Koopmans spectral functionals: theory and recent developments

Nicola Colonna

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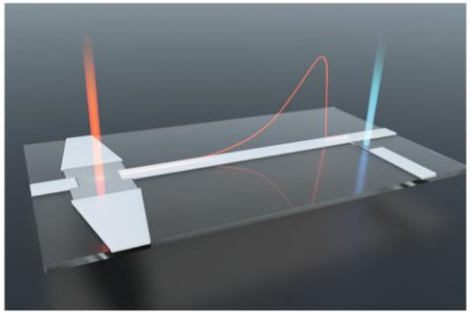
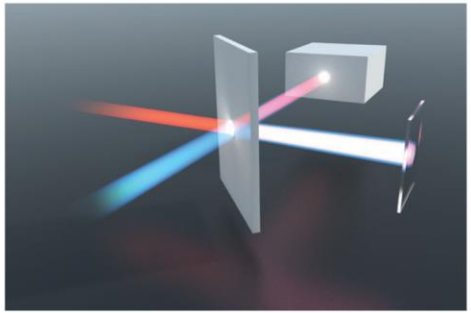
Spectral properties of materials

- Response of a system to external stimuli
- Connected to macroscopic materials properties



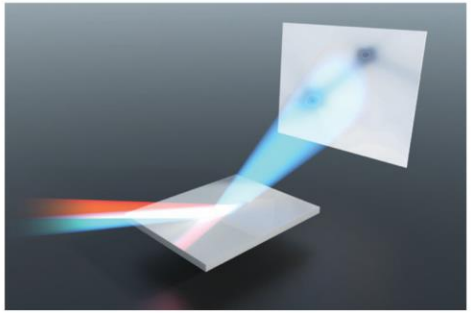
Transport

- Conductivity
- Carriers mobility



Optical probes

- Dielectric properties



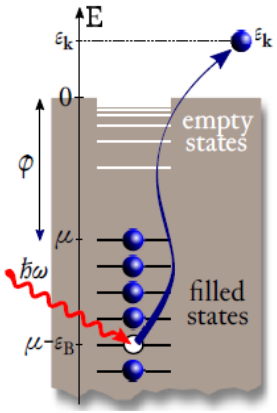
Scattering probes

- Structural properties
- Electronic degrees of freedom

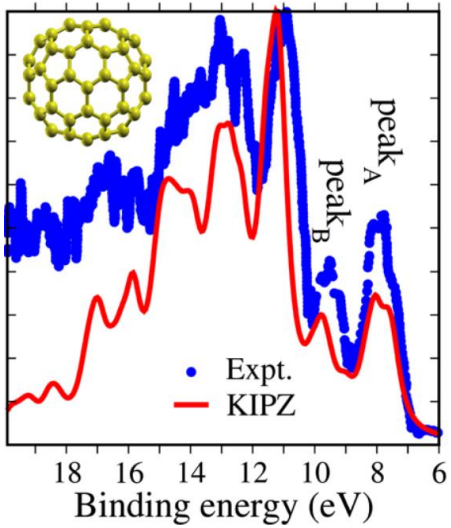
Rev. Mod. Phys. **93**, 041002 (2021)

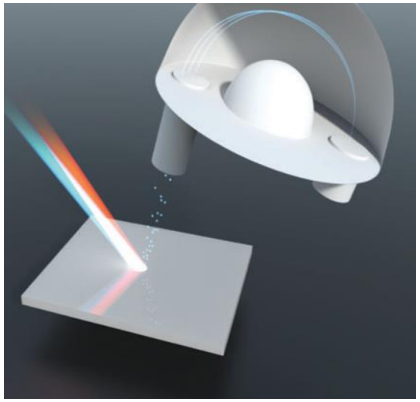
Spectral properties of materials

- Ultimately related to the underlying **electronic band structure**
- Band structure: directly probed with **photoemission spectroscopy**

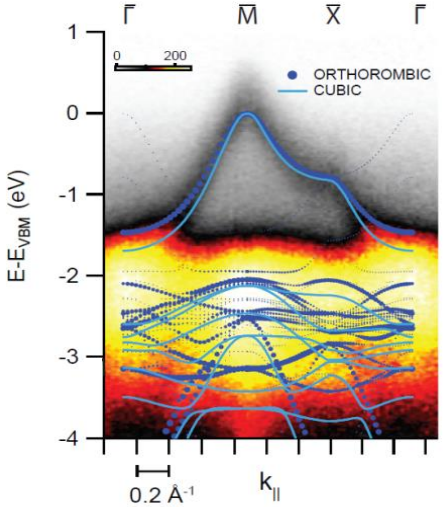


PES





Angle-resolved PES



Picture courtesy of Dr. Marco Vanzini
N.L. Nguyen *et al.* PRL **114**, 166405 (2015)

Rev. Mod. Phys. **93**, 041002 (2021)
M. Puppin, S. Polishchuk, **NC** *et al.* PRL **124**, 206402 (2020)

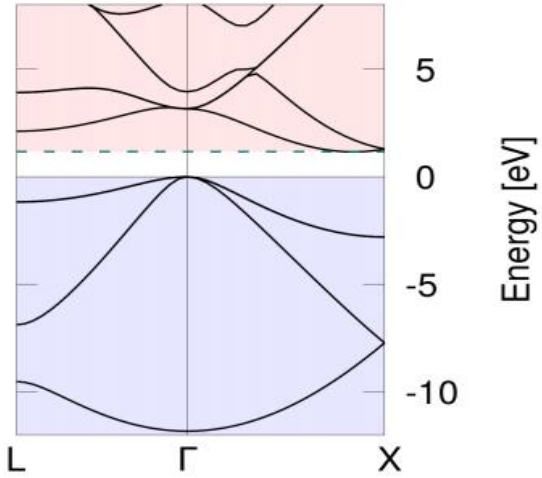
Density functional theory vs Green's functions

- **GW is accurate but complex** (non-local, and frequency dependent) and perturbative

GW

Green's function $G(\mathbf{r},\mathbf{r}',\omega)$

Silicon:
Exp. gap: 1.17 eV
G_0W_0 gap: 1.1-1.3 eV



Density functional theory vs Green's functions

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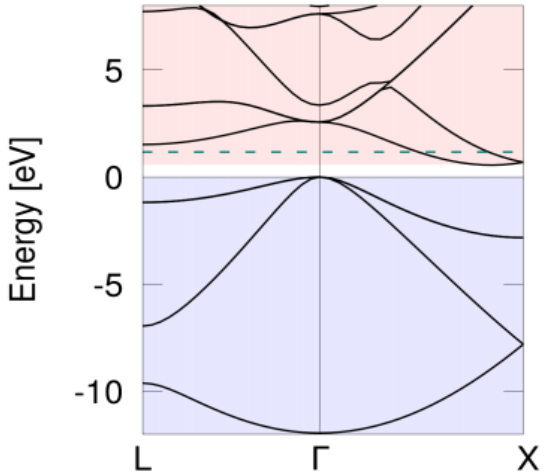
- **KS-DFT is simple** (local) but not rigorously justified (although frequently used)

DFT

Ground-state density $\rho(\mathbf{r})$



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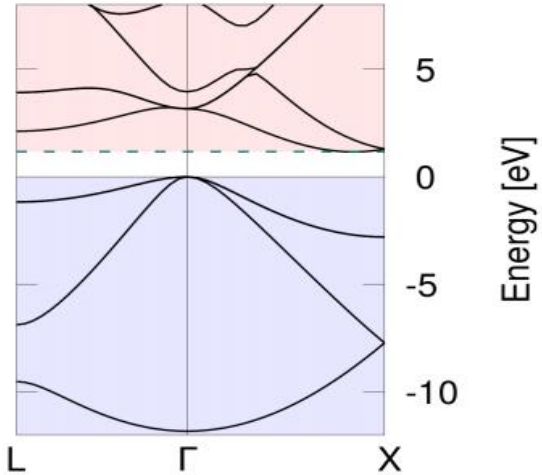

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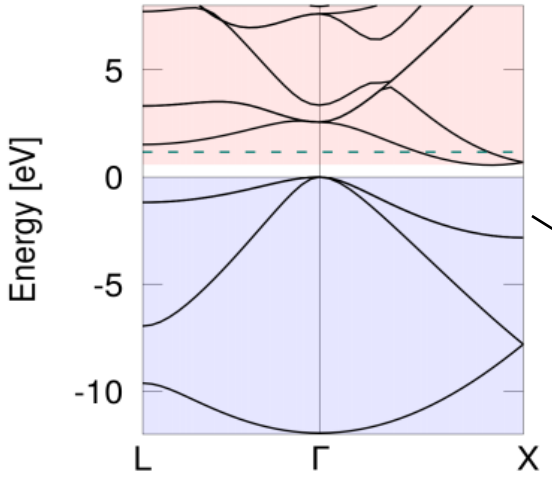

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Spectral functionals:
DFT efficiency +
GW accuracy

GW

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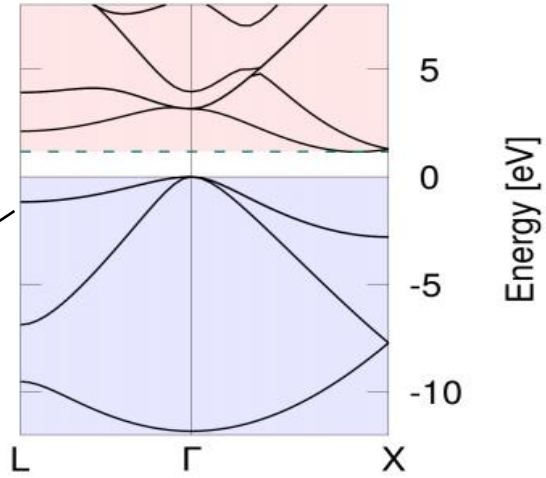
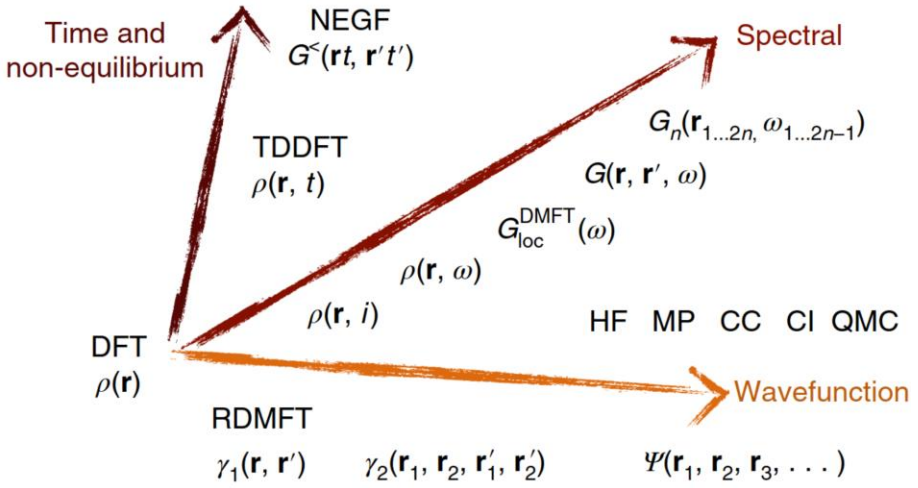


Goal: Spectral functionals

- **Spectral properties within a functional theory**
  (achieving for electronic excitations what DFT has achieved for GS properties)

- Need to go **beyond DFT**: a functional of the local static density $\rho(\boldsymbol{r})$ can only give total energy



Marzari, Ferretti, and Wolverton Nature Materials **20**, 736 (2021)

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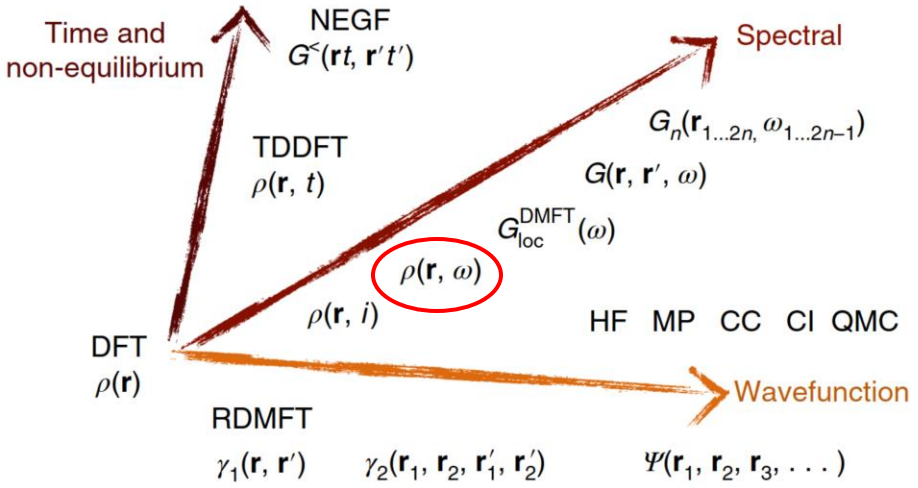

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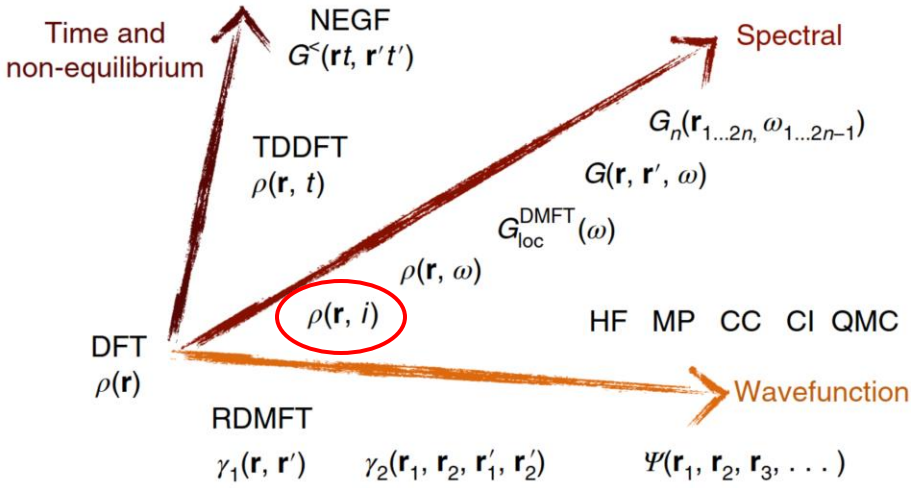
- In a quasi particle picture, $\rho(\boldsymbol{r},\omega) \rightarrow \rho(\boldsymbol{r},i)$: **orbital-density-dependent functionals**



Marzari, Ferretti, and Wolverton Nature Materials **20**, 736 (2021)

Koopmans-compliant spectral functionals

CORE IDEA:

For every orbital the expectation value

$$\varepsilon_i = \frac{dE}{df_i} = \langle \phi_i | \hat{H} | \phi_i \rangle$$

is **independent on its own occupation** and equal to

$$\varepsilon_i = E_i^{N\pm1} - E^N$$

I. Dabo *et al.* arXiv0910.2637 (2009)
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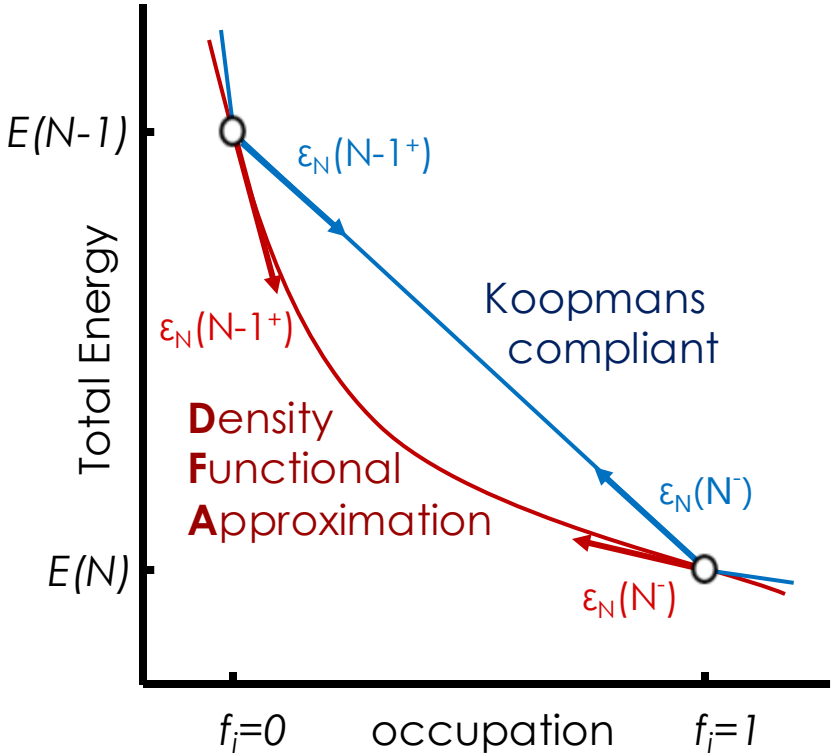

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Linearization

I. Dabo *et al.* PRB **82**, 115121 (2010); Borghi et *al.* PRB **90**, 075135 (2014)

$$E^{\mathrm{KC}} = E^{\mathrm{DFT}} + \sum_i \left[- \int_0^{f_i} ds \, \langle \phi_i | H^{\mathrm{DFT}}(s) | \phi_i \rangle + f_i \eta_i \right]$$

Remove the non-linear term

Add a Koopmans' term

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Basic variables: orbital densities

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correct leading quadratic error [N. Colonna *et al.*, JCTC **14**, 2549 (2018)]

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Similar to +U correction in DFT+U
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Similar to +U correction in DFT+U
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*Other KC flavors: **KI, KIPZ, pKIPZ***
(see Edward's talk)

Screening

I. Dabo *et al.* PRB **82**, 115121 (2010); N.L. Nguyen *et al.* PRX **8**, 021051 (2018); N. Colonna *et al.* JCTC **14**, 2549 (2018)

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Define an orbital-dependent **screening coefficient**:

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Alternatively, from finite differences (see Edward's talk): $\alpha_i = \dfrac{\Delta E_i^{\mathrm{DFT}} - H_{ii}^{\alpha=0}}{H_{ii}^{\alpha=1} - H_{ii}^{\alpha=0}}$

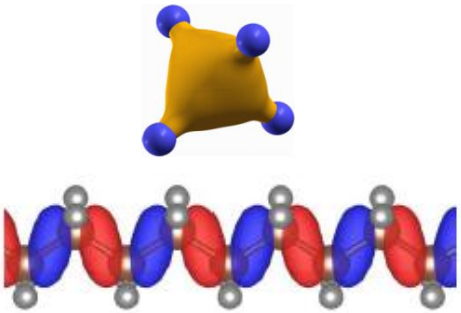
Localization

$$E_{gs}^{KC} = \min_{\{\phi_i\}} \left\{ E^{KC}[\{\rho_i\}] - \sum_{ij} \Lambda_{ji}(\langle\phi_i|\phi_j\rangle - \delta_{ji}) \right\}$$

At the minimum: $\langle\phi_j|\hat{h}_i^{KC}|\phi_i\rangle = \langle\phi_j|\hat{h}_j^{KC}|\phi_i\rangle$ ⇨ Λ is Hermitian

M. Pederson *et al.* JCP **80**, 1972 (1984)

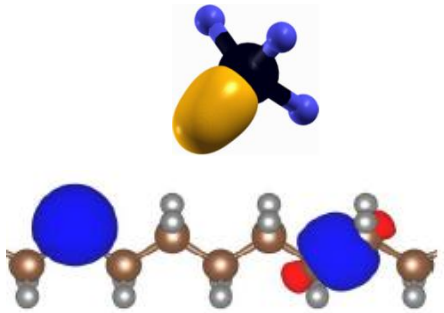
CANONICAL



$$\lambda_m = \sum_{ij} U_{mj}\Lambda_{ji}U_{im}^{\dagger}$$

$$|\psi_m\rangle = \sum_{i} |\phi_i\rangle U_{im}^{\dagger}$$

VARIATIONAL



Localization: key feature for application to extended systems!

Koopmans spectral functionals: Summary

$$E^{\mathrm{KC}}[\rho,\{\rho_i\}] = E^{\mathrm{DFT}}[\rho] + \sum_i \alpha_i \Pi_i^{\mathrm{KC}}[\rho_i]$$

- **Orbital densities** as fundamental variables: $\rho_i(\mathbf{r}) = f_i|\phi_i(\mathbf{r})|^2$
- **Linearization**: $\dfrac{dE}{df_i} = E_i^{N\pm1} - E^N$

I. Dabo *et al.* arXiv0910.2637 (2009); I. Dabo *et al.* PRB **82**, 115121 (2010)

- **Screening/Relaxation** upon electron addition/removal: $\alpha_i = \dfrac{\langle n_i|\varepsilon^{-1} f_{\mathrm{Hxc}}^{\mathrm{DFT}}|n_i\rangle}{\langle n_i|f_{\mathrm{Hxc}}^{\mathrm{DFT}}|n_i\rangle}$

I. Dabo *et al.* PRB **82**, 115121 (2010); N. Colonna *et al.* JCTC **14**, 2549 (2018)

- **Localization** (key feature for extended system applications)

N.L. Nguyen *et al.* PRX **8**, 021051 (2018)

Comparison with DFT+U

	DFT+U	Koopmans
Seeks to correct …	Erroneous global curvature in total energy w.r.t. N	Erroneous global curvature in total energy w.r.t. **canonical** occupancies

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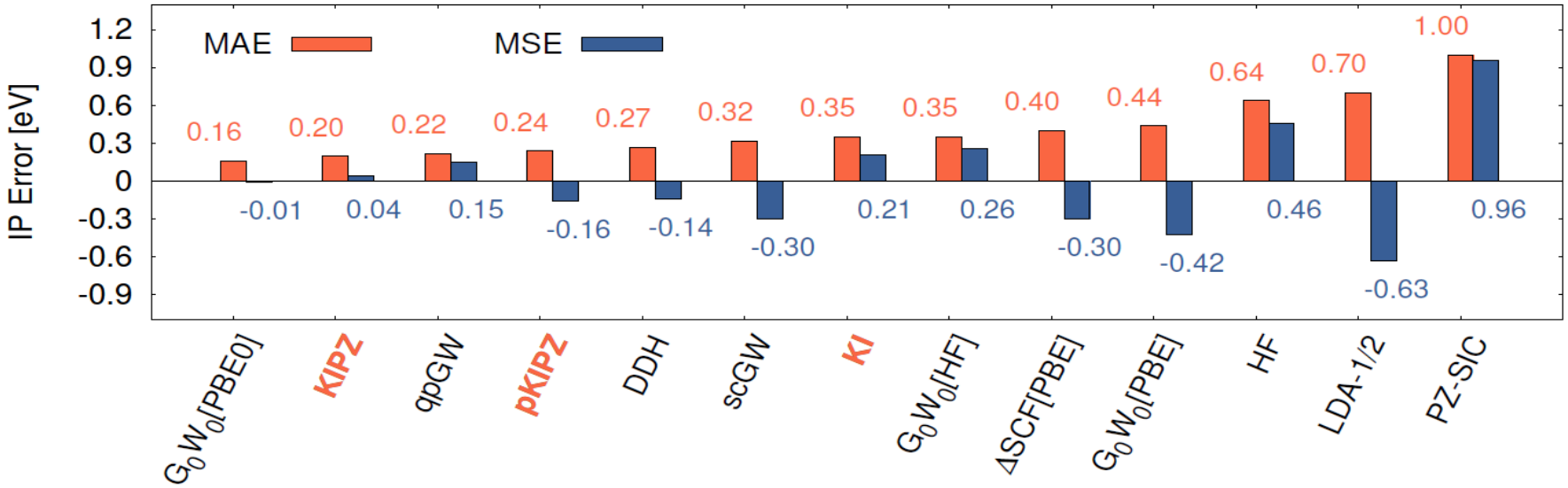
Parametrized by …	Hubbard paramenters: $\{U_I\}$	Screening coefficients: $\{a_i\}$

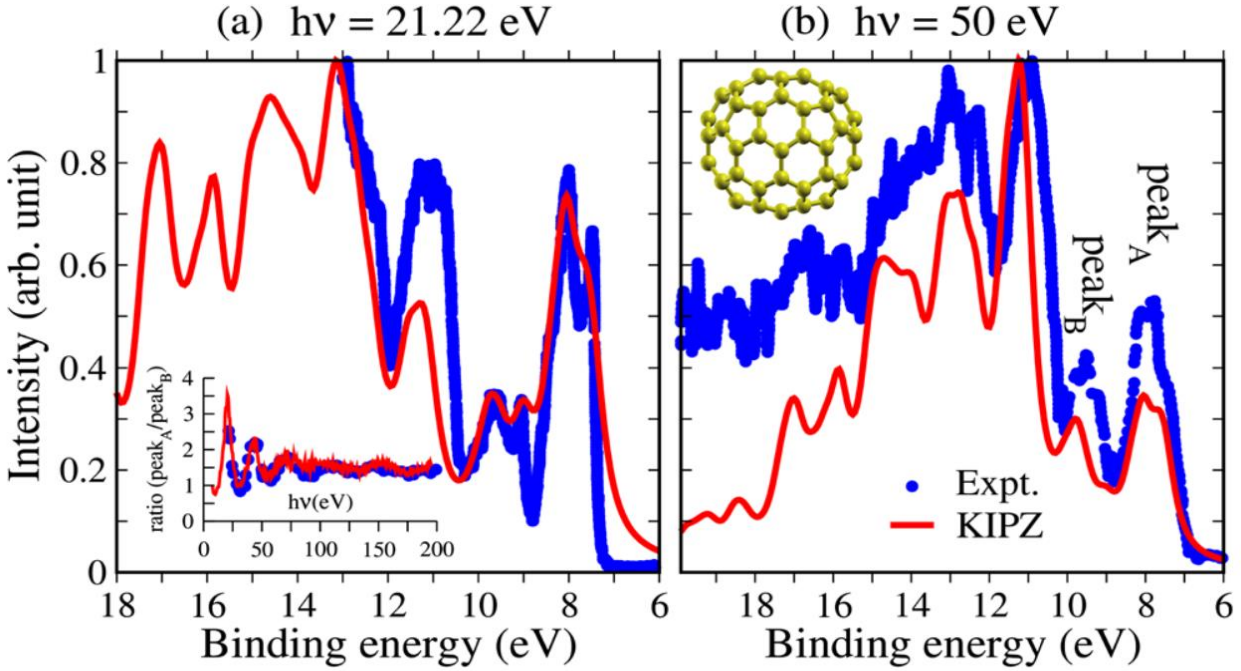
Benchmarks: GW100 Test Set



Method	***Basic variable***	***Complexity***
LDA-1/2	$\rho(\mathbf{r})$	*Local*
KI / KIPZ	$\rho_i(\mathbf{r})$	*Local and orbital-dependent*
HF / DDH	$\gamma(\mathbf{r},\mathbf{r'})$	*Non-local*
GW	$G(\mathbf{r},\mathbf{r'},\omega)$	*Non-local and frequency dependent*

N. Colonna *et al.* JCTC **15**, 1905 (2019)

Photo-emission of molecules: C_{70} fullerene

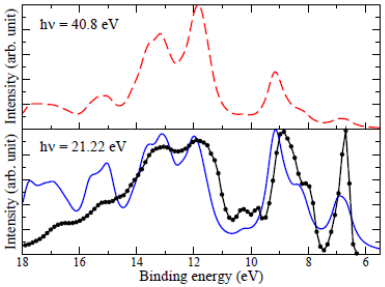


	PBE	scf-GW	KIPZ	Exp
$Peak_A$ (eV)	5.60	7.45	**7.42**	**7.48**

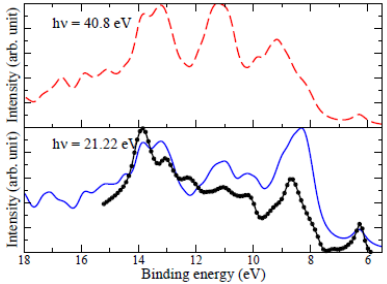
N.L. Nguyen et al. PRL **114**, 166405 (2015)

Photo-emission of molecules

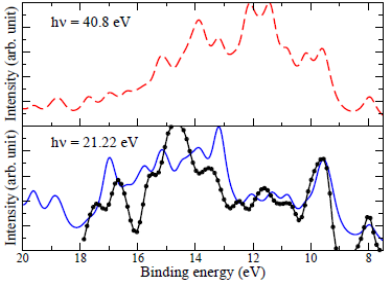
Porphyne



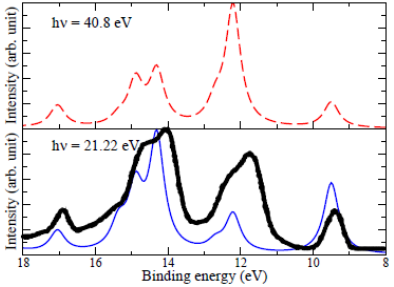
Phthalocyanine



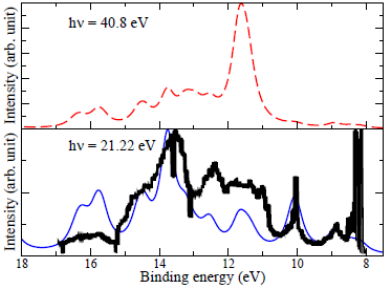
PTCDA



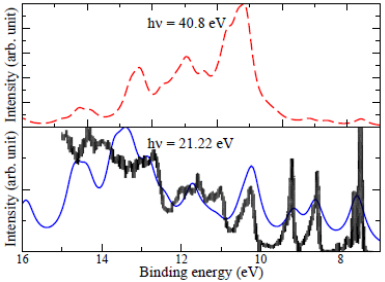
Benzene



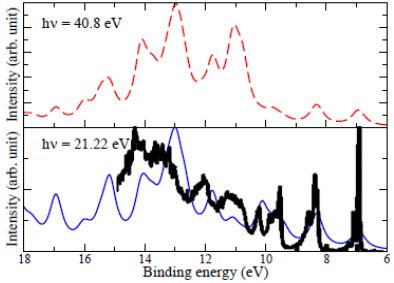
Naphthalene



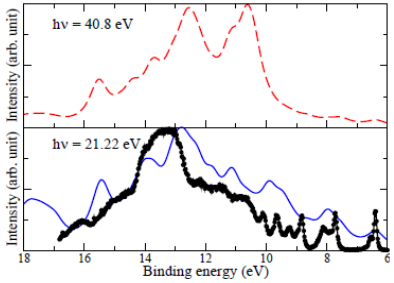
Antracene



Tetracene

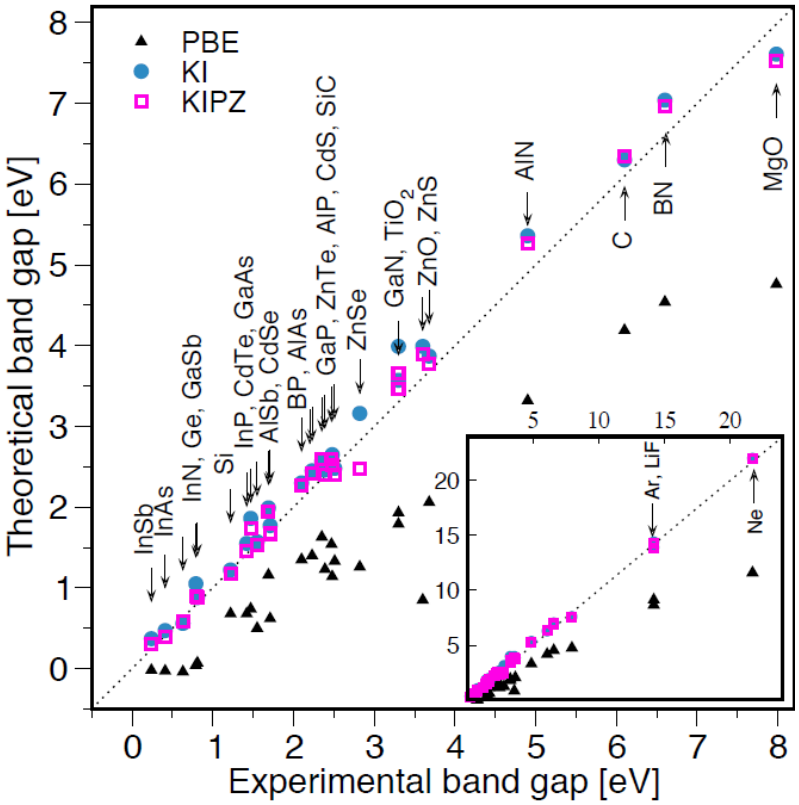


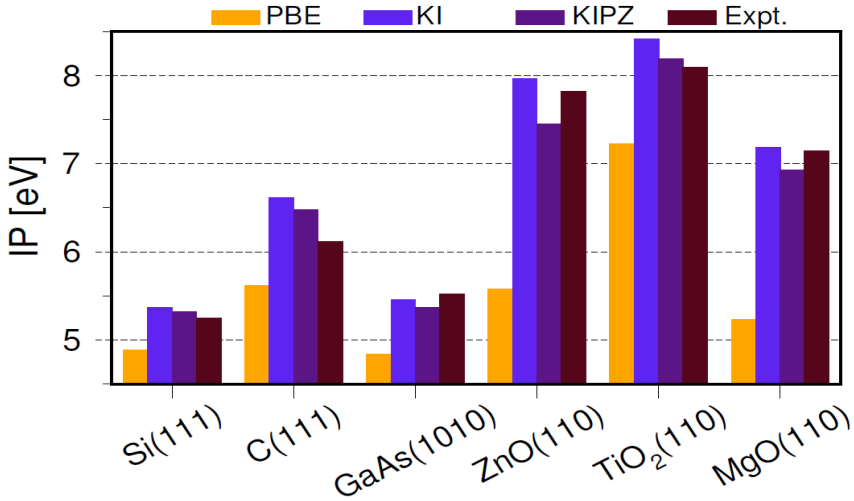
Pentacene



N.L. Nguyen *et al.* PRL **114**, 166405 (2015)

Band gaps and IPs in semiconductors



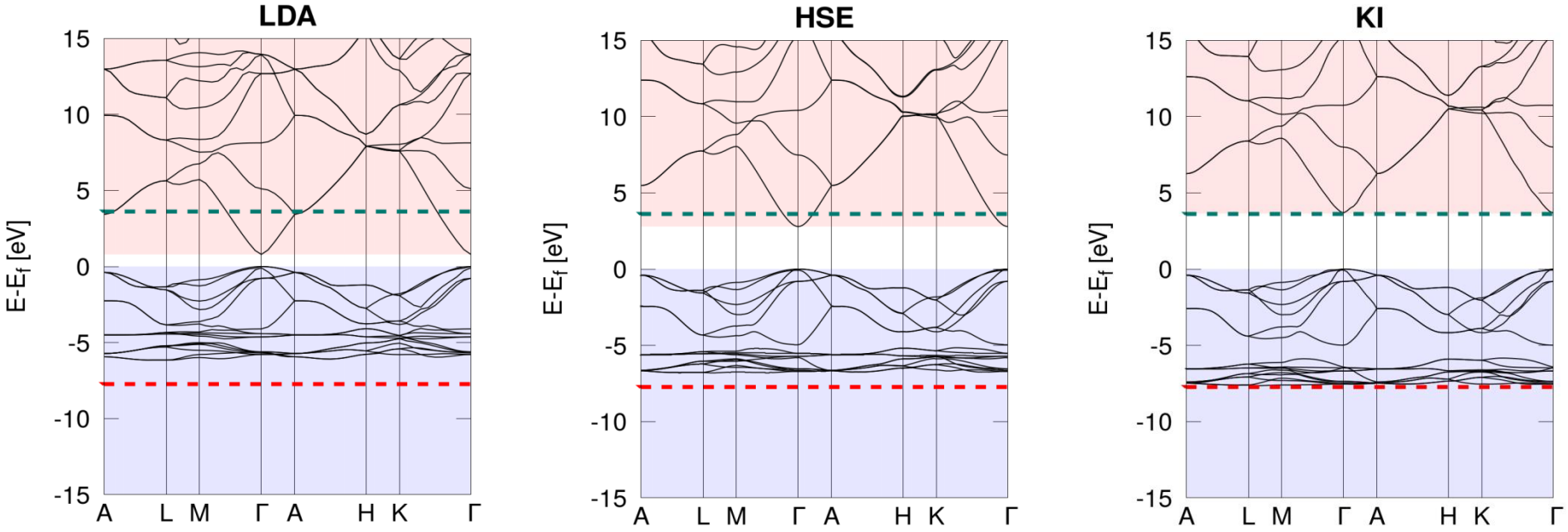


MAE (eV)

	G_0W_0	QSG$\widetilde{W}$	KI	KIPZ
GAP	0.56	**0.18**	0.27	**0.22**
IP	**0.39**	0.49	0.19	**0.21**

N.L. Nguyen, **NC** *et al.* PRX **8**, 021051 (2018)

ZnO band structure



	LDA	HSE	GW_0	$scGW\tilde{W}$	KI	Exp
E_g (eV)	0.79	2.79	3.0	3.2	**3.62**	**3.60**
ε_d (eV)	-5.1	-6.1	-6.4	-6.7	**-6.9**	**[-7.5;-8.0]**
IP[110](eV)		7.11	7.17	8.24	**7.97**	**7.82**

N. Colonna *et al.* JCTC **18**, 5435 (2022)

Non-collinear extension

Requires an extension of the theory:

$$n_i(\mathbf{r}) \rightarrow \boldsymbol{n}_i(\mathbf{r}) = \underline{\{n_i(\mathbf{r}), m_x^i(\mathbf{r}), m_y^i(\mathbf{r}), m_z^i(\mathbf{r})\}}$$

$$n_i(\mathbf{r}) = \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})$$

$$\boldsymbol{m}_i(\mathbf{r}) = \mu_B \psi_i^\dagger(\mathbf{r})\boldsymbol{\sigma}\psi_i(\mathbf{r})$$

A. Marrazzo and N. Colonna, PRR **6**, 033085 (2024)

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1. Energy correction:

$$\Pi_i^{\mathrm{qKI}} = \frac{1}{2} f_i(1-f_i)\langle n_i|f_{\mathrm{Hxc}}|n_i\rangle \quad \Rightarrow \quad \Pi_i^{\mathrm{qKI}} = \frac{1}{2} f_i(1-f_i)\langle \boldsymbol{n}_i|\boldsymbol{f}_{\mathrm{Hxc}}|\boldsymbol{n}_i\rangle$$

$$f_{\mathrm{Hxc}}(\boldsymbol{r},\boldsymbol{r}') = \frac{\delta E_{\mathrm{Hxc}}^{\mathrm{DFT}}}{\delta\rho(\boldsymbol{r})\delta\rho(\boldsymbol{r}')} \quad \Rightarrow \quad \boldsymbol{f}_{Hxc}(\boldsymbol{r},\boldsymbol{r}') = \frac{\delta E_{\mathrm{Hxc}}^{\mathrm{DFT}}}{\delta\boldsymbol{\rho}(\boldsymbol{r})\delta\boldsymbol{\rho}(\boldsymbol{r}')} = \begin{pmatrix} f_{Hxc}^{\rho,\rho} & f_{xc}^{\rho,m_x} & f_{xc}^{\rho,m_y} & f_{xc}^{\rho,m_z} \\ f_{xc}^{m_x,\rho} & f_{xc}^{m_x,m_x} & f_{xc}^{m_x,m_y} & f_{xc}^{m_x,m_z} \\ f_{xc}^{m_y,\rho} & f_{xc}^{m_y,m_x} & f_{xc}^{m_y,m_y} & f_{xc}^{m_y,m_z} \\ f_{xc}^{m_z,\rho} & f_{xc}^{m_z,m_x} & f_{xc}^{m_z,m_y} & f_{xc}^{m_z,m_z} \end{pmatrix}$$

A. Marrazzo and N. Colonna, PRR **6**, 033085 (2024)

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$$n_i(\mathbf{r}) = \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})$$

$$\boldsymbol{m}_i(\mathbf{r}) = \mu_B \psi_i^\dagger(\mathbf{r})\boldsymbol{\sigma}\psi_i(\mathbf{r})$$

2. Screening coefficients

$$\alpha_i = \frac{\langle n_i|\epsilon^{-1} f_{\mathrm{Hxc}}|n_i\rangle}{\langle n_i|f_{\mathrm{Hxc}}|n_i\rangle} \quad \Rightarrow \quad \alpha_i = \frac{\langle \boldsymbol{n}_i|\boldsymbol{\epsilon}^{-1} \boldsymbol{f}_{\mathrm{Hxc}}|\boldsymbol{n}_i\rangle}{\langle \boldsymbol{n}_i|\boldsymbol{f}_{\mathrm{Hxc}}|\boldsymbol{n}_i\rangle}$$

$$\epsilon^{-1} = 1 + f_{\mathrm{Hxc}}\chi \quad \Rightarrow \quad \boldsymbol{\epsilon}^{-1} = \mathbf{1} + \boldsymbol{f}_{\mathrm{Hxc}}\boldsymbol{\chi}$$

$$\boldsymbol{\chi}(\boldsymbol{r}, \boldsymbol{r}') = \begin{pmatrix} \chi^{\rho,\rho} & \chi^{\rho,m_x} & \chi^{\rho,m_y} & \chi^{\rho,m_z} \\ \chi^{m_x,\rho} & \chi^{m_x,m_x} & \chi^{m_x,m_y} & \chi^{m_x,m_z} \\ \chi^{m_y,\rho} & \chi^{m_y,m_x} & \chi^{m_y,m_y} & \chi^{m_y,m_z} \\ \chi^{m_z,\rho} & \chi^{m_z,m_x} & \chi^{m_z,m_y} & \chi^{m_z,m_z} \end{pmatrix}$$

A. Marrazzo and N. Colonna, PRR **6**, 033085 (2024)

Non-collinear extension

$$\mathcal{V}_i^{KI(2)}(\mathbf{r}) = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\boldsymbol{n}_i(\mathbf{r})\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}')\boldsymbol{n}_i(\mathbf{r}')\sigma_0 + (1-f_i)\sum_\alpha \int d\mathbf{r}' \left[\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}')\boldsymbol{n}_i(\mathbf{r}')\right]_\alpha \sigma_\alpha$$

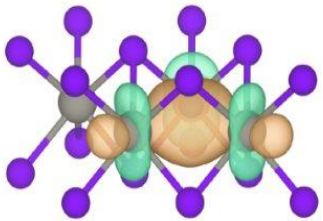
Wannier function charge density / Wannier function spin density

$$\left(n_\rho(\mathbf{r}), n_{m_x}(\mathbf{r}), n_{m_y}(\mathbf{r}), n_{m_z}(\mathbf{r})\right) \cdot \begin{pmatrix} \mathbb{F}_{Hxc}^{\rho,\rho} & \mathbb{F}_{xc}^{\rho,m_x} & \mathbb{F}_{xc}^{\rho,m_y} & \mathbb{F}_{xc}^{\rho,m_z} \\ \mathbb{F}_{xc}^{m_x,\rho} & \mathbb{F}_{xc}^{m_x,m_x} & \mathbb{F}_{xc}^{m_x,m_y} & \mathbb{F}_{xc}^{m_x,m_z} \\ \mathbb{F}_{xc}^{m_y,\rho} & \mathbb{F}_{xc}^{m_y,m_x} & \mathbb{F}_{xc}^{m_y,m_y} & \mathbb{F}_{xc}^{m_y,m_z} \\ \mathbb{F}_{xc}^{m_z,\rho} & \mathbb{F}_{xc}^{m_z,m_x} & \mathbb{F}_{xc}^{m_z,m_y} & \mathbb{F}_{xc}^{m_z,m_z} \end{pmatrix} \cdot \begin{pmatrix} n_\rho(\mathbf{r}) \\ n_{m_x}(\mathbf{r}) \\ n_{m_y}(\mathbf{r}) \\ n_{m_z}(\mathbf{r}) \end{pmatrix}$$

charge-charge interaction; charge-spin interaction; spin-spin interaction

screened interaction = un-screened interaction + interacting response function

$$\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}') = \mathbf{F}_{Hxc}(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}''\mathbf{F}_{Hxc}(\mathbf{r},\mathbf{r}'')\int d\mathbf{r}'''\chi(\mathbf{r}'',\mathbf{r}''')\mathbf{F}_{Hxc}(\mathbf{r}''',\mathbf{r}')$$



charge-charge; charge-spin; spin-spin

$$\begin{pmatrix} \chi^{\rho,\rho} & \chi^{\rho,m_x} & \chi^{\rho,m_y} & \chi^{\rho,m_z} \\ \chi^{m_x,\rho} & \chi^{m_x,m_x} & \chi^{m_x,m_y} & \chi^{m_x,m_z} \\ \chi^{m_y,\rho} & \chi^{m_y,m_x} & \chi^{m_y,m_y} & \chi^{m_y,m_z} \\ \chi^{m_z,\rho} & \chi^{m_z,m_x} & \chi^{m_z,m_y} & \chi^{m_z,m_z} \end{pmatrix} \cdot \begin{pmatrix} F_{Hxc}^{\rho,\rho} & F_{xc}^{\rho,m_x} & F_{xc}^{\rho,m_y} & F_{xc}^{\rho,m_z} \\ F_{xc}^{m_x,\rho} & F_{xc}^{m_x,m_x} & F_{xc}^{m_x,m_y} & F_{xc}^{m_x,m_z} \\ F_{xc}^{m_y,\rho} & F_{xc}^{m_y,m_x} & F_{xc}^{m_y,m_y} & F_{xc}^{m_y,m_z} \\ F_{xc}^{m_z,\rho} & F_{xc}^{m_z,m_x} & F_{xc}^{m_z,m_y} & F_{xc}^{m_z,m_z} \end{pmatrix}$$

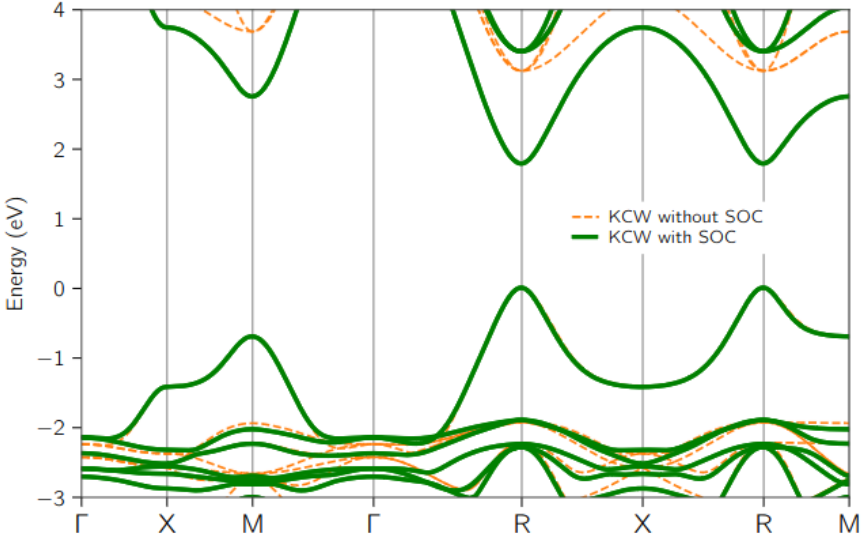
Spin-dependent interactions and **screening** effects **beyond** the random phase approximation (GW)

Available in QE v7.4: **`KCW`** package

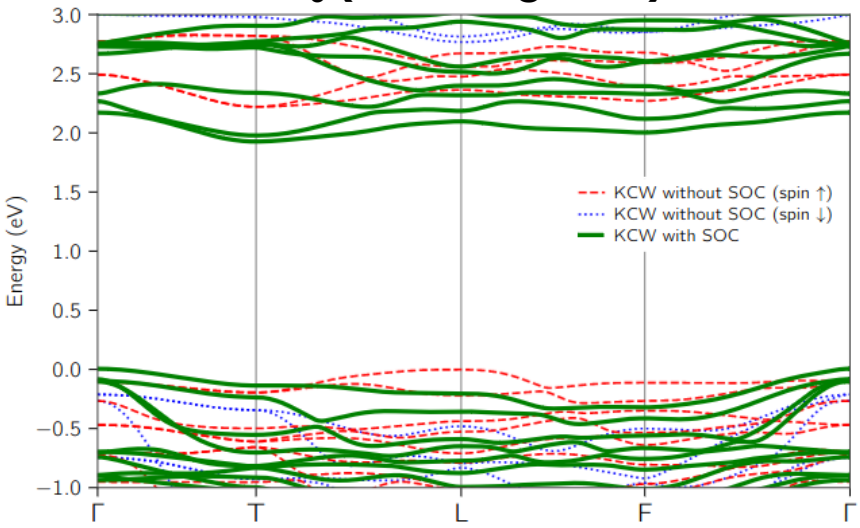
A. Marrazzo and N. Colonna, PRR **6**, 033085 (2024)

Non-collinear extension

$CsPbBr_3$ (non magnetic)



CrI_3 (ferromagnetic)



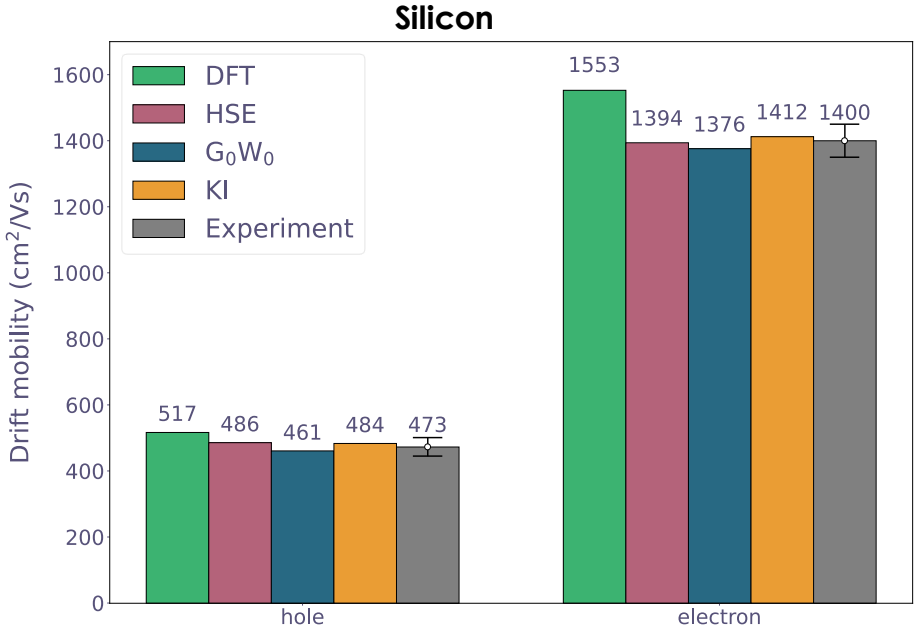
	LDA	HSE	G_0W_0	QSGW*	KI	Exp.
$CsPbBr_3$	0.18	0.78	0.94	1.53	**1.78**	**1.85**
CrI_3	0.43	1.65	1.99	2.2 - 2.5	**1.92**	**2.2**

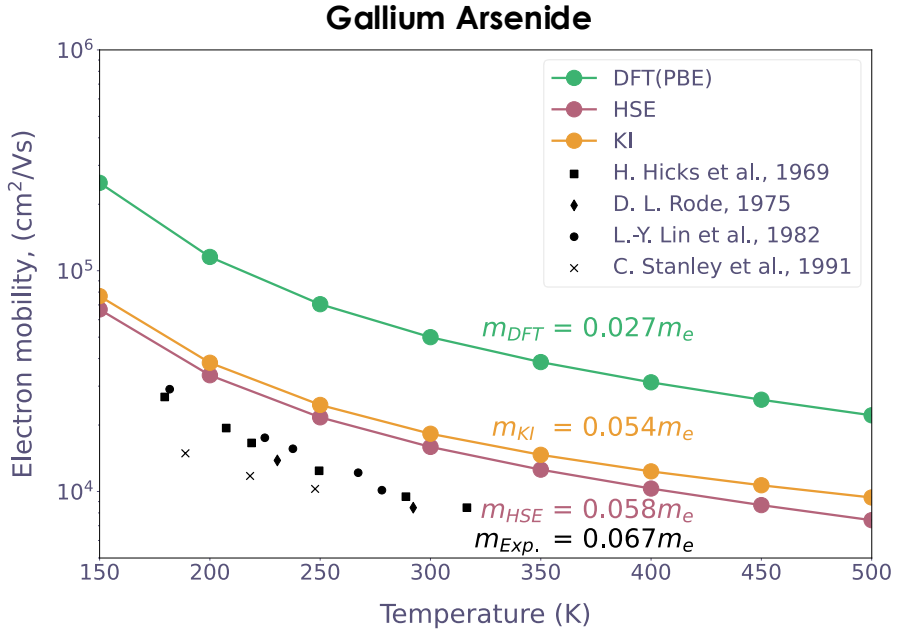
Results as good as state-of-the-art GW (QSGW plus vertex corrections)

A. Marrazzo and N. Colonna, PRR **6**, 033085 (2024)

Interaction with the nuclei

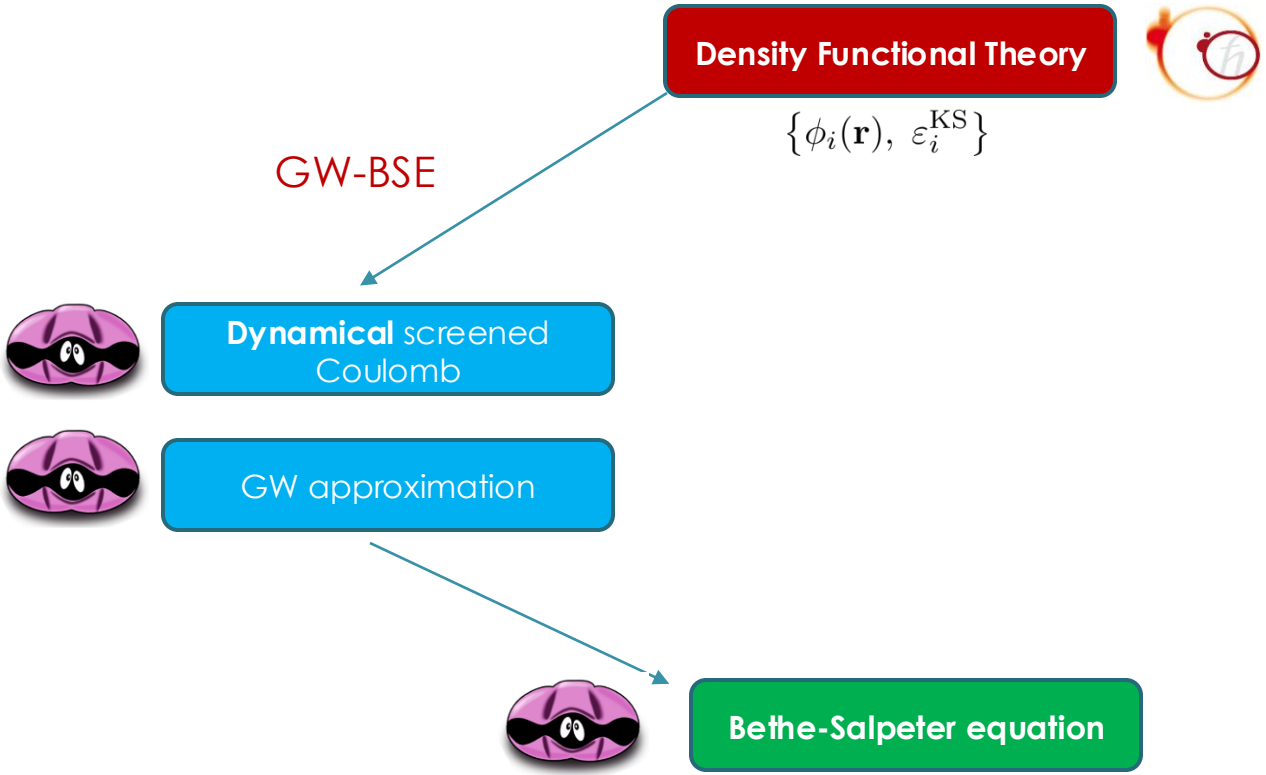
Electron-phonon interaction
(temperature dependence, **transport**,
BCS superconductivity, …)





A. Poliukhin, **NC** *et al.* npj Comp. Mat. **12**, 151 (2026)

Optical spectra: Koopmans meets Bethe-Salpeter



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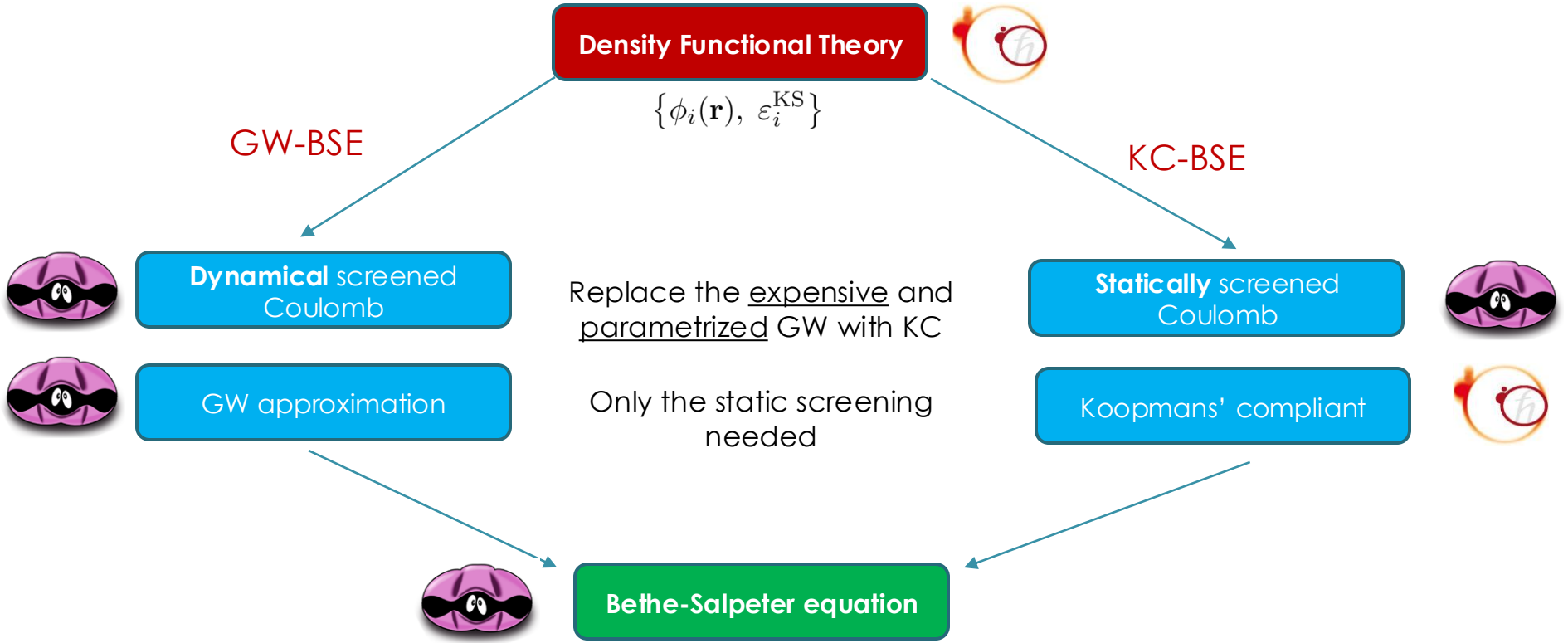


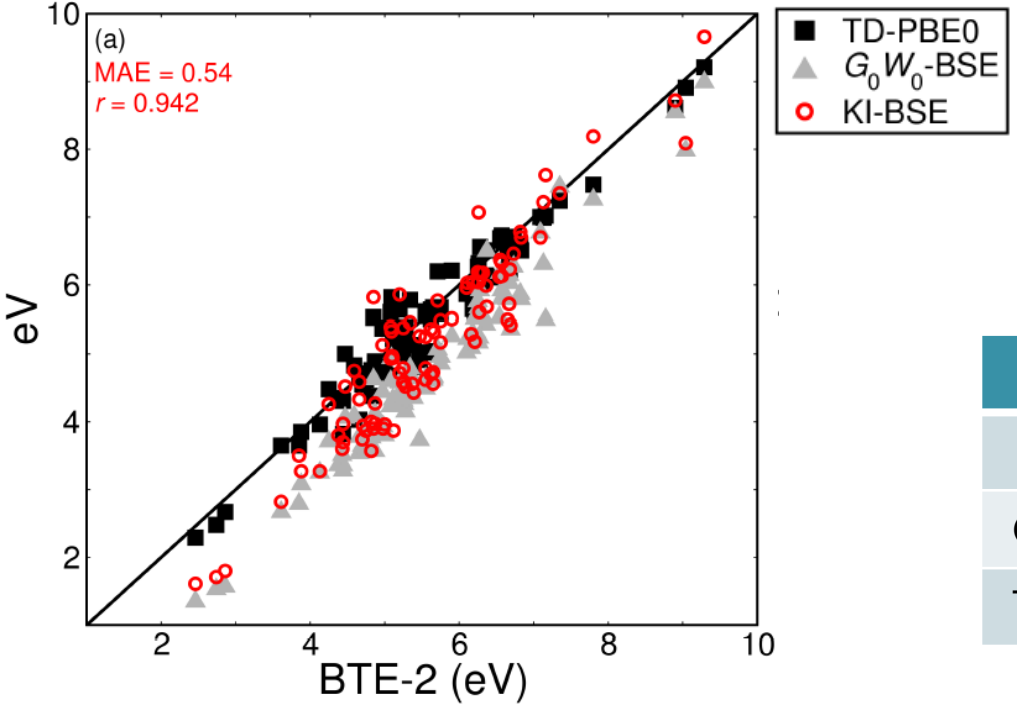
J. Elliott, **N. Colonna**, *et al.* JCTC **15**, 3710 (2019); M. Bonacci *et al. in preparation* (2026)

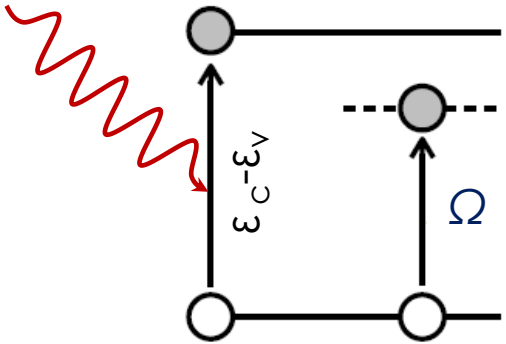
Finite systems: Thiel's set benchmark

BTE-2: Schreiber et al. J. Chem. Phys **128**, 134110 (2008)

G_0W_0: Bruneval et al., J. Chem. Phys. **142** , 244101 (2015)

TD-PBE0: Jaquemin et al., J. Chem. Theory Comput. **5**, 2420 (2009)





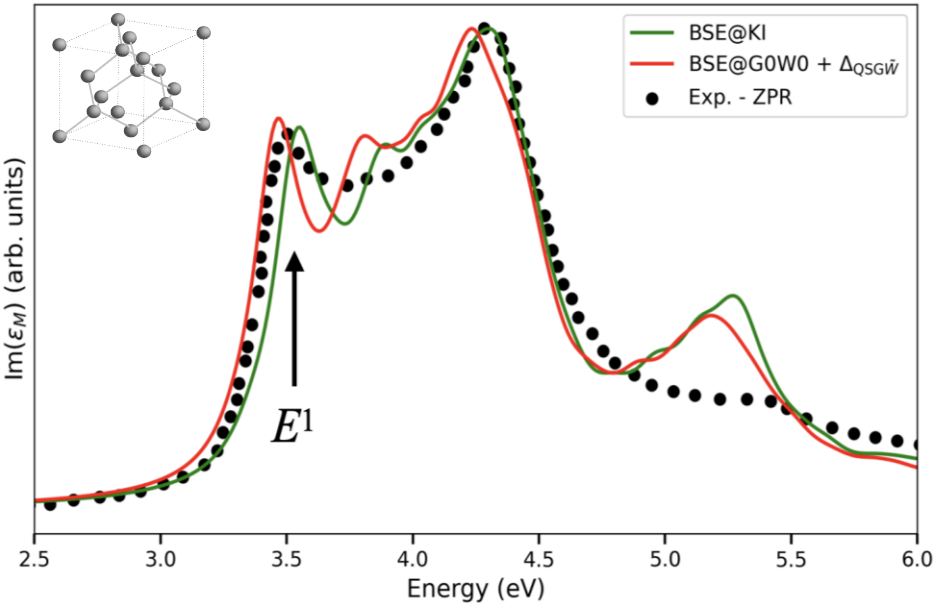
Average performance

	MAE	MA%E	MSE
KI-BSE	**0.54**	**10.6**	**-0.43**
GW-BSE	0.83	16.1	-0.83
TD-PBE0	0.26	4.72	0.04

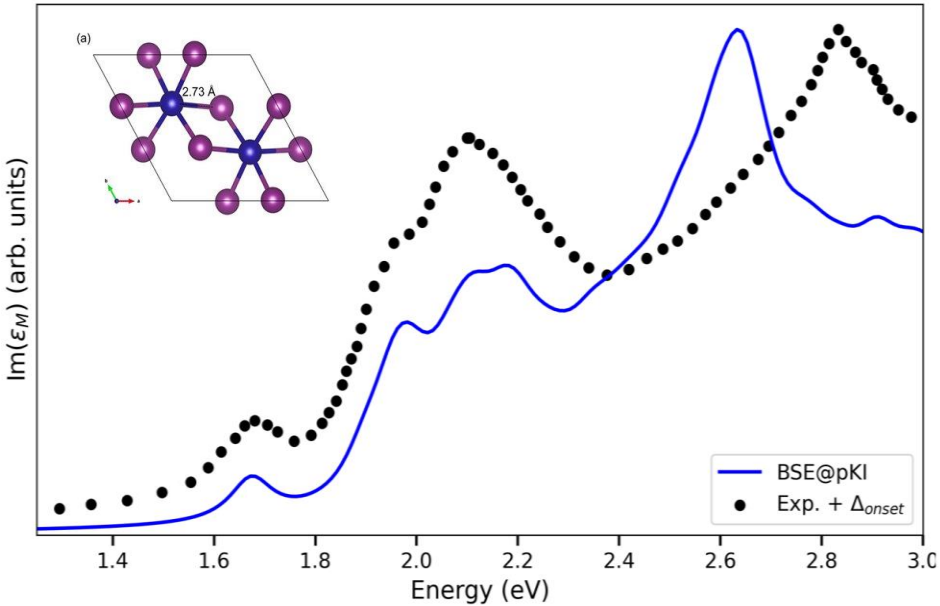
J. Elliott, **N. Colonna**, *et al.* JCTC **15**, 3710 (2019)

Applications to extended systems

Silicon



CrI_3



M. Bonacci, *et al*. in *preparation* (2026)

Real-time propagation

Time-dependent spectroscopies and non-linear phenomena
(Transient absorption, time-resolved ARPES,
pump/probe, ultrafast, HHG, …)

$$\frac{\partial \hat{\rho}}{\partial t} = i\hbar \left[\hat{H}^{\mathrm{eff}}(t), \hat{\rho}(t) \right]$$

$$\hat{H}^{\mathrm{eff}}(t) = \hat{H}^{0} + \hat{U}(t) + \Sigma^{\mathrm{e-e}}[\Delta\hat{\rho}](t)$$

quasi-particle H

el-el interaction

external electric field

C. Attaccalite et al. PRB **84**, 245110 (2011)

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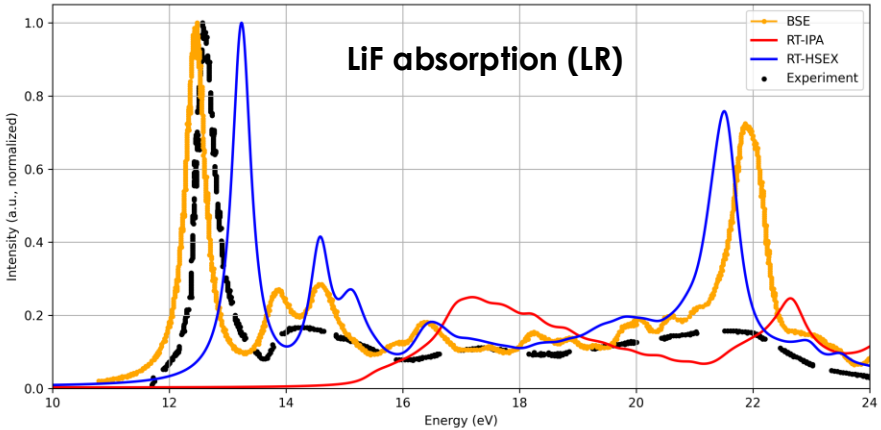
EDUS +

quasi-particle H

el-el interaction (HSEX)

external electric field



G. Cistaro, … , **NC** *in preparation* (2026)

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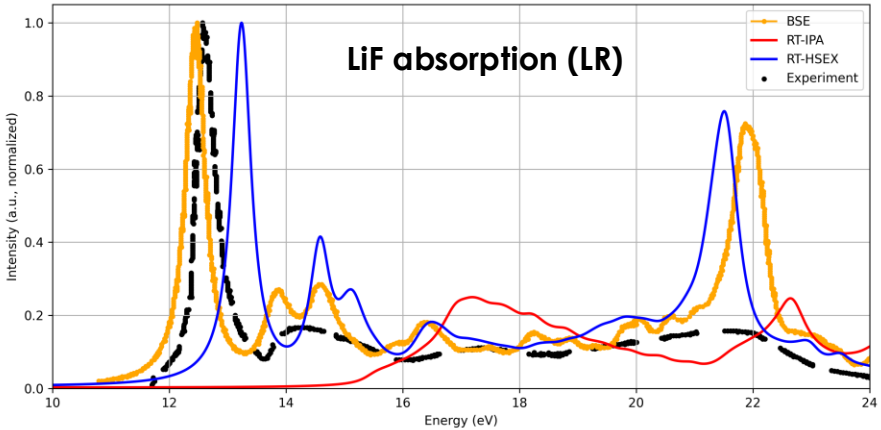
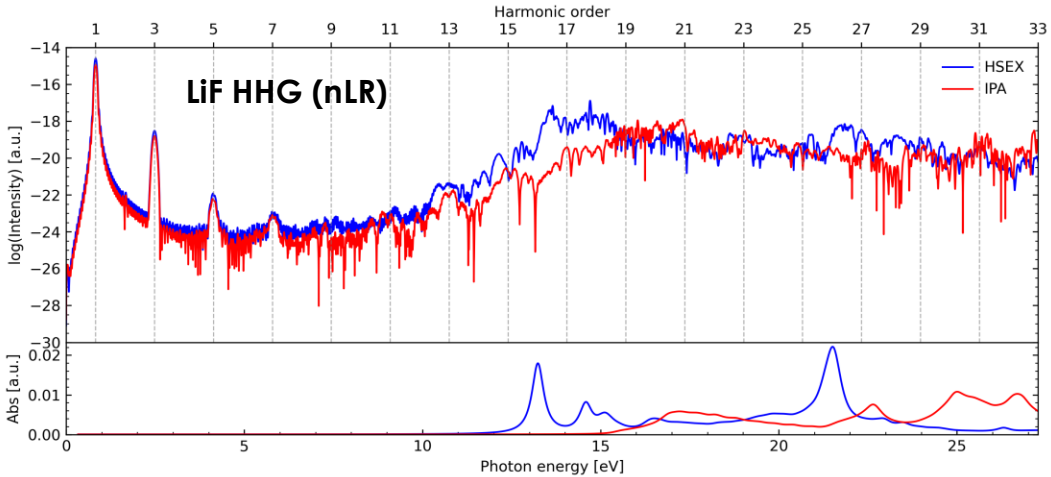
EDUS +

quasi-particle H

el-el interaction (HSEX)

external electric field





G. Cistaro, … , **NC** *in preparation* (2026)

KC potentials vs self-energies

Orbital-density dependent functionals (KC but also, e.g., PZ-SIC):

$$[h_0 + \bar{v}^{\mathrm{KC}}_{\mathrm{xc},m}]|\psi_m\rangle = \lambda_m|\psi_m\rangle$$

$\bar{v}^{\mathrm{KC}}_{\mathrm{xc},m}(\mathbf{r})$: **real**, **local** and **state-dependent**

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This is reminiscent of Green's function theory:

$$[h_0 + \Sigma^{\mathrm{QP}}_m]|\psi^{\mathrm{QP}}_m\rangle = z^{\mathrm{QP}}_m|\psi^{\mathrm{QP}}_m\rangle$$

$\Sigma^{\mathrm{QP}}_m(\mathbf{r},\mathbf{r}')$: **complex**, **non-local** and **state-dependent**

KC potentials vs self-energies (Hartree-Fock)

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Hartree-Fock Self energy (in the localized representation of the variational orbitals)

$$\Sigma_{\mathrm{x}}(\mathbf{x},\mathbf{x}') = -\sum_{k\sigma}^{\mathrm{occ}} \psi_{k\sigma}(\mathbf{x})\psi^*_{k\sigma}(\mathbf{x}')f_{\mathrm{H}}(\mathbf{r},\mathbf{r}') \qquad \langle i\sigma|\Sigma_{\mathrm{x}}|j\sigma'\rangle \simeq -\langle\phi_{i\sigma}|v_{\mathrm{H}}[n_{i\sigma}]|\phi_{i\sigma}\rangle\delta_{ij}\delta_{\sigma\sigma'}$$

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$$\Sigma_{\mathrm{x}}(\mathbf{x},\mathbf{x}') = -\sum_{k\sigma}^{\mathrm{occ}} \psi_{k\sigma}(\mathbf{x})\psi^*_{k\sigma}(\mathbf{x}') f_{\mathrm{H}}(\mathbf{r},\mathbf{r}') \qquad \langle i\sigma|\Sigma_{\mathrm{x}}|j\sigma'\rangle \simeq \boxed{-\langle\phi_{i\sigma}|v_{\mathrm{H}}[n_{i\sigma}]|\phi_{i\sigma}\rangle\delta_{ij}\delta_{\sigma\sigma'}}$$

KIPZ@Hartree and **NO screening** (v_{xc}=0, f_{Hxc}= f_H, ε^{-1} = 1)

$$\langle i\sigma|v^{\mathrm{KIPZ}}_{j\sigma',\mathrm{xc}}|j\sigma'\rangle \simeq \delta_{ij}\delta_{\sigma\sigma'}\left\{\left(\frac{1}{2} - f_{i\sigma}\right)\langle n_{i\sigma}|f_{\mathrm{H}}|n_{i\sigma}\rangle - E_{\mathrm{H}}[n_{i\sigma}]\right\} \simeq \boxed{-\langle\phi_{i\sigma}|v_{\mathrm{H}}[n_{i\sigma}]|\phi_{i\sigma}\rangle\delta_{ij}\delta_{\sigma\sigma'}}$$

A. Ferretti *et al.* , PRB **89**, 195134 (2014); N. Colonna *et al.* JCTC **15**, 1905 (2019)

KC potentials vs self-energies (COHSEX)

Screened Exchange plus Coulomb hole (COHSEX): $\Sigma_{\rm xc}^{\rm COHSEX} = \Sigma_{\rm xc}^{\rm COH} + \Sigma_{\rm xc}^{\rm SEX}$

$$\Sigma_{\rm xc}^{\rm SEX}(\mathbf{x},\mathbf{x}') = -\sum_{k\sigma}^{\rm occ} \psi_{k\sigma}(\mathbf{x})\psi_{k\sigma}^*(\mathbf{x}')W(\mathbf{r},\mathbf{r}')$$

$$\Sigma_{\rm xc}^{\rm COH}(\mathbf{x},\mathbf{x}') = \frac{1}{2}\delta(\mathbf{x},\mathbf{x}')\left[W(\mathbf{r},\mathbf{r}') - f_{\rm H}(\mathbf{r},\mathbf{r}')\right]$$

In the localized representation of the variational orbitals

$$\langle i\sigma|\Sigma_{\rm xc}^{\rm COHSEX}|j\sigma'\rangle \simeq \delta_{ij}\delta_{\sigma\sigma'}\left\{\left(\frac{1}{2} - f_{i\sigma}\right)\langle n_{i\sigma}|W|n_{i\sigma}\rangle - E_{\rm H}[n_{i\sigma}]\right\}$$

N. Colonna *et al.* JCTC **15**, 1905 (2019)

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KIPZ@Hartree plus **RPA screening** (v_{xc}=0, f_{Hxc}= f_H, ε^{-1} = RPA)

$$\langle i\sigma|v_{j\sigma',\rm xc}^{\rm KIPZ}|j\sigma'\rangle \simeq \delta_{ij}\delta_{\sigma\sigma'}\left\{\left(\frac{1}{2} - f_{i\sigma}\right)\langle n_{i\sigma}|W|n_{i\sigma}\rangle - E_{\rm H}[n_{i\sigma}]\right\}$$

N. Colonna *et al.* JCTC **15**, 1905 (2019)

KC potentials vs self-energies (static $GW\Gamma_{xc}$)

KIPZ@DFT (v_{xc}=DFT, f_{Hxc}= DFT, ε^{-1} = DFT)

$$\mathcal{F}_{\mathrm{Hxc}} = \varepsilon^{-1}_{\mathrm{t-e}} f_{\mathrm{Hxc}}$$

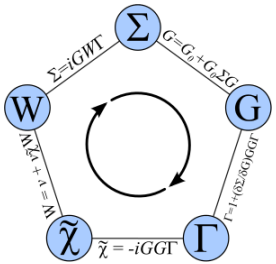
$$\langle i\sigma|v^{\mathrm{KIPZ}}_{j\sigma',\mathrm{xc}}|j\sigma'\rangle \simeq \delta_{ij}\delta_{\sigma\sigma'}\left\{\langle\phi_{i\sigma}|v^{\mathrm{DFT}}_{\sigma,\mathrm{xc}}|\phi_{i\sigma}\rangle + \left(\frac{1}{2} - f_{i\sigma}\right)\langle n_{i\sigma}|\mathcal{F}^{\sigma\sigma}_{\mathrm{Hxc}}|n_{i\sigma}\rangle - E_{\mathrm{Hxc}}[n_{i\sigma}]\right\}$$

$GW\Gamma_{xc}$: including local (DFT based) vertex corrections

$$\Sigma^{GW\Gamma_{\mathrm{xc}}}_{\mathrm{xc}}(1,2) = iG(1,2)W_{t-e}(1,2)$$

$$W_{t-e} = \varepsilon^{-1}_{t-e} f_{\mathrm{H}} = [1 - f_{\mathrm{Hxc}}\chi_0]^{-1} f_{\mathrm{H}}$$

$$\Sigma^{(0)}_{\mathrm{xc}}(1,2) = \delta(1,2)V_{\mathrm{xc}}(1)$$



Hybertsen and Louie, Phys Rev B, **35** 5585 (1987); Del Sole *et al*. Phys. Rev. B, **49** 8024 (1994)

$$\langle i\sigma|\Sigma^{\mathrm{GW}\Gamma_{\mathrm{xc}}}_{\mathrm{xc}}|j\sigma'\rangle \simeq \delta_{ij}\delta_{\sigma\sigma'}\left\{\left(\frac{1}{2} - f_{i\sigma}\right)\langle n_{i\sigma}|W_{t-e}|n_{i\sigma}\rangle - E_{\mathrm{H}}[n_{i\sigma}]\right\}$$

N. Colonna *et al.* JCTC **15**, 1905 (2019)

Resonance with other efforts

- **Wannier transition-state method** (Anisimov and Kozhevnikov)
  - V. I. Anisimov and A. V. Kozhevnikov Phys. Rev. B **72**, 075125 (2005)
  - V. I. Anisimov *et al*. J. Phys.: Condens. Matter **16** 106206 (2007)
- **Ensemble-DFT** (E. Kraisler & L. Kronik)
  - E. Kraisler and L. Kronik PRL **110** 126403 (2013)
- **Dielectric-dependent hybrid functionals** (G. Galli, A. Pasquarello, …)
  - J.H. Skone et *al.* Phys. Rev. B **89** 195112 (2014)
- **LOSC functionals** (W. Yang)
  - C. Li *et al*. Phys. Rev. Lett. **114**, 053001 (2015)
  - C. Li *et al*. National Science Review **5,** 203 (2018)
- **Koopmans-Wannier** (Lin-Wang Wang)
  - J. Ma and L.-W. Wang Scientific Report **6** 24924 (2016)
- **Optimally tuned hybrid functionals** (L. Kronik, A. Pasquarello, …)
  - D. Wing et *al.* PNAS **18**, e2104556118 (2021)

Conclusions

- **Paradigm shift**; conceptually similar to DFT but with a **functional theory of orbital densities** (quasiparticle discretization of a spectral functional theory [Ferretti and Marzari arXiv:2508.17245])

DFT: Ground State properties

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

Koopmans: Charged excitations

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \quad \longrightarrow \quad \rho(\mathbf{r}, i)$$

- **Accuracy comparable to stat-of-the-art Greens function methods** at a **reduced computational** cost and **complexity**, and within a **functional framework**
- **Linearization, Screening and Localization** as key features
- **Spin-dependent screening effects and interactions** beyond standard diagrammatic techniques
- **Open source**: available in the official QE release and at koopmans-functionals.org

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- *N. Colonna et al. JCTC **14**, 2549 (2018)*
- *N. Colonna et al. JCTC **15**, 1905 (2019)*
- *N.L. Nguyen, et al. PRX **8**, 021051 (2018)*
- *J. Elliott, et al. JCTC **15**, 3710 (2019) KC+BSE*
- *R. De Gennaro et. al PRB **106** 035106 (2022)*
- *N. Colonna et al. JCTC **18**, 5435 (2022)*
- *E. Linscott et al. JCTC **19**, 7097 (2023)*
- *A. Marrazzo and N. Colonna PRR **6**, 033085 (2024)*
- *Y. Schubert et al. npj Comp. Mat. **10**, 2997 (2024)*

- Theoretical framework
- Theoretical framework
- KC as a spectral theory
- Screening/Relaxation
- Connection with the GW approximation
- Application to extended systems (band gaps)
- KC+BSE for finite systems
- Bloch's symmetry and band structures
- KCW code: Implementation of KC in PBC
- `Koopmans` package
- Non-collinear extension
- Machine learning the screening coefficients

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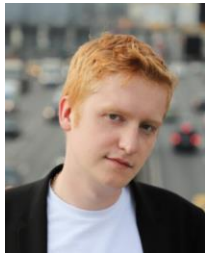

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