

TDDFT in linear response

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"small"



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"small"

$$\chi(\mathbf{r}, \mathbf{r}', \omega)$$

polarizability :: linear response function

TDDFT in linear response

$$v_{ext}(\mathbf{r}, t) = v_{ext}(\mathbf{r}, 0) + \delta v_{ext}(\mathbf{r}, t)$$

$$\chi(\mathbf{r}, \mathbf{r}', \omega)$$

polarizability :: linear response function

Section 2 :: Linear Response approach



excitations energies
Absorption spectrum
Electron Energy Loss
refraction index
Inelastic X-ray Scattering
Compton Scattering
Reflectivity
Surface differential reflectivity
Reflectance Anisotropy spectroscopy

Section 2 :: Linear Response approach

$$v_{ext}(\mathbf{r}, t) = v_{ext}(\mathbf{r}, 0) + \delta v_{ext}(\mathbf{r}, t)$$

$$n(\mathbf{r}, t) = n(\mathbf{r}, 0) + \delta n(\mathbf{r}, t) + \delta^{(2)} n(\mathbf{r}, t) + \dots$$

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$$\delta n(\mathbf{r}, t) = \int d\mathbf{r}' dt' \chi(\mathbf{r}, \mathbf{r}', t - t') \delta v_{ext}(\mathbf{r}', t')$$

polarizability

Section 2 :: Linear Response approach

polarizability :: density-density response function

$$\chi(\mathbf{r}, \mathbf{r}', t - t') = i \langle \Psi_0 | [\hat{n}(\mathbf{r}, t), \hat{n}(\mathbf{r}', t')] | \Psi_0 \rangle$$

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polarizability :: density-density response function

$$\chi(\mathbf{r}, \mathbf{r}', t - t') = i \langle \Psi_0 | [\hat{n}(\mathbf{r}, t), \hat{n}(\mathbf{r}', t')] | \Psi_0 \rangle$$

$$\hat{n}(\mathbf{r}, t) = e^{-iHt} \hat{n}(\mathbf{r}) e^{iHt} \qquad \hat{n}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$$

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polarizability :: density-density response function

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$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \sum_I \left[\frac{\langle \Psi_0 | \hat{n}(\mathbf{r}) | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}') | \Psi_0 \rangle}{\omega - (E_I - E_0) + i0^+} - \frac{\langle \Psi_0 | \hat{n}(\mathbf{r}') | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}) | \Psi_0 \rangle}{\omega + (E_I - E_0) + i0^+} \right]$$



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polarizability :: density-density response function

$$\chi(\mathbf{r}, \mathbf{r}', t - t') = i \langle \Psi_0 | [\hat{n}(\mathbf{r}, t), \hat{n}(\mathbf{r}', t')] | \Psi_0 \rangle$$

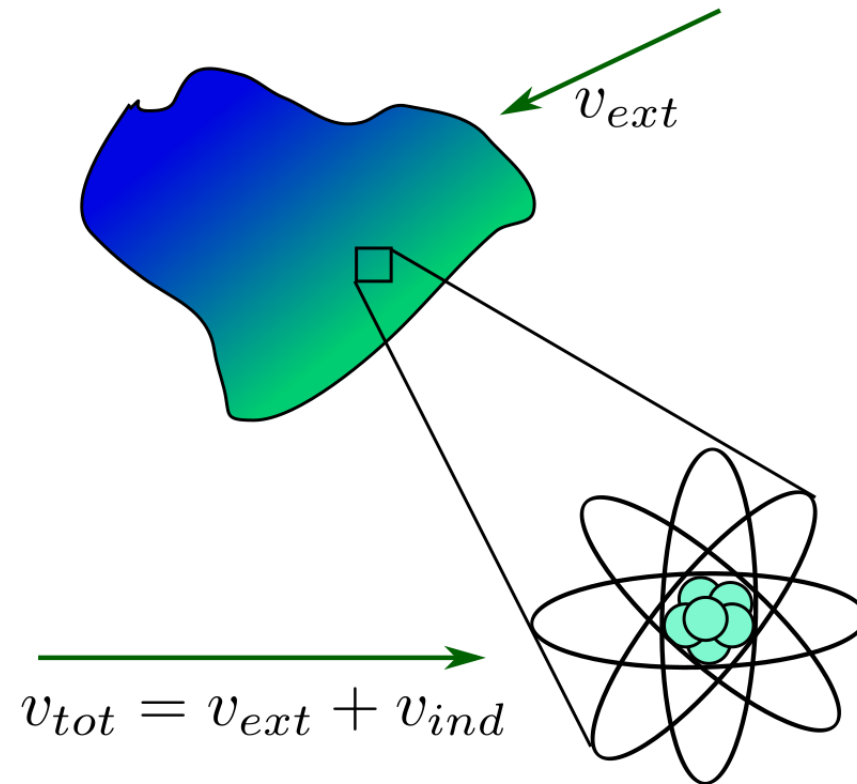
$$\hat{n}(\mathbf{r}, t) = e^{-iHt} \hat{n}(\mathbf{r}) e^{iHt} \qquad \hat{n}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$$

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \sum_I \left[\underbrace{\frac{\langle \Psi_0 | \hat{n}(\mathbf{r}) | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}') | \Psi_0 \rangle}{\omega - (E_I - E_0) + i0^+}}_{\Omega_I \text{ excitations energies}} - \frac{\langle \Psi_0 | \hat{n}(\mathbf{r}') | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}) | \Psi_0 \rangle}{\omega + (E_I - E_0) + i0^+} \right]$$



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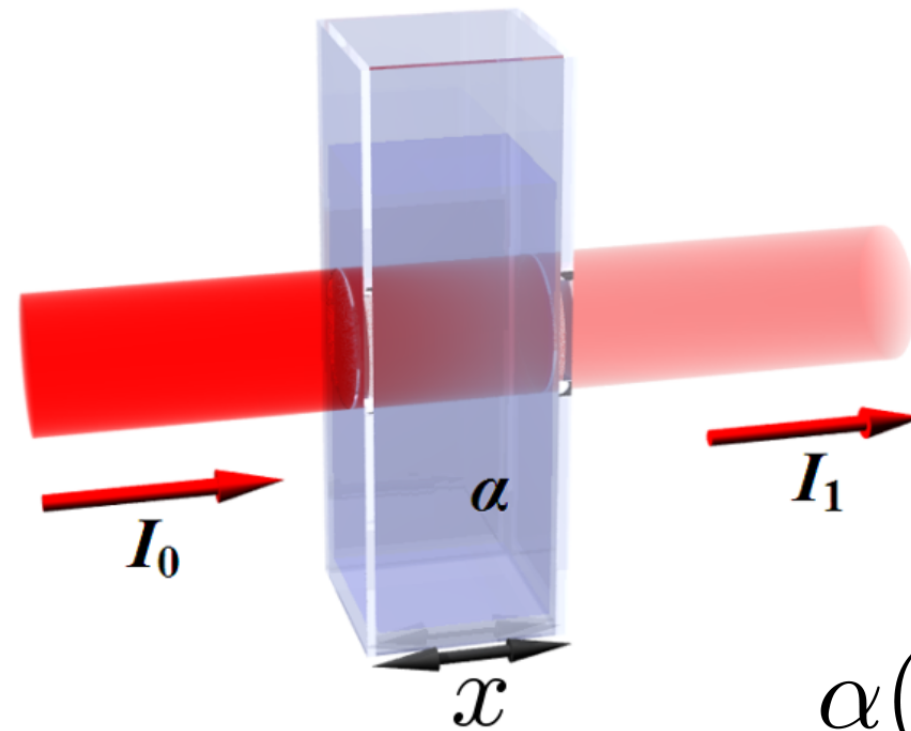
Connection to spectroscopies :: inverse dielectric function



$$v_{tot} = \epsilon^{-1} v_{ext}$$

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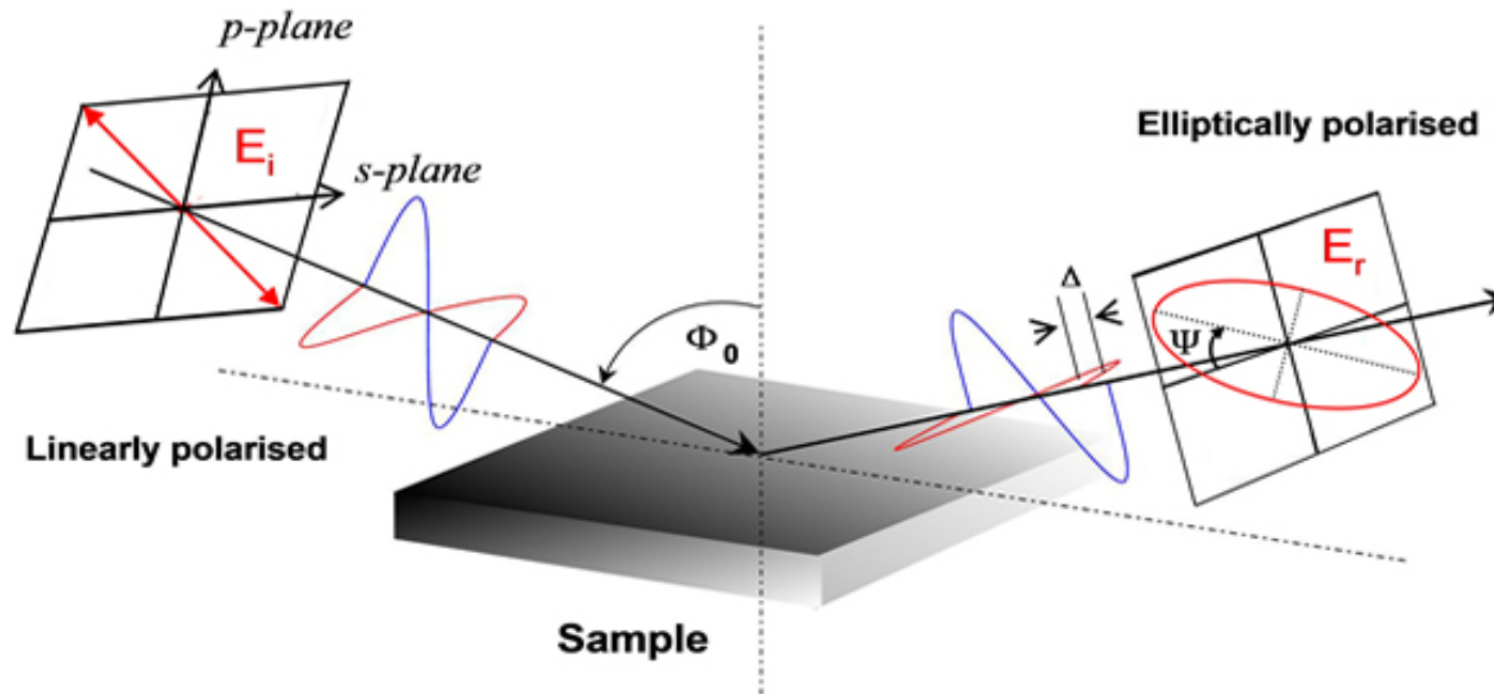
Connection to spectroscopies :: optical absorption



$$\alpha(\omega) = \text{Im} [\varepsilon_M(\omega)]$$

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Connection to spectroscopies :: optical absorption

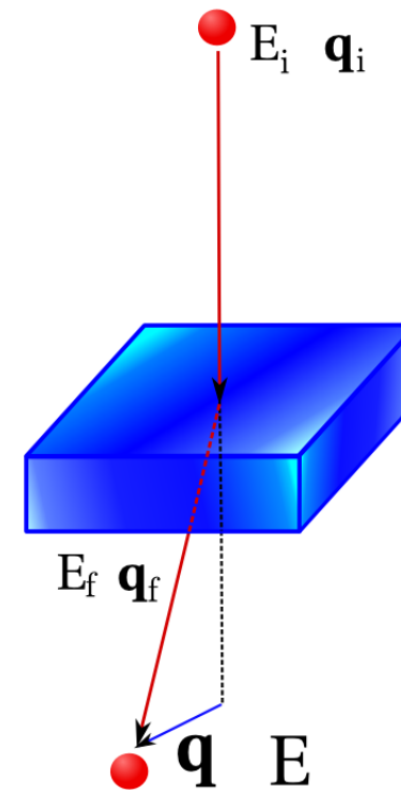


$$\varepsilon_M = \sin^2 \Phi + \sin^2 \Phi \tan^2 \Phi \left(\frac{1 - \frac{E_r}{E_i}}{1 + \frac{E_r}{E_i}} \right)$$

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Connection to spectroscopies :: electron energy loss (EELS)

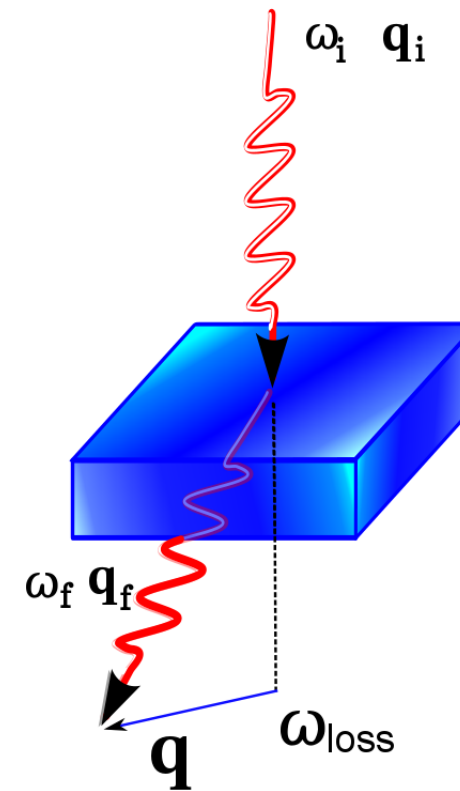
$$\frac{d^2\sigma}{d\Omega d\omega} \propto \text{Im} [\varepsilon^{-1}(\mathbf{q}, \omega)]$$



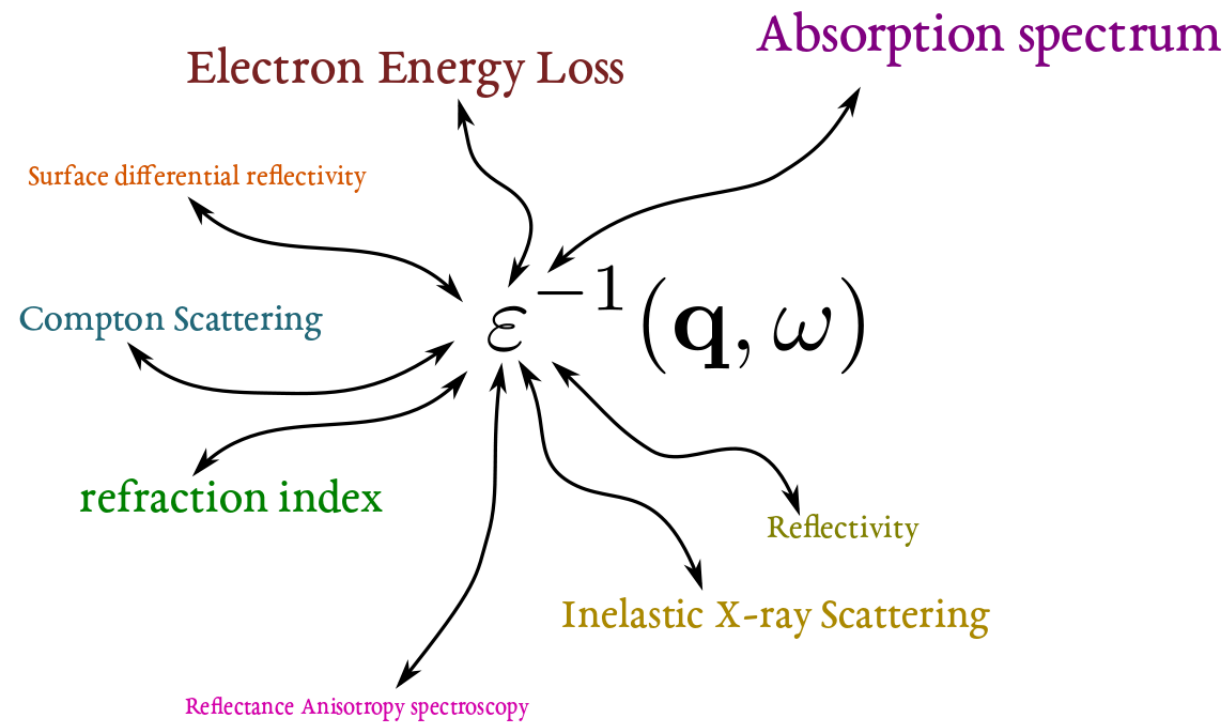
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Connection to spectroscopies :: inelastic X-ray scattering (IXS)

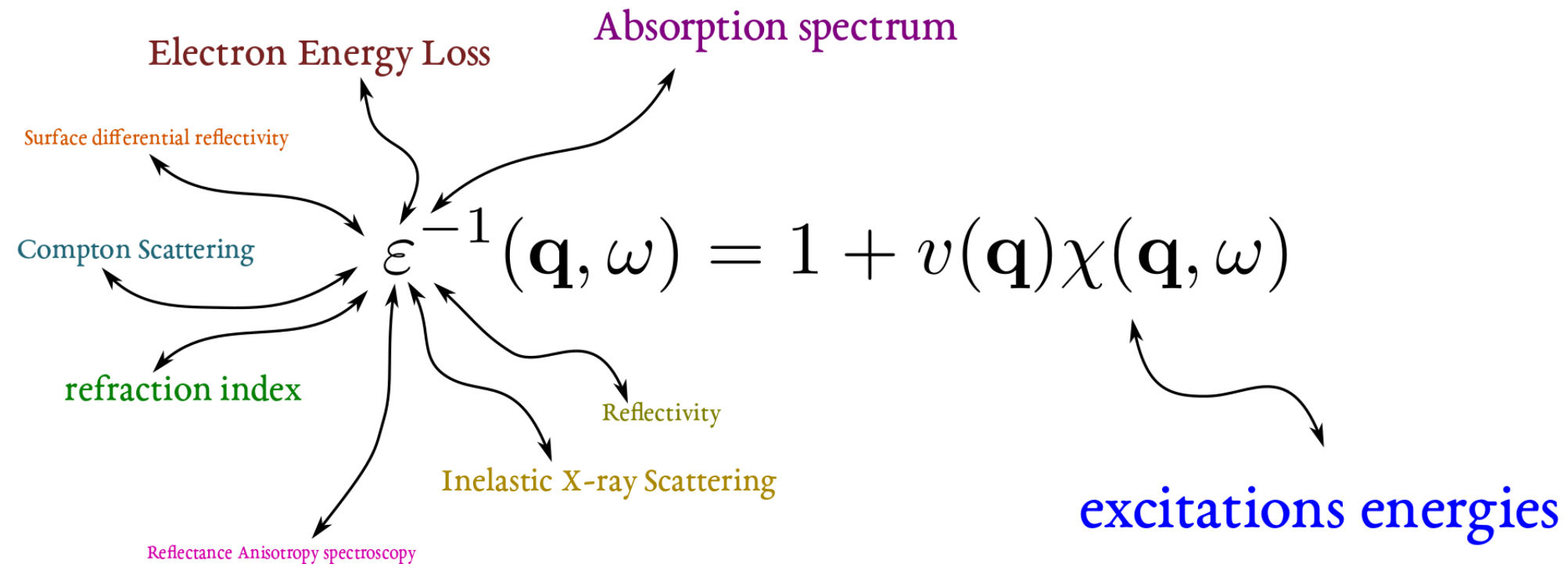
$$\frac{d^2\sigma}{d\Omega d\omega} \propto \text{Im} [\varepsilon^{-1}(\mathbf{q}, \omega)]$$



Section 2 :: Linear Response approach



Section 2 :: Linear Response approach



Section 2 :: Linear Response approach

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \sum_I \left[\frac{\langle \Psi_0 | \hat{n}(\mathbf{r}) | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}') | \Psi_0 \rangle}{\omega - (E_I - E_0) + i0^+} - \frac{\langle \Psi_0 | \hat{n}(\mathbf{r}') | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}) | \Psi_0 \rangle}{\omega + (E_I - E_0) + i0^+} \right]$$

Polarizability of an independent-particle system

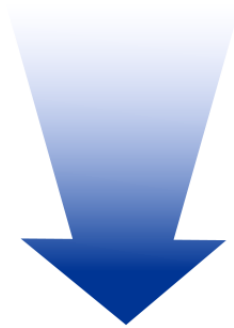
$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \sum_I \left[\frac{\langle \Psi_0 | \hat{n}(\mathbf{r}) | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}') | \Psi_0 \rangle}{\omega - (E_I - E_0) + i0^+} - \frac{\langle \Psi_0 | \hat{n}(\mathbf{r}') | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}) | \Psi_0 \rangle}{\omega + (E_I - E_0) + i0^+} \right]$$

Ψ_0  single determinant

Polarizability of an independent-particle system

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \sum_I \left[\frac{\langle \Psi_0 | \hat{n}(\mathbf{r}) | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}') | \Psi_0 \rangle}{\omega - (E_I - E_0) + i0^+} - \frac{\langle \Psi_0 | \hat{n}(\mathbf{r}') | \Psi_I \rangle \langle \Psi_I | \hat{n}(\mathbf{r}) | \Psi_0 \rangle}{\omega + (E_I - E_0) + i0^+} \right]$$

Ψ_0



single determinant



$$\chi^0(\mathbf{r}, \mathbf{r}', \omega) = \sum_{ij} (f_i - f_j) \left[\frac{\psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) \psi_i(\mathbf{r}') \psi_j^*(\mathbf{r}')}{\omega - (\epsilon_j - \epsilon_i) + i0^+} - \frac{\psi_i(\mathbf{r}) \psi_j^*(\mathbf{r}) \psi_i^*(\mathbf{r}') \psi_j(\mathbf{r}')}{\omega + (\epsilon_j - \epsilon_i) + i0^+} \right]$$



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$$\delta n = \chi^0 \delta v_{eff} \qquad \delta n :$$

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$$\delta n = \chi^0 \delta v_{eff}$$

$$\delta n = \chi \delta v_{ext}$$

Section 2 :: Linear Response approach

$$\delta n = \chi^0 \delta v_{eff}$$

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$$\chi \delta v_{ext} \stackrel{\text{DFT}}{=} \chi^0 \delta v_{eff}$$

Section 2 :: Linear Response approach

$$\delta n = \chi^0 \delta v_{eff} \qquad \delta n = \chi \delta v_{ext}$$

$$\chi \delta v_{ext} \stackrel{\text{DFT}}{=} \chi^0 \delta v_{eff}$$

$$\delta v_{eff} = \delta v_{ext} + \delta v_H + \delta v_{xc}$$

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Dyson equation for the polarizability

$$\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$$

● evalu

● f

Section 2 :: Linear Response approach

Dyson equation for the polarizability

$$\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$$

● evalu

● f_{xc} :

● appro

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \chi^0(\mathbf{r}, \mathbf{r}', \omega) +$$

$$+ \int d\mathbf{r}_1 d\mathbf{r}_2 \chi^0(\mathbf{r}, \mathbf{r}_1, \omega) [v(\mathbf{r}_1, \mathbf{r}_2) + f_{xc}(\mathbf{r}_1, \mathbf{r}_2, \omega)] \chi(\mathbf{r}_2, \mathbf{r}', \omega)$$

Section 2 :: Linear Response approach

Dyson equation for the polarizability

$$\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$$

● evaluate

● f_{xc}

● approximation

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \chi^0(\mathbf{r}, \mathbf{r}', \omega) +$$

$$+ \int d\mathbf{r}_1 d\mathbf{r}_2 \chi^0(\mathbf{r}, \mathbf{r}_1, \omega) [v(\mathbf{r}_1, \mathbf{r}_2) + f_{xc}(\mathbf{r}_1, \mathbf{r}_2, \omega)] \chi(\mathbf{r}_2, \mathbf{r}', \omega)$$

$$f_{xc} = \frac{\delta v_{xc}}{\delta n} \quad \text{exchange-correlation kernel}$$

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- evaluation of χ knowing χ^0 (ground state calculation)
- f_{xc} functional of the ground-state density
- approximations for f_{xc}

)

$$\left. \begin{array}{l} \bullet f_{xc} = 0 \\ \bullet f_{xc} = \frac{\delta v_{xc}^{gs}}{\delta n} \\ \bullet \text{any other } f_{xc} \end{array} \right\} \text{coherence vs freedom}$$

Section 2 :: Linear Response approach

Practical procedure for χ and ε^{-1} Scal

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Practical procedure for χ and ε^{-1} Scalings

- DFT-KS calculation ψ_i, ϵ_i (approx :: v_{xc}, V_{ion}^{ps}) $o(N^{1\div 3})$

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Practical procedure for χ and ε^{-1} Scalin

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- creation of $\chi^0 = \sum_{ij} \frac{\psi_i^*(\mathbf{r})\psi_j(\mathbf{r})\psi_i(\mathbf{r}')\psi_j^*(\mathbf{r}')}{\omega - (\epsilon_j - \epsilon_i) + i0^+}$ $o(N^4)$

Section 2 :: Linear Response approach

Practical procedure for χ and ε^{-1} Scalin

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- determination of $\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$ (approx :: f_{xc}) $o(N^{2\div 3})$

Section 2 :: Linear Response approach

Practical procedure for χ and ε^{-1} Scaling

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Absorption spectrum Inelastic X-ray Scattering refraction index Surface differential reflectivity

Section 2 :: Linear Response approach

Practical procedure for χ and ε^{-1} Scaling

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Absorption spectrum Inelastic X-ray Scattering refraction index Surface differential reflectivity
Compton Scattering Reflectivity Electron Energy Loss Reflectance Anisotropy spectroscopy

Section 2 :: Linear Response approach

Practical procedure for χ and ε^{-1}

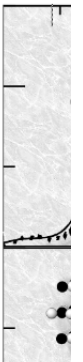
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Absorption spectrum Inelastic X-ray Scattering refraction index Surface differential reflectivity
Compton Scattering Reflectivity Electron Energy Loss Reflectance Anisotropy spectroscopy

Scaling (with N_{atoms})

$$o(N^{1\div 3})$$

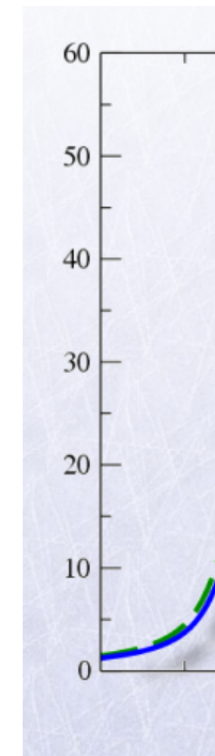
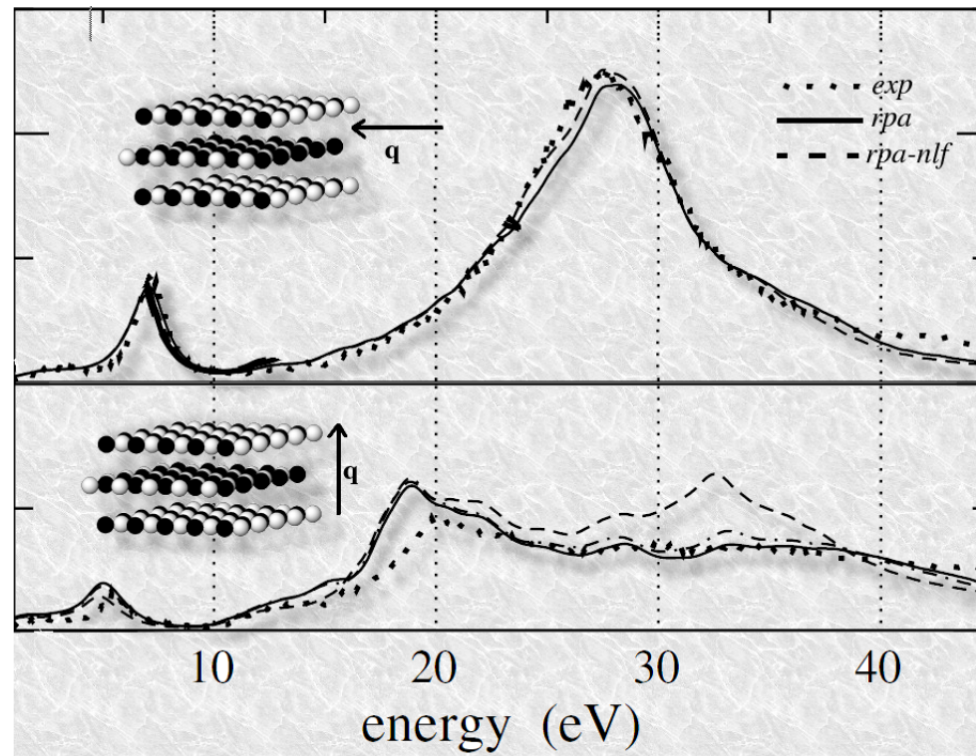
$$o(N^4)$$

$$o(N^{2\div 3})$$



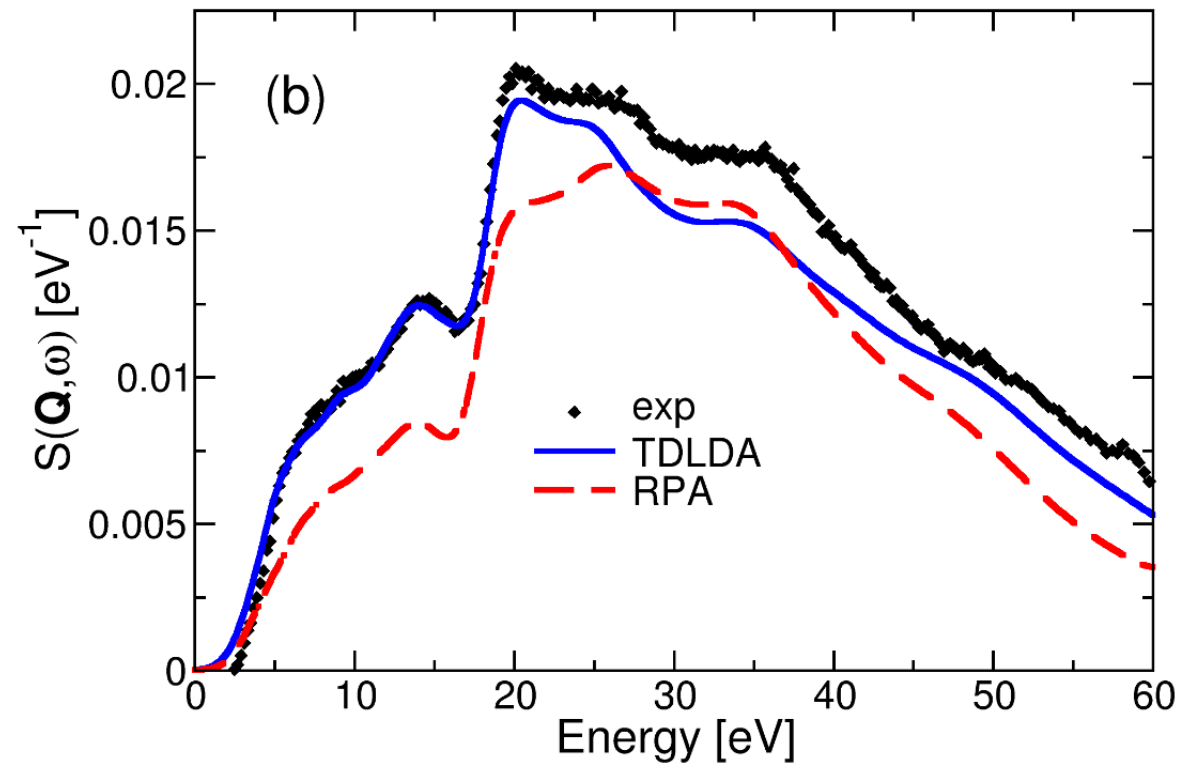
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EELS of graphite



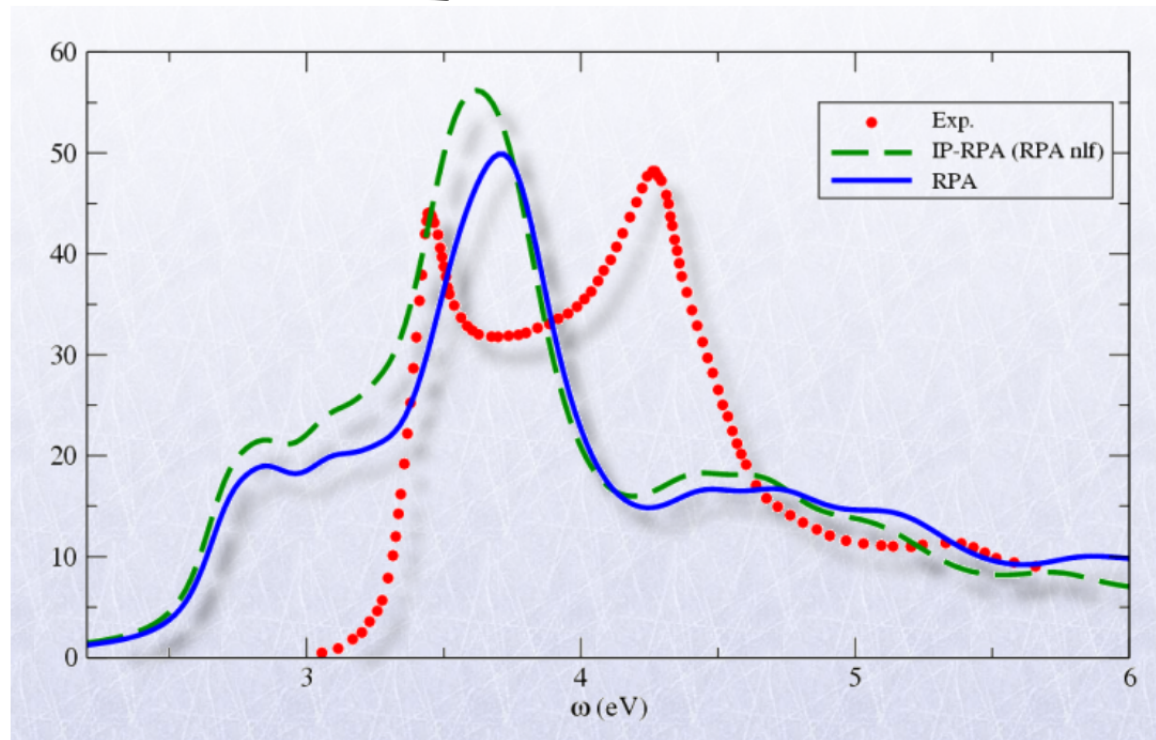
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IXS of Silicon



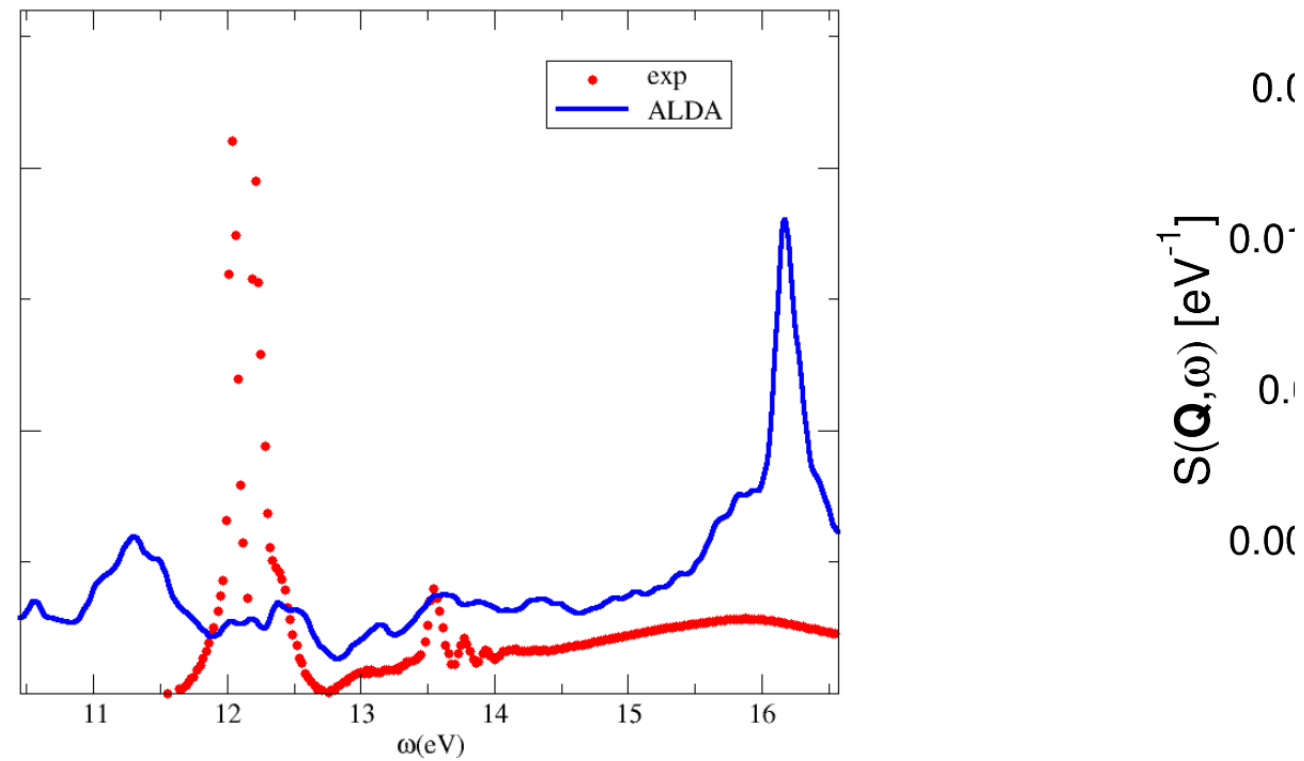
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Absorption of Silicon

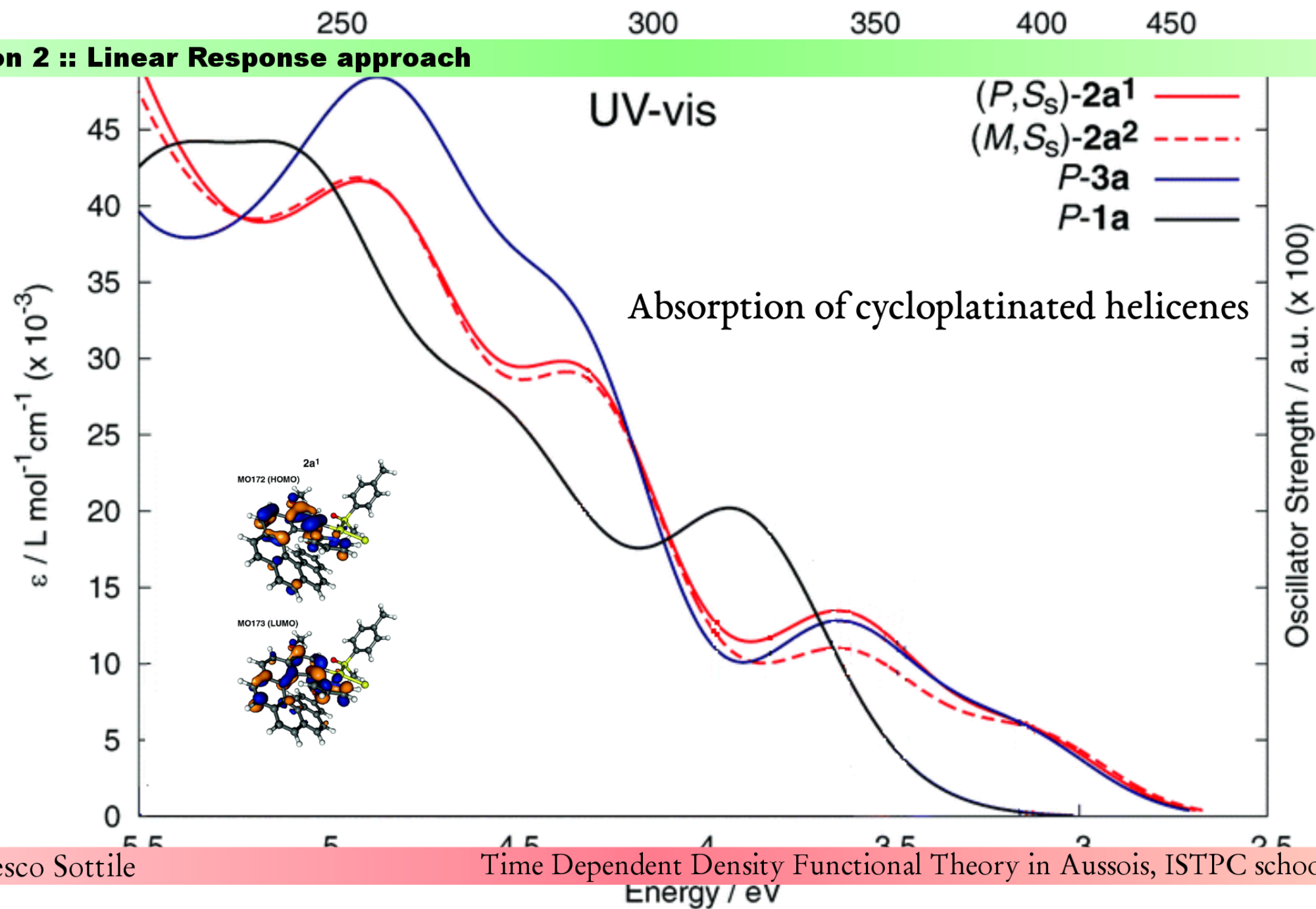


Section 2 :: Linear Response approach

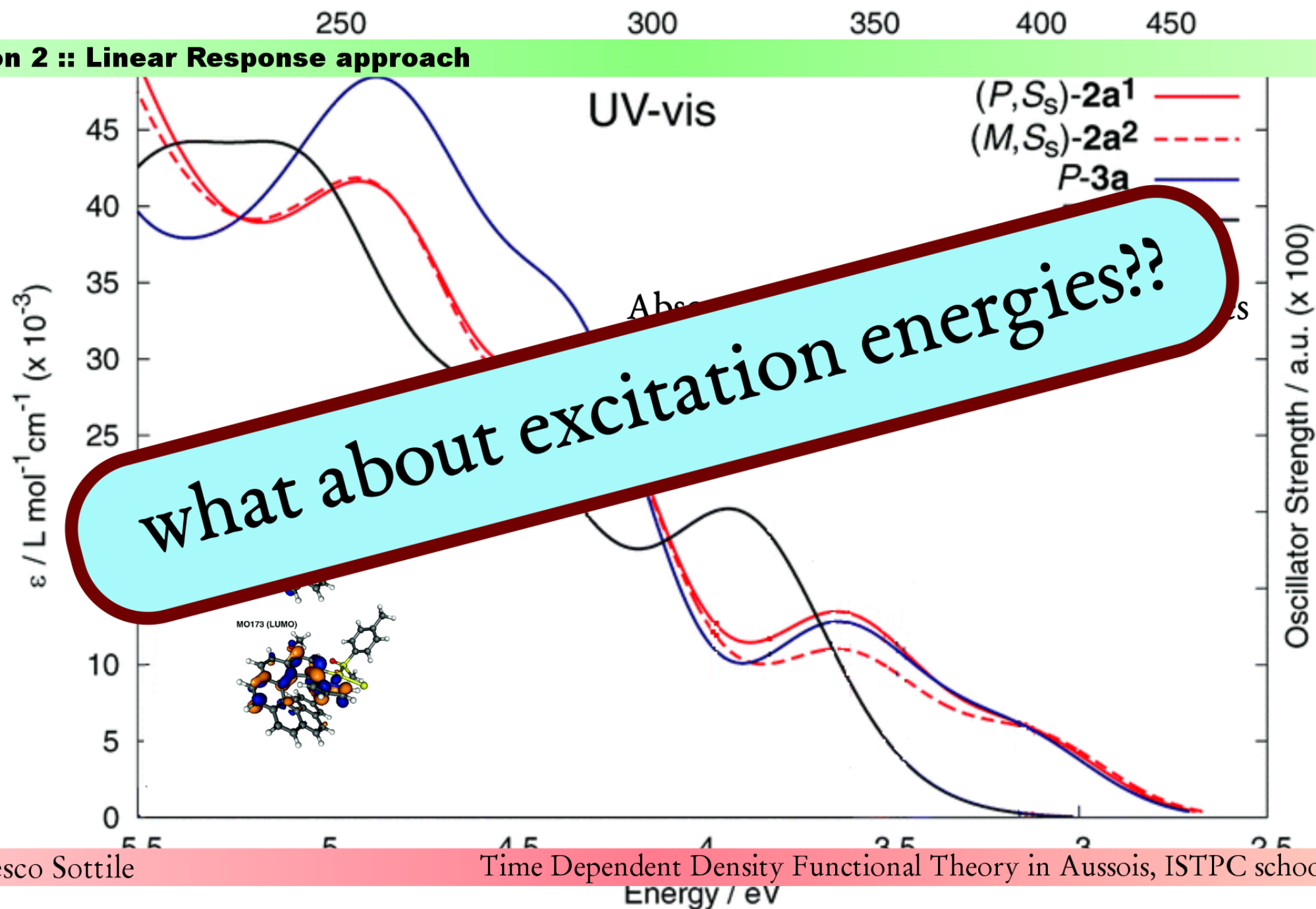
Absorption of Argon



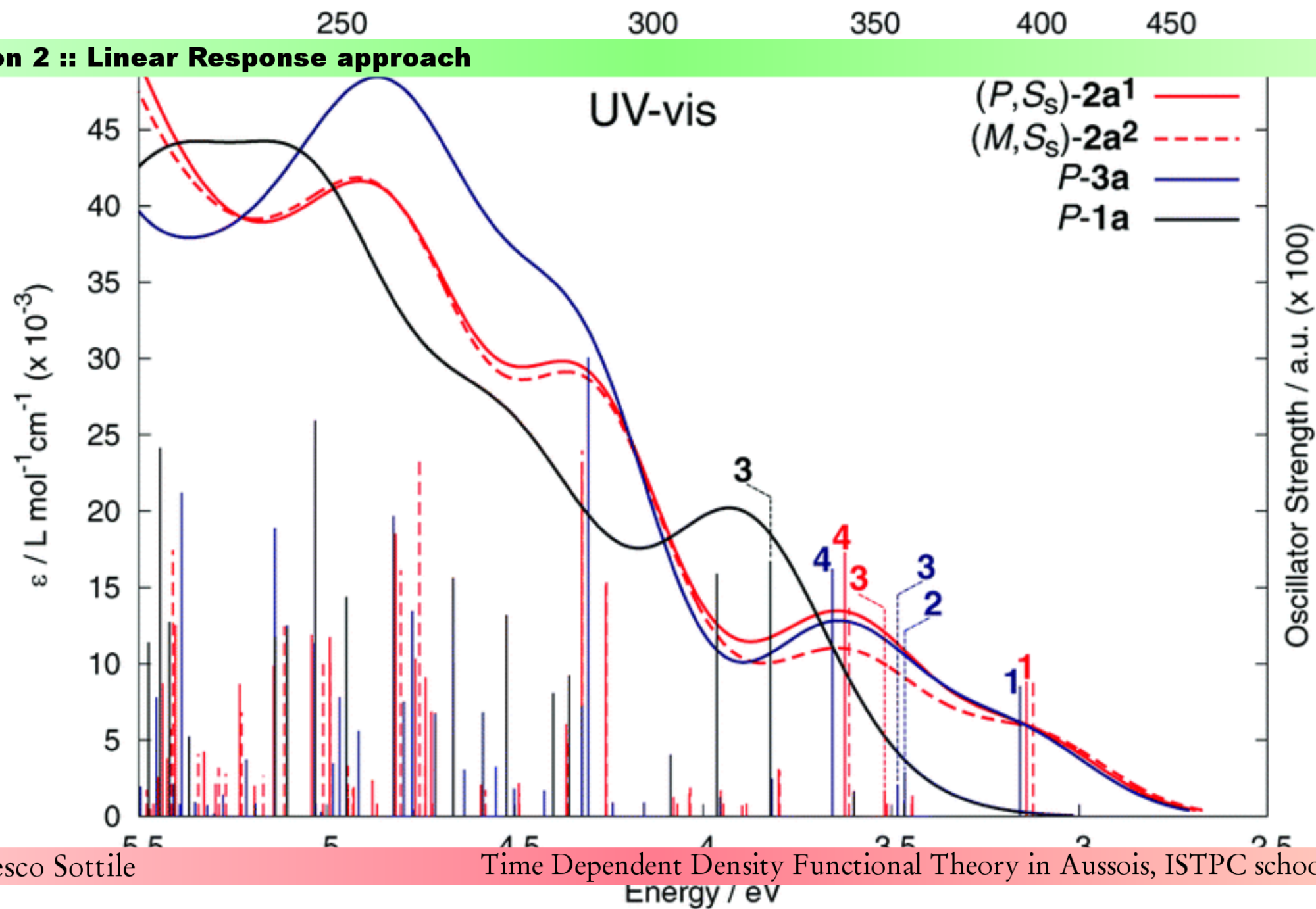
Section 2 :: Linear Response approach



Section 2 :: Linear Response approach



Section 2 :: Linear Response approach



Section 2 :: Linear Response approach

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \chi^0(\mathbf{r}, \mathbf{r}', \omega) + \\ + \int d\mathbf{r}_1 d\mathbf{r}_2 \chi^0(\mathbf{r}, \mathbf{r}_1, \omega) [v(\mathbf{r}_1, \mathbf{r}_2) + f_{xc}(\mathbf{r}_1, \mathbf{r}_2, \omega)] \chi(\mathbf{r}_2, \mathbf{r}', \omega)$$

Section 2 :: Linear Response approach

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \chi^0(\mathbf{r}, \mathbf{r}', \omega) + \\ + \int d\mathbf{r}_1 d\mathbf{r}_2 \chi^0(\mathbf{r}, \mathbf{r}_1, \omega) [v(\mathbf{r}_1, \mathbf{r}_2) + f_{xc}(\mathbf{r}_1, \mathbf{r}_2, \omega)] \chi(\mathbf{r}_2, \mathbf{r}', \omega)$$

basis change

$$f_{ij}^{kl} = \iint \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) \psi_k(\mathbf{r}') \psi_l^*(\mathbf{r}') f(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}'$$

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$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \chi^0(\mathbf{r}, \mathbf{r}', \omega) + \\ + \int d\mathbf{r}_1 d\mathbf{r}_2 \chi^0(\mathbf{r}, \mathbf{r}_1, \omega) [v(\mathbf{r}_1, \mathbf{r}_2) + f_{xc}(\mathbf{r}_1, \mathbf{r}_2, \omega)] \chi(\mathbf{r}_2, \mathbf{r}', \omega)$$

basis change

$$f_{ij}^{kl} = \iint \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) \psi_k(\mathbf{r}') \psi_l^*(\mathbf{r}') f(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}'$$

$$\chi_{ij}^{kl} = [\chi^0]_{ij}^{kl} + \sum_{mnop} [\chi^0]_{ik}^{mn} \left[v_{mn}^{op} + [f_{xc}]_{mn}^{op} \right] \chi_{op}^{kl}$$

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$$[\chi^0]_{ij}^{kl} = \frac{(f_i - f_j)\delta_{ik}\delta_{jl}}{\omega - (\epsilon_j - \epsilon_i)} \quad \text{diagonal in } ij, kl$$

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$$\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$$



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

Section 2 :: Linear Response approach

$$\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$$



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

$$\chi = \left[(\chi^0)^{-1} - K \right]^{-1}$$

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$$\chi =$$

$$\chi_{ij}^{kl}$$

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$$\chi_{ij}^{kl} = \left[(x^0)^{-1} \right]_{\omega - (\epsilon_j - \epsilon_i)\delta_{ik}\delta_{jl}}$$

Section 2 :: Linear Response approach

$$\chi = \left[(\chi^0)^{-1} - K \right]^{-1}$$

χ_{ij}^{kl} $\omega - (\epsilon_j - \epsilon_i)\delta_{ik}\delta_{jl}$ $K_{ij}^{kl} = \iint \psi_i^*(\mathbf{r})\psi_j(\mathbf{r})\psi_i(\mathbf{r}')\psi_j^*(\mathbf{r}')K(\mathbf{r},\mathbf{r}') d\mathbf{r}d\mathbf{r}'$

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$$\chi = \frac{1}{H^{\text{EXC}} - \omega} = \sum_{\lambda\lambda'} \frac{|V_\lambda\rangle S_\lambda^{\lambda'} \langle V_\lambda|}{E_\lambda - \omega}$$

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$$\chi = \frac{1}{H^{\text{EXC}} - \omega} = \sum_{\lambda} \frac{|V_{\lambda}\rangle \langle V_{\lambda}|}{E_{\lambda} - \omega}$$

Section 2 :: Linear Response approach

$$H^{\text{EXC}} = \begin{bmatrix} \vdots & & & & \\ & (\epsilon_j - \epsilon_i) \delta_{ik} \delta_{jl} & & & \\ & & \vdots & & \\ & & & (\epsilon_j - \epsilon_i) \delta_{ik} \delta_{jl} & \\ & K_{ij}^{kl} & & & K_{ij}^{kl} \\ & & & & & K_{ij}^{kl} \\ & & & & & & K_{ij}^{kl} \\ & & & & & & & (\epsilon_j - \epsilon_i) \delta_{ik} \delta_{jl} \end{bmatrix}$$

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$$H^{\text{EXC}} = \begin{matrix} & kl & ij \\ & \left[\begin{array}{c|c} \begin{array}{c} \text{Diagram 1: } i \rightarrow j \text{ (blue up), } k \rightarrow l \text{ (blue up)} \\ \text{Diagram 2: } i \rightarrow l \text{ (red down), } j \rightarrow k \text{ (blue up)} \end{array} & \begin{array}{c} \text{Diagram 3: } i \rightarrow j \text{ (blue up), } k \rightarrow l \text{ (red down)} \\ \text{Diagram 4: } i \rightarrow l \text{ (red down), } j \rightarrow k \text{ (red down)} \end{array} \end{array} \right] \end{matrix}$$

The diagrams illustrate four possible excitation pathways between two sets of orbitals (solid lines) and virtual orbitals (dashed lines). In each diagram, the initial occupied orbitals are labeled i and j , and the final virtual orbitals are labeled k and l . Blue arrows represent excitations from occupied to virtual orbitals, while red arrows represent de-excitations from virtual to occupied orbitals.

- Diagram 1 (Top Left):** Two blue arrows show excitations from $i \rightarrow j$ and $k \rightarrow l$.
- Diagram 2 (Bottom Left):** A red arrow shows a de-excitation from $i \rightarrow l$, and a blue arrow shows an excitation from $j \rightarrow k$.
- Diagram 3 (Top Right):** A blue arrow shows an excitation from $i \rightarrow j$, and a red arrow shows a de-excitation from $k \rightarrow l$.
- Diagram 4 (Bottom Right):** Two red arrows show de-excitations from $i \rightarrow l$ and $j \rightarrow k$.

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$$H^{\text{EXC}} = \begin{matrix} & kl & ij \\ \begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix} \end{matrix}$$

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$$\left[\begin{array}{c|c} A & B \\ \hline -B^* & -A^* \end{array} \right] \begin{bmatrix} X \\ Y \end{bmatrix} = E_\lambda \begin{bmatrix} X \\ Y \end{bmatrix}$$

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$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{B} \\ \hline \mathbf{B}^* & \mathbf{A}^* \end{array} \right] \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} = E_\lambda \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & -1 \end{array} \right] \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix}$$

Section 2 :: Linear Response approach

$$H^{\text{EXC}} = \begin{matrix} & \begin{matrix} ij \\ kl \end{matrix} \\ \begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix} \end{matrix}$$

Tamm-Dancoff approx

Section 2 :: Linear Response approach

$$H^{\text{EXC}} = \begin{matrix} & \begin{matrix} i & j \\ k & l \end{matrix} \end{matrix} \left[\begin{array}{c|c} \begin{array}{c} \text{Diagram 1: Blue arrows showing transitions } i \rightarrow j \text{ and } k \rightarrow l \end{array} & \begin{array}{c} \text{Diagram 2: Faded diagram with blue arrow } i \rightarrow j \text{ and red arrow } k \rightarrow l \end{array} \\ \hline \begin{array}{c} \text{Diagram 3: Faded diagram with red arrow } i \rightarrow j \text{ and blue arrow } k \rightarrow l \end{array} & \begin{array}{c} \text{Diagram 4: Red arrows showing transitions } i \rightarrow j \text{ and } k \rightarrow l \end{array} \end{array} \right]$$

Tamm-Dancoff approx

Section 2 :: Linear Response approach

		
$\chi = \chi^0 + \chi^0 [v + f_{xc}] \chi$	full spectrum N^4 scaling	excitations energies
$\left[\begin{array}{c c} A & B \\ \hline -B^* & -A^* \end{array} \right] \begin{bmatrix} X \\ Y \end{bmatrix} = E_\lambda \begin{bmatrix} X \\ Y \end{bmatrix}$	few excitations energies iterative techniques analysis	N^6 scaling