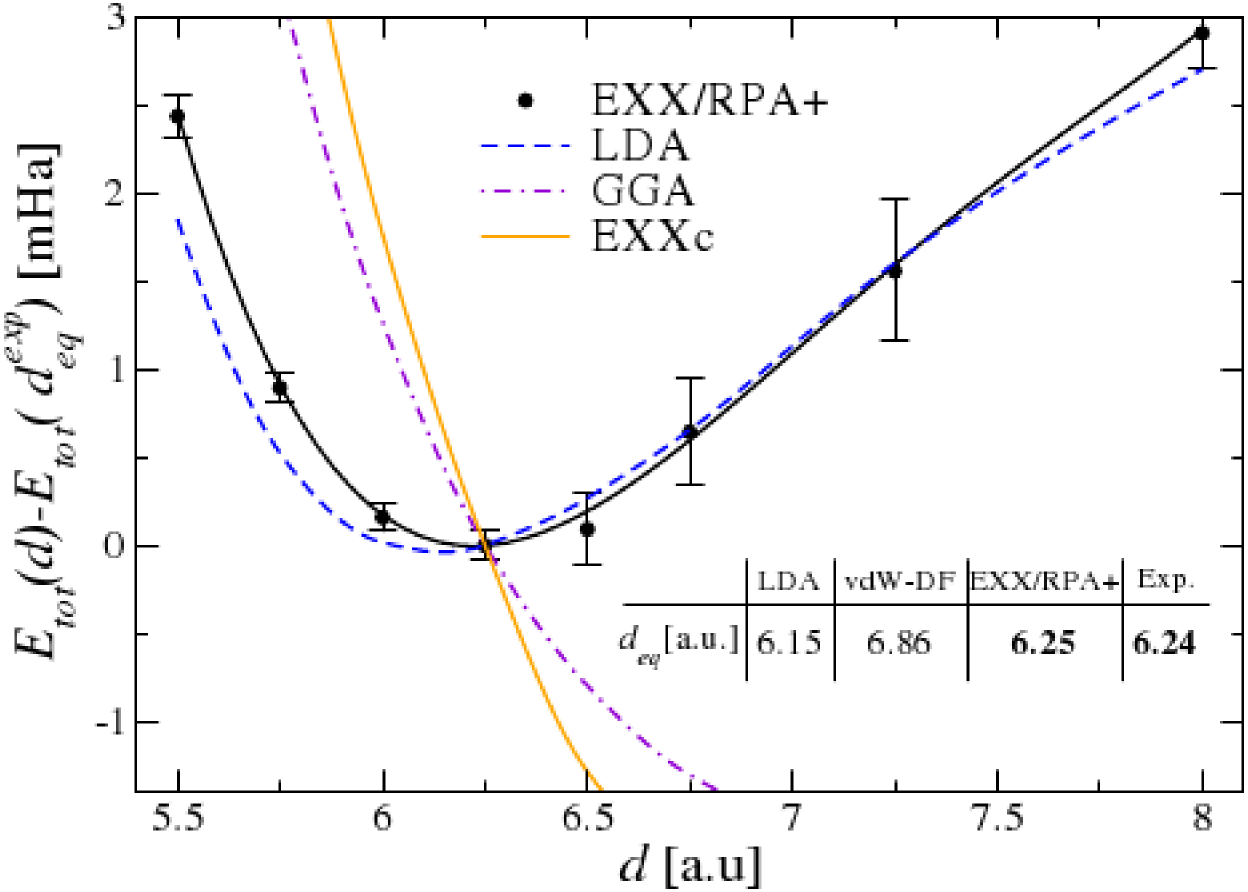
$$= \langle\Psi_s|\hat{H}|\Psi_s\rangle + \frac{1}{2}Tr\left[v_cG_sG_s + ln(1 - v_cG_sG_s)\right]$$

.......evaluated at G=G_s, equivalent to RPA ACFDT

PRL **96,** 136404 (2006) PHYSICAL REVIEW LETTERS week ending 7 APRIL 2006

First-Principles Description of Correlation Effects in Layered Materials

Andrea Marini,[1] P. García-González,[2] and Angel Rubio[3,4]



	LDA	vdW-DF	EXX/RPA+	Exp.
d_{eq}[a.u.]	6.15	6.86	**6.25**	**6.24**

RPA+ : because RPA has deficiencies

Uniform gas correlation energy too negative.

Can be corrected by LDA like term.

S. Kurth and J. P. Perdew, Phys. Rev. B 59, 10 461 (1999); M. Lein, E. K. U. Gross, and J. P. Perdew, Phys. Rev. B 61, 13 431 (2000).

Conclusions

RPA = simplest way to include response
=== a lot of physics!!!

Spectra: plasmons, crystal LFE, but e.g. no excitons
(Hartree only!!!)

Many-body effects:
renormalization of energies,
lifetimes
plasmon satellites
but no "strong correlation"

Total energies: long range contributions, improved correlation energies

Conclusions

RPA = simplest way to include response
=== a lot of physics!!!

Spectra: plasmons, crystal LFE, but e.g. no excitons

RPA = excellent starting point for doing better

Many-body effects:
renormalization of energies,
lifetimes
plasmon satellites
but no "strong correlation"

Total energies: long range contributions, improved correlation energies

Palaiseau Theoretical Spectroscopy Group

ETSF

Thank you!!!