Real Space Visualization of Collective Excitation in Sr_2CuO_3

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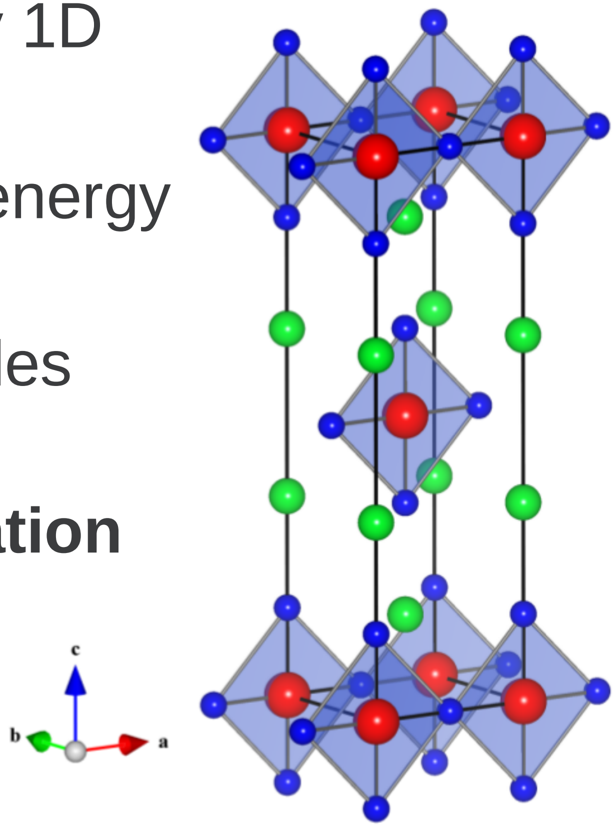
Introduction

- Sr_2CuO_3 is hallmark material to study 1D physics.
- Collective excitation appears in low energy spectrum.
- Calculate excitation from first principles using local basis.
- **Collective excitation is a 3D excitation (2 chain physics)**

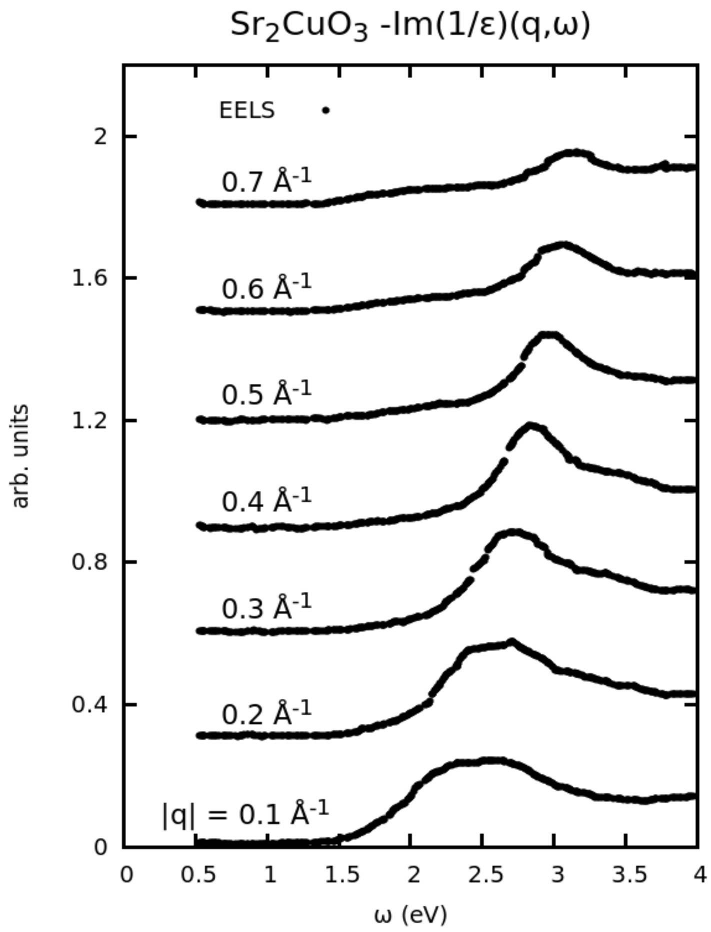


Experimental Motivation

Electron Energy Loss Spectroscopy (EELS)

- Scattering due to beam of fast electrons
- Probes longitudinal density excitations
- Measures Loss function

$$Im\left(\frac{-1}{\varepsilon(\vec{q},\omega)}\right)\sim Im(\chi(\vec{q},\omega))$$

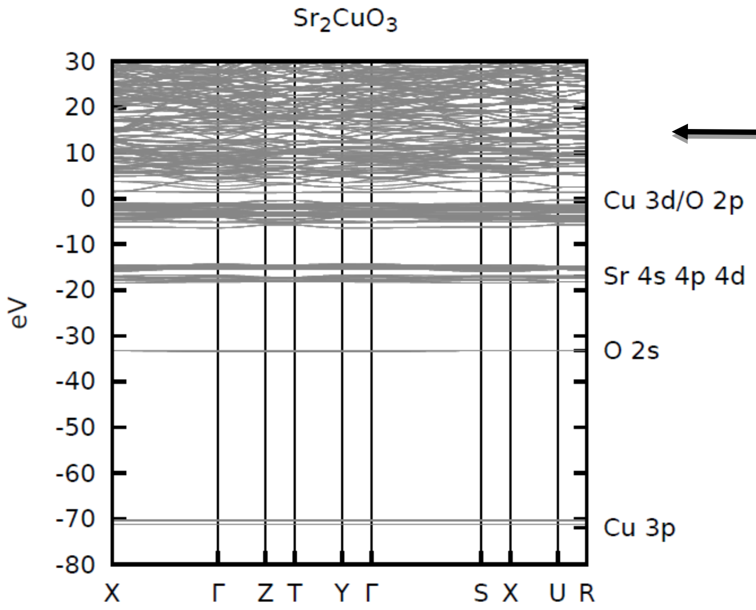


J. Fink et al. Journal of Electron spectroscopy 117-118 (2001) 287-309

Time-Dependent Density Functional Theory (TD-DFT)

- *Ab-initio* method of doing spectroscopy (0K) from Kohn-Sham band structure.

GGA+U band structure:
U =4 eV J = 1 eV



Entire Hilbert Space (e-HS)

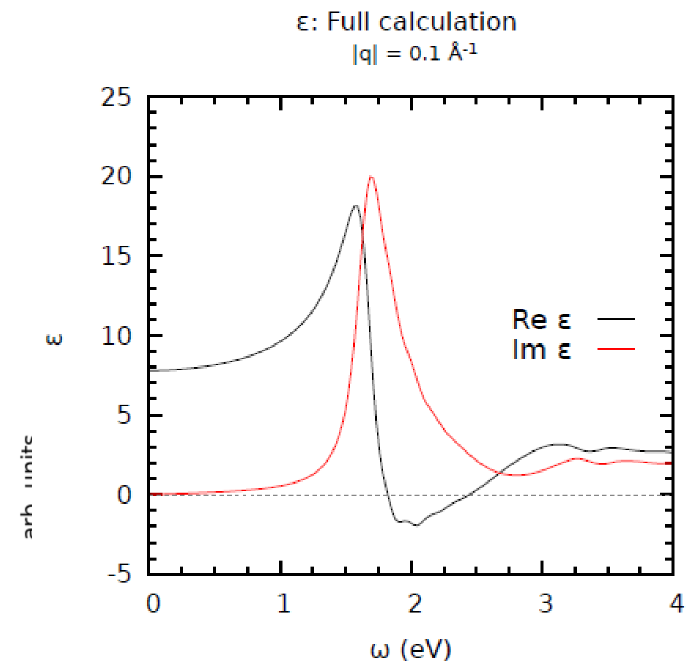
$$(\chi_s)_{\vec{G}\,\vec{G}'}(\vec{q},\omega) = \frac{1}{V_{BvK}} \sum_{\vec{k}}^{1BZ} \sum_{jj'} \left\langle \vec{k}j \right| e^{-i(\vec{q}+\vec{G})\cdot\hat{x}} \left| \vec{k}+\vec{q}\,j' \right\rangle \frac{f_{\vec{k}j} - f_{\vec{k}+\vec{q}\,j'}}{\varepsilon_{\vec{k}j} - \varepsilon_{\vec{k}+\vec{q}\,j'} + \hbar(\omega + i\eta^{+})} \left\langle \vec{k}+\vec{q}j' \right| e^{i(\vec{q}+\vec{G}')\cdot\hat{x}} \left| \vec{k}j \right\rangle$$

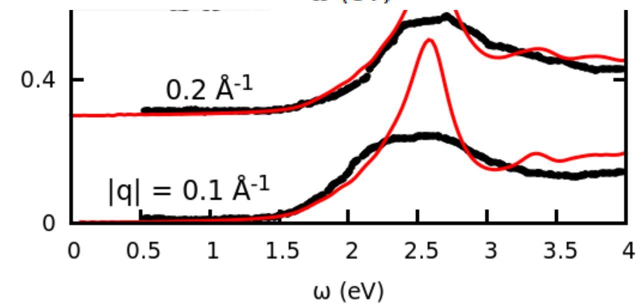
TD-DFT 2

TD-DFT Matrix equation:

$$\chi_{\vec{G}\vec{G}'}(\vec{q},\omega) = \sum_{\vec{G}_1} (\chi_s)_{\vec{G}\vec{G}_1}(\vec{q},\omega)\left[1 - \left(v(\vec{q}) + f_{xc}(\vec{q},\omega)\right)\right]^{-1}_{\vec{G}_1\vec{G}'}$$

- Random Phase Approximation (RPA) ($f_{xc} = 0$).





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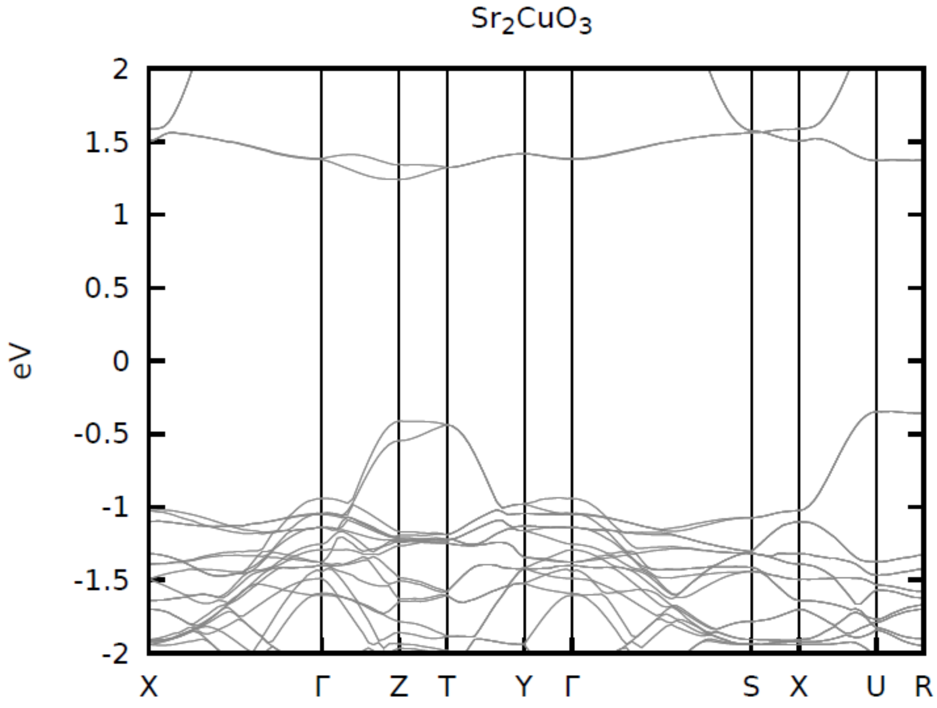
Downfolded Response

TD-DFT equation for downfolded response (d-HS):

$$\chi_{\vec{G}\vec{G}'}(\vec{q},\omega) = \sum_{\vec{G}_1}(\chi_s)_{\vec{G}\vec{G}_1}(\vec{q},\omega)\,[1 - V(\vec{q},\omega)\chi_s(\vec{q},\omega)]^{-1}_{\vec{G}_1\vec{G}'}$$

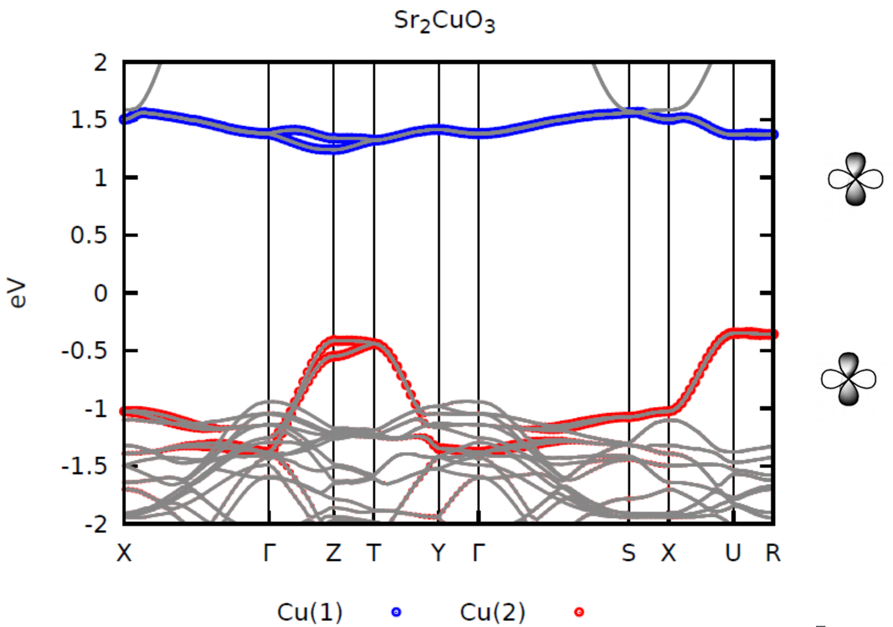


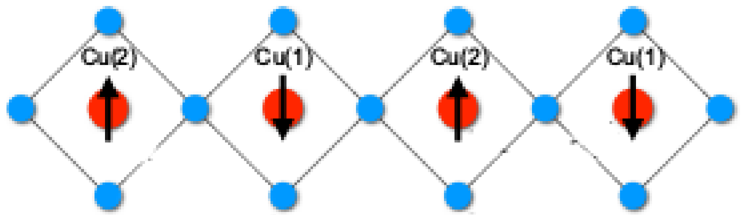
Downfolded Hilbert Space

Wannier functions:

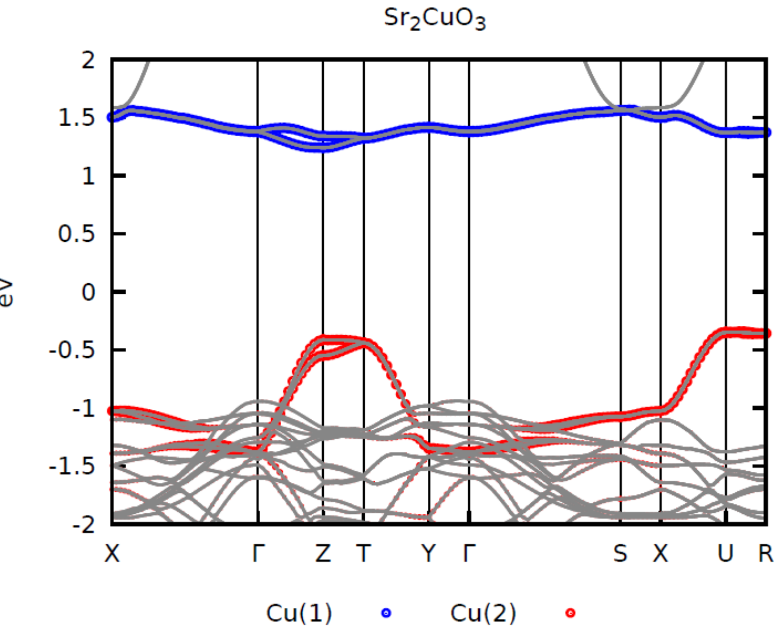
$$W_{n\sigma}(\vec{x}-\vec{R}) = \frac{1}{N_{BvK}} \sum_{\vec{k}}^{1BZ} e^{-i\vec{k}\cdot\vec{R}} \sum_{j=n_1(\vec{k})}^{n_2(\vec{k})} a_{nj\sigma}(\vec{k})\psi_{\vec{k}j\sigma}(\vec{x})$$

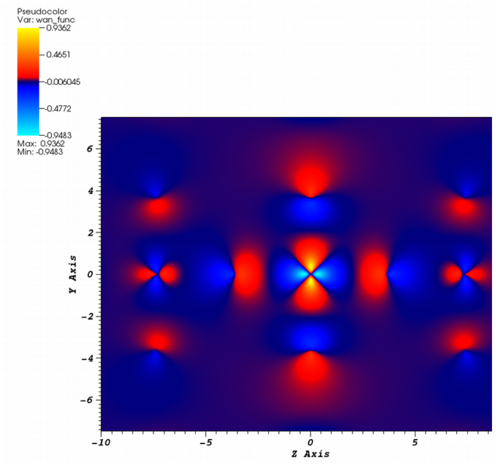
$$a_{nj\sigma}(\vec{k}) = \langle \vec{k}j\sigma | lm \rangle_\alpha$$

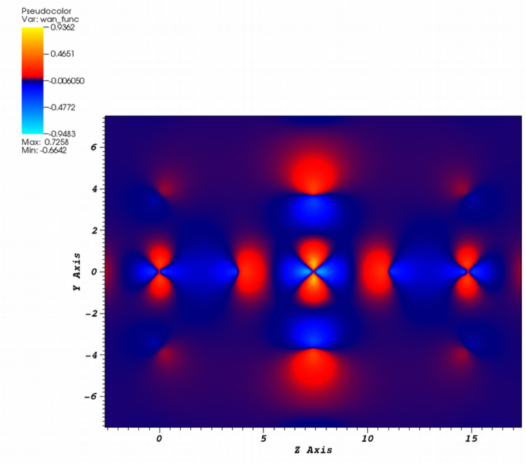


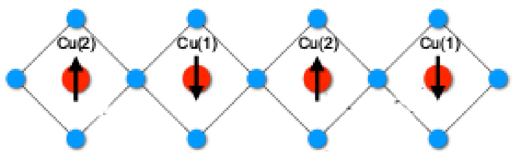


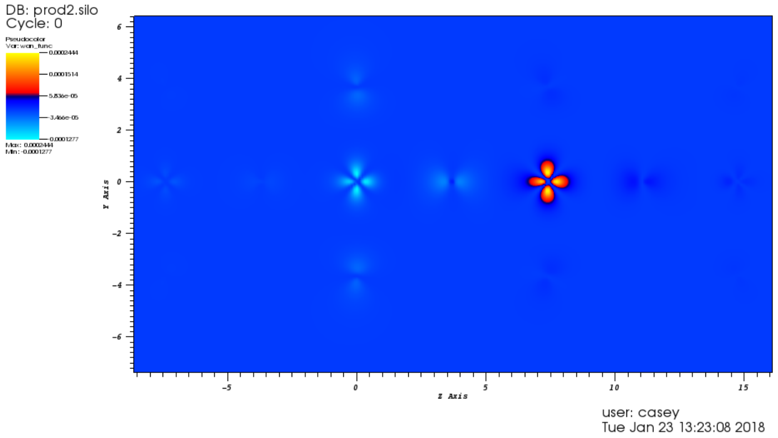
Downfolded Hilbert Space





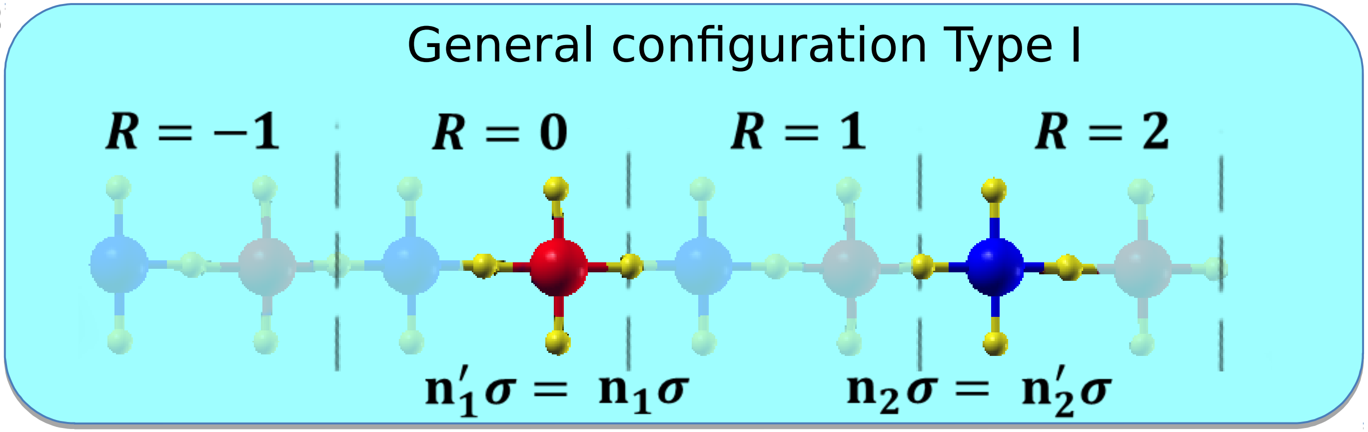


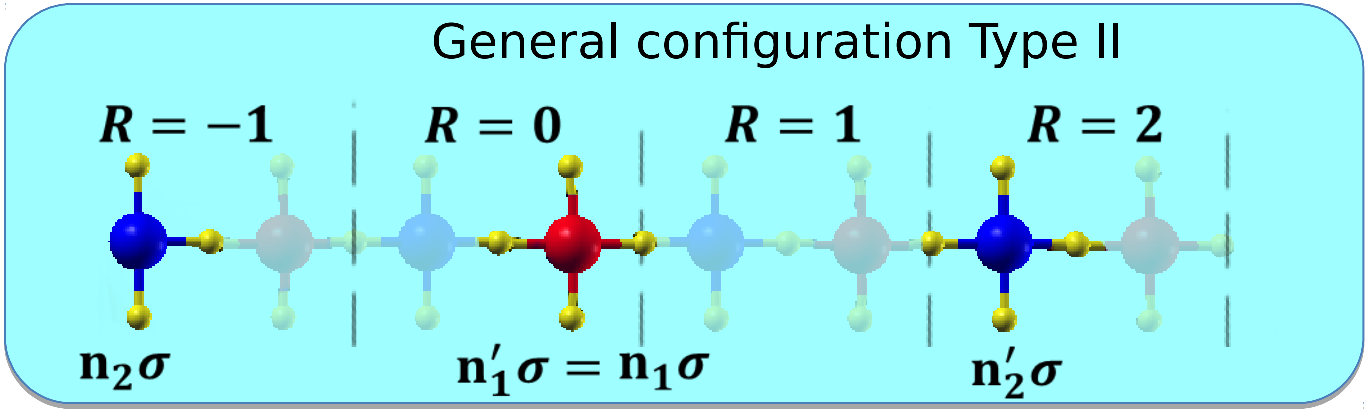




$$(\chi_s)_{\vec{G}\vec{G}'}(\vec{q},\omega)$$

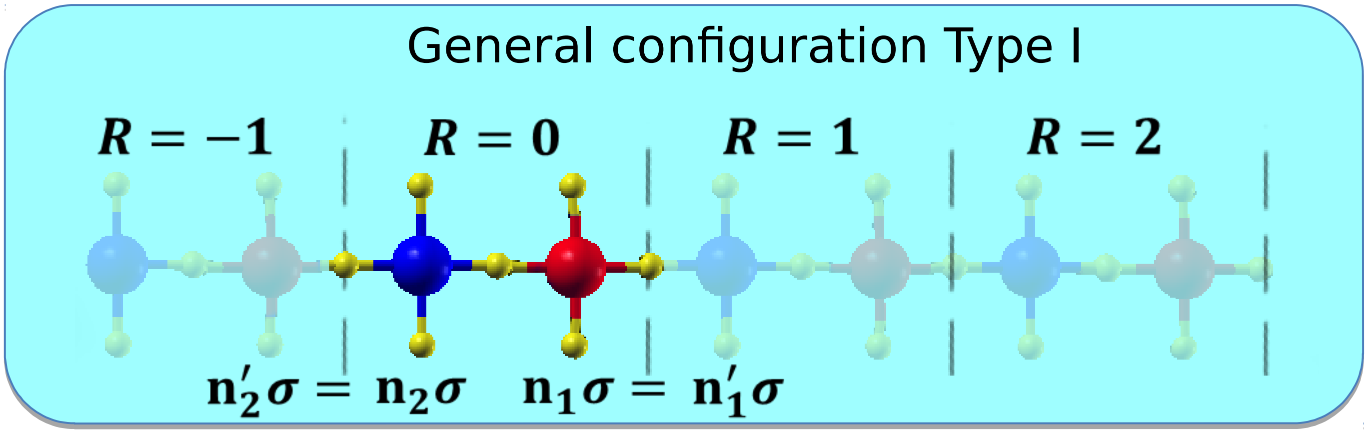
$$= \sum_{\vec{R}\,\vec{R}'} \sum_{\substack{n_1 n_2 \\ n'_1 n'_2}} \sum_{\sigma} A_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q}+\vec{G})(\tilde{\chi}_s)_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}^{\vec{0}\,n'_1\sigma;\vec{R}'\,n'_2\sigma}(\vec{q},\omega)A^{*}_{\vec{0}\,n'_1\sigma\,;\vec{R}'\,n'_2\sigma}(\vec{q}+\vec{G}')$$

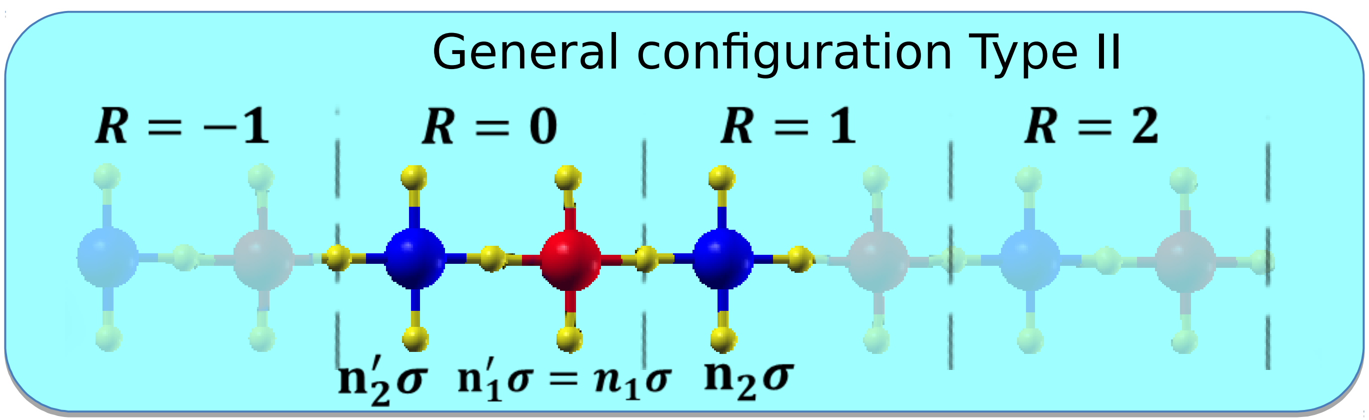




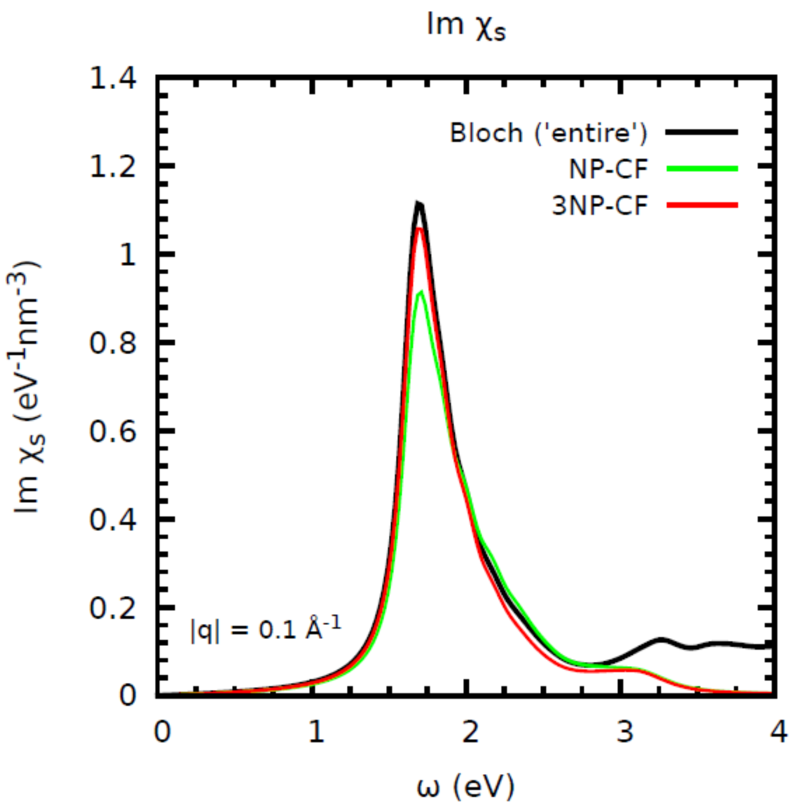
$$(\chi_s)_{\vec{G}\vec{G}'}(\vec{q},\omega)$$

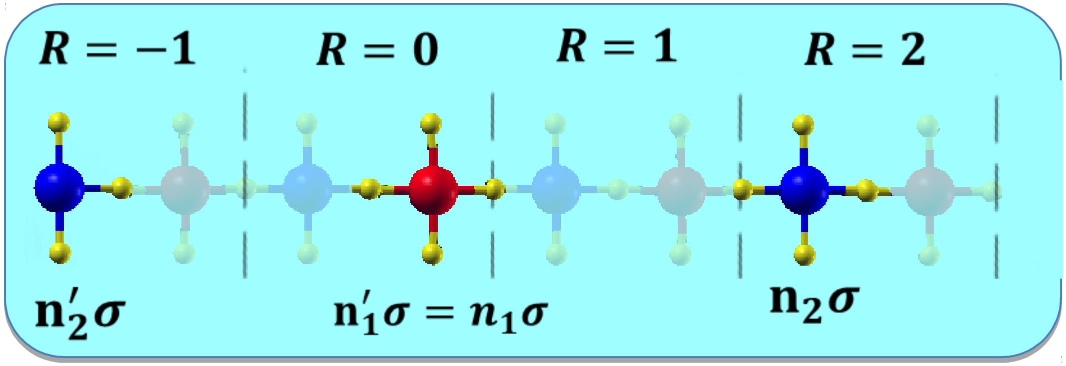
$$= \sum_{\vec{R}\,\vec{R}'} \sum_{\substack{n_1 n_2 \\ n_1' n_2'}} \sum_{\sigma} A_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q}+\vec{G})(\tilde{\chi}_s)^{\vec{0}\,n_1'\sigma;\vec{R}'n_2'\sigma}_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q},\omega)A^{*}_{\vec{0}\,n_1'\sigma\,;\vec{R}'\,n_2'\sigma}(\vec{q}+\vec{G}')$$





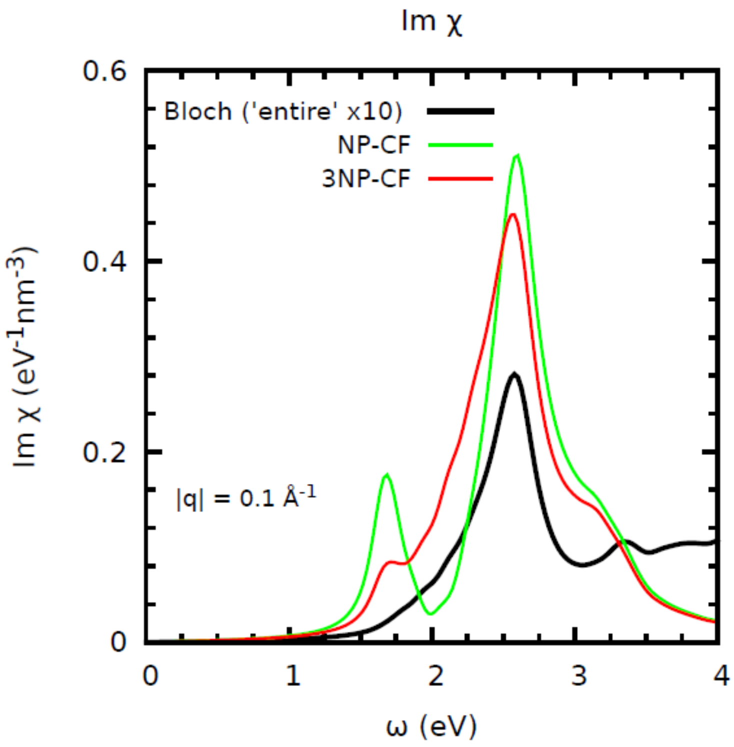
Nearest Plaquette Charge Fluctuations (NP-CF)

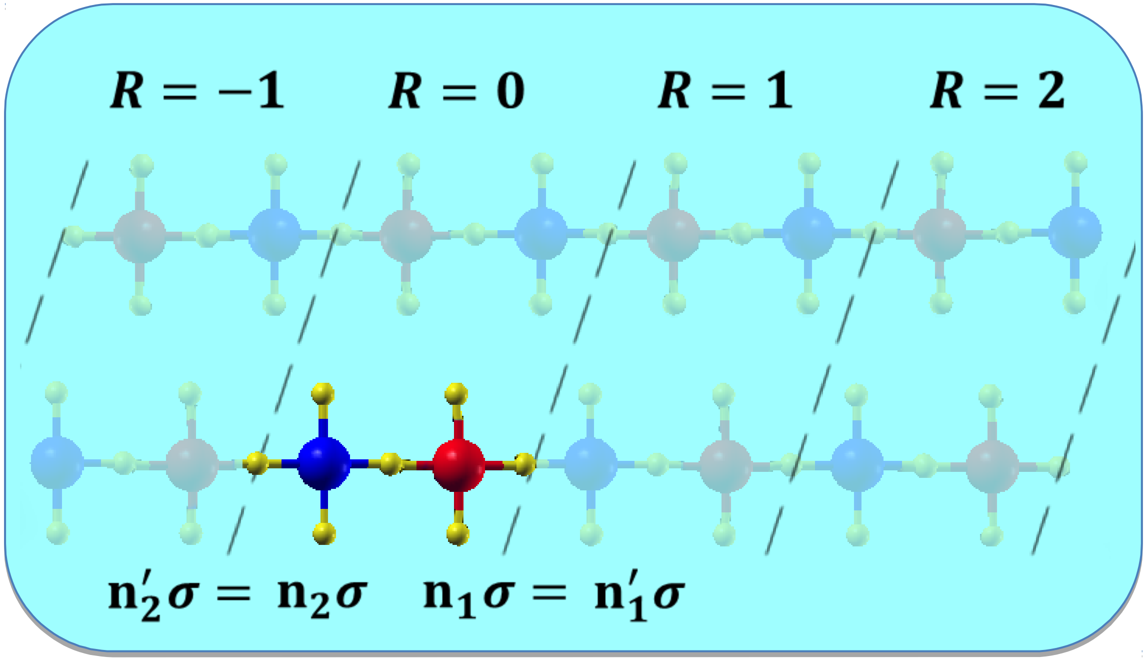




$$(\chi)_{\vec{G}\vec{G}'}(\vec{q},\omega)$$

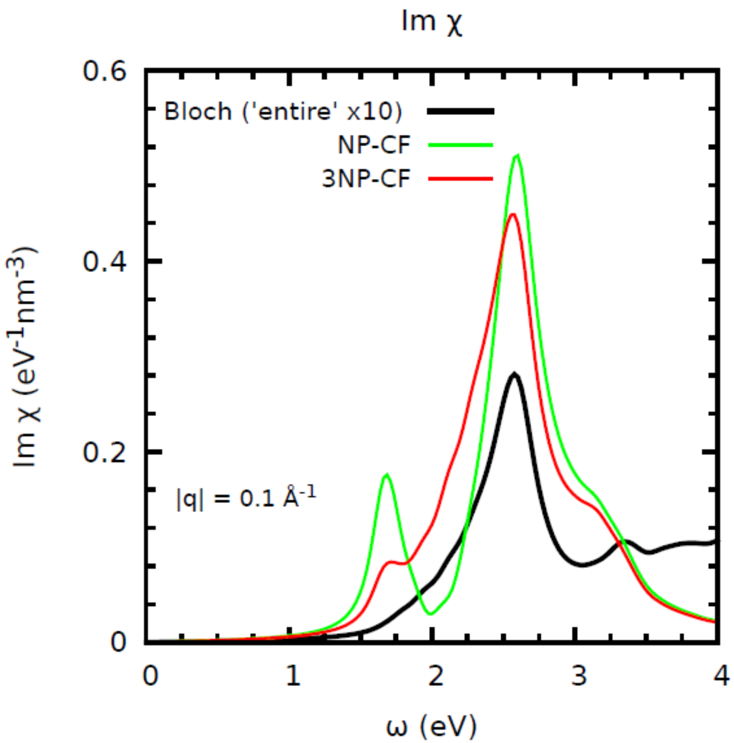
$$=\sum_{\vec{R}\,\vec{R}'}\sum_{\substack{n_1 n_2\\ n_1' n_2'}}\sum_{\sigma\sigma'} A_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q}+\vec{G})(\tilde{\chi})^{\vec{0}\,n_1'\sigma';\vec{R}'n_2'\sigma'}_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q},\omega)A^{*}_{\vec{0}\,n_1'\sigma'\,;\vec{R}'\,n_2'\sigma'}(\vec{q}+\vec{G}')$$

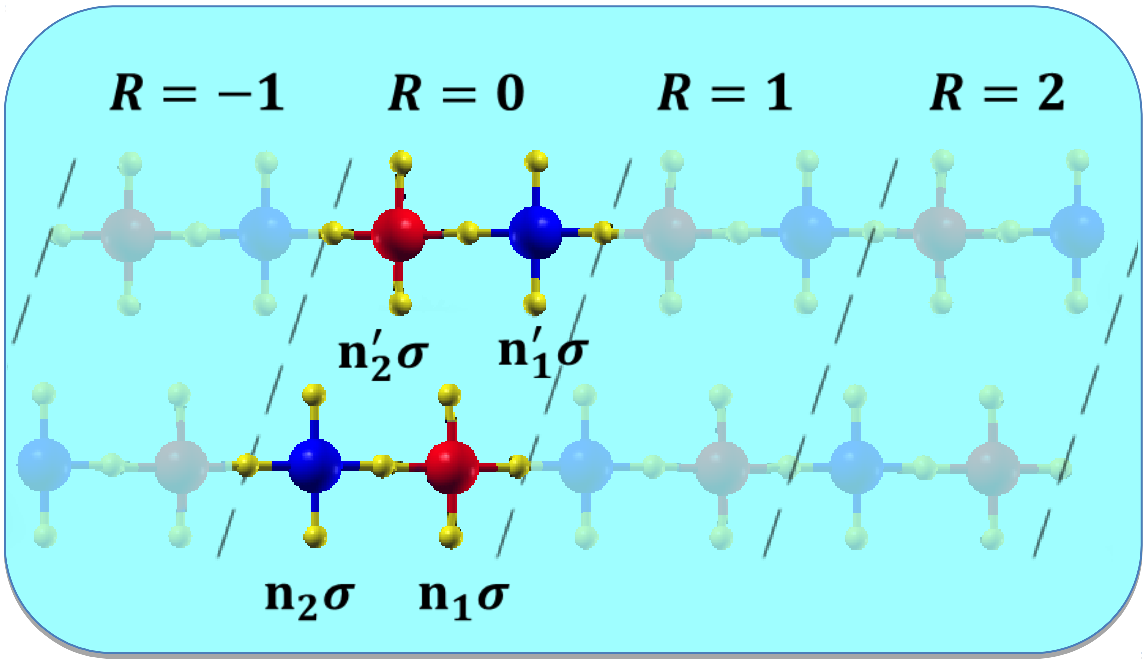




$$(\chi)_{\vec{G}\vec{G}'}(\vec{q},\omega)$$

$$= \sum_{\vec{R}\,\vec{R}'} \sum_{\substack{n_1 n_2 \\ n_1' n_2'}} \sum_{\sigma\sigma'} A_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q}+\vec{G})(\tilde{\chi})^{\vec{0}\,n_1'\sigma';\vec{R}'n_2'\sigma'}_{\vec{0}\,n_1\sigma\,;\vec{R}\,n_2\sigma}(\vec{q},\omega)A^{*}_{\vec{0}\,n_1'\sigma'\,;\vec{R}'\,n_2'\sigma'}(\vec{q}+\vec{G}')$$

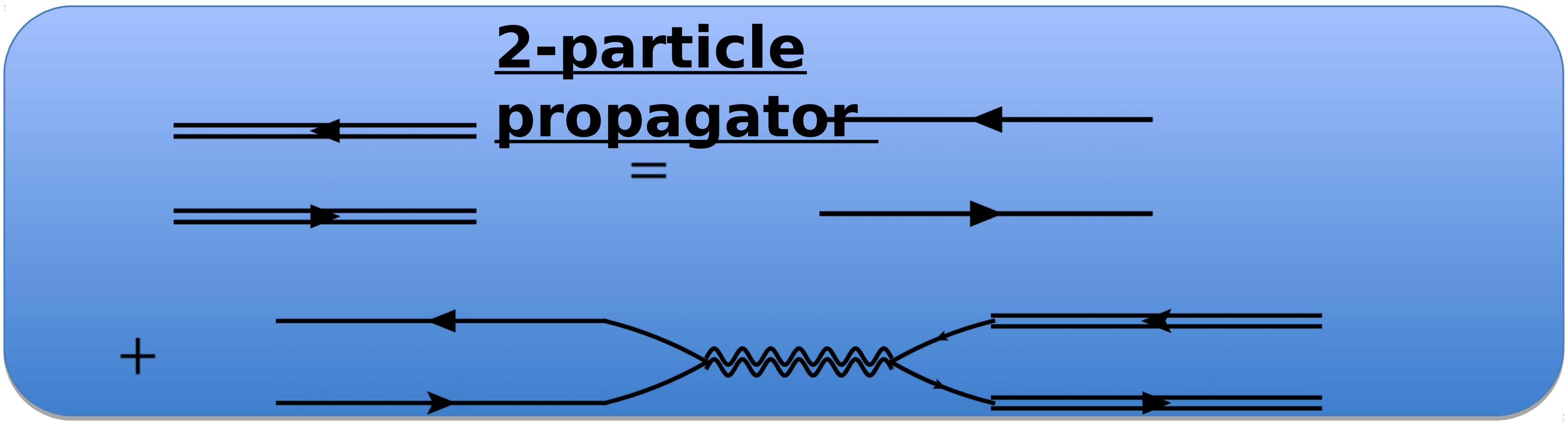




Understanding $\tilde{\chi}$

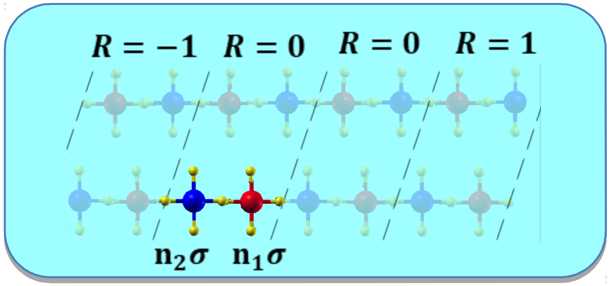
Understanding

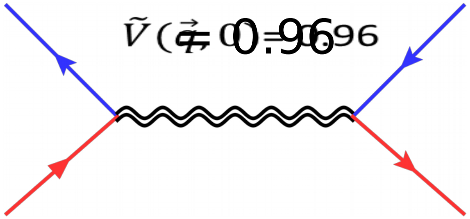
- $$(\tilde{\chi})^{\vec{0}\,n_1'\sigma';\vec{R}'n_2'\sigma'}_{\vec{0}\,n_1\sigma;\vec{R}\,n_2\,\sigma}(\vec{q},\omega) = \sum_{\vec{R}_1\vec{R}_1'}\sum_{\substack{n_3n_4\\n_3'n_4'}}\sum_{\sigma_1\sigma_1'}(\tilde{\chi}_s)^{\vec{0}\,n_3'\sigma;\vec{R}'n_4'\sigma}_{\vec{0}\,n_1\sigma;\vec{R}\,n_2\,\sigma}(\vec{q},\omega)\,[\{1-\tilde{V}(\vec{q},\omega)\tilde{\chi}_s(\vec{q},\omega)\}^{-1}]^{\vec{0}\,n_1'\sigma;\vec{R}'n_2'\sigma}_{\vec{0}\,n_1\sigma;\vec{R}\,n_2\,\sigma}$$



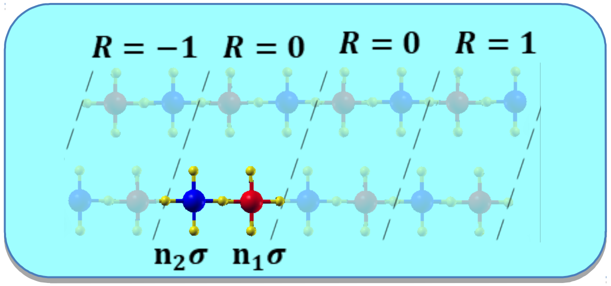
Effective interactions

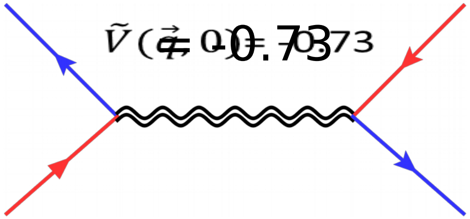
Particle-hole pair 2

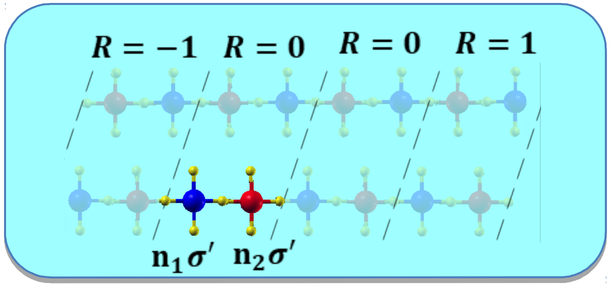


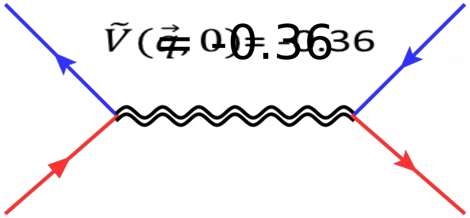


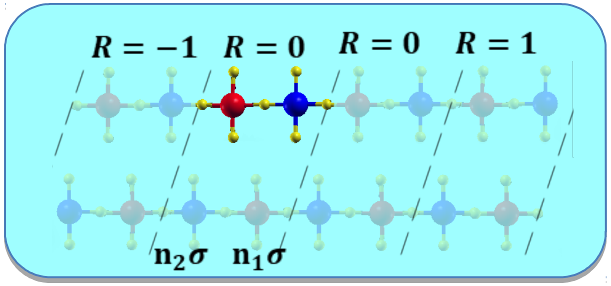
Particle-hole pair 1











Results for χ

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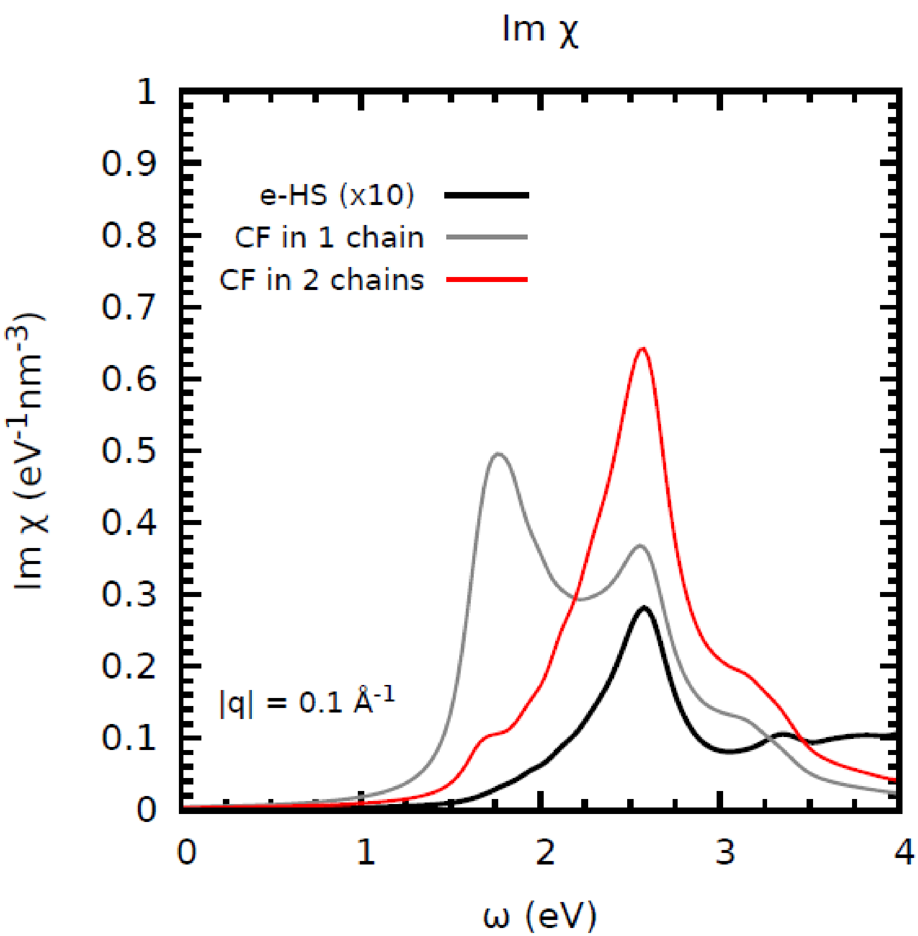

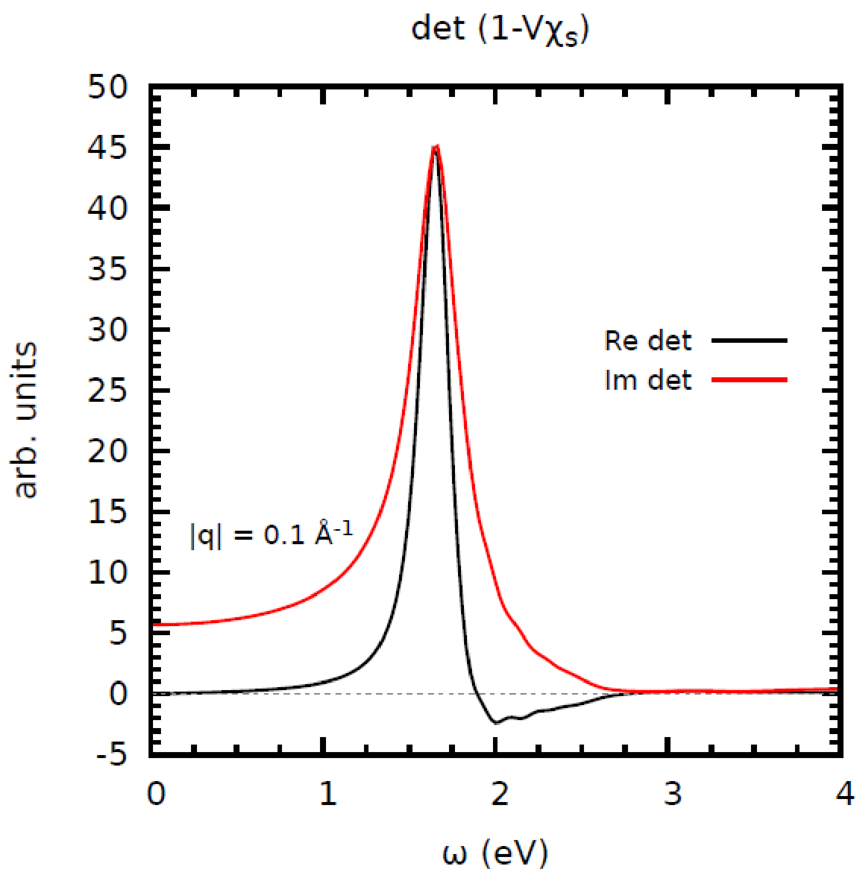

Conclusions

- We understood collective excitation using real space physics using TD-DFT.
- **Collective excitation is localized but is localized to 2 chains.**

Collaborators

Adolfo Eguiluz

Robert Van Wesep

Anton Kozhevnikov