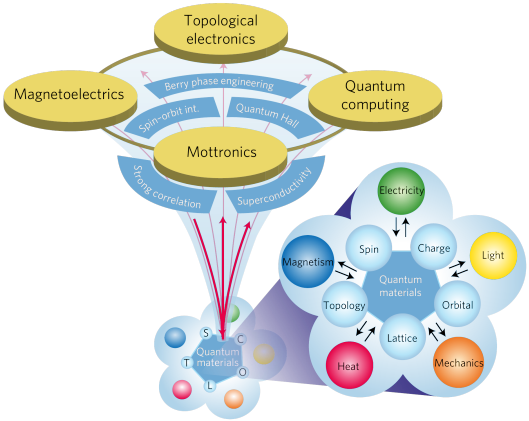
International Summer School on Computational Quantum Materials 2024

# Ab initio description of strongly correlated materials: combining density functional theory plus and dynamical mean-field theory

Sophie Beck

27th May 2024

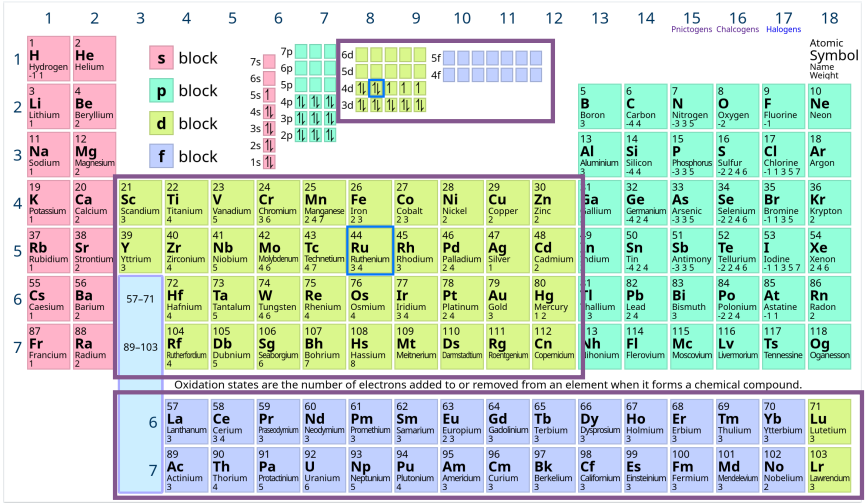
# Strongly correlated materials - next generation electronics?




- sensitive to small changes in external parameters:
  - temperature
  - pressure
  - doping
  - ...
- emerging phenomena:
  - high $T_C$ superconductivity
  - colossal magnetoresistance
  - Mott physics
  - ...

Y. Tokura, M. Kawasaki, and N. Nagaosa, Nat. Phys. 13, 1056 (2017)

# Correlated $d$-/$f$-shells



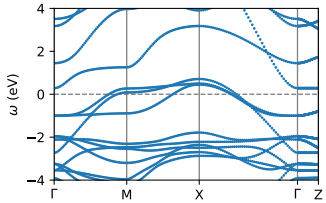

https://ptable.com

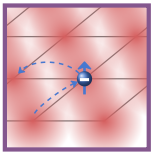
# Weak versus strong correlation

**weakly correlated systems**

- effective single-particle picture
- density functional theory

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}}\{\chi_1(\mathbf{x}_1)\chi_2(\mathbf{x}_2) - \chi_1(\mathbf{x}_2)\chi_2(\mathbf{x}_1)\}$$
$$= \frac{1}{\sqrt{2}}\begin{vmatrix} \chi_1(\mathbf{x}_1) & \chi_2(\mathbf{x}_1) \\ \chi_1(\mathbf{x}_2) & \chi_2(\mathbf{x}_2) \end{vmatrix},$$



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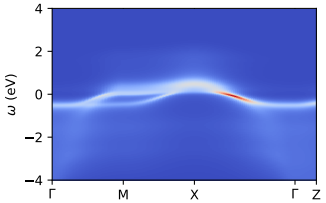
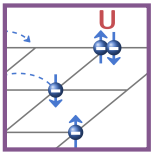
**strongly correlated systems**

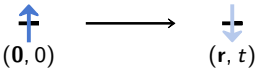
- breakdown of single-particle picture
- large local Coulomb interaction $U$
- between ionic localization and itinerant behavior



# Spectral function $A(\mathbf{k}, \omega)$

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\,\mathrm{Im}\int \mathrm{d}\mathbf{r}\int \mathrm{d}t\, e^{\mathrm{i}(\mathbf{kr}-\omega t)}\underbrace{\mathrm{i}\theta(t)\left\langle[\Psi(\mathbf{r},t),\Psi^{\dagger}(\mathbf{0},0)]\right\rangle}_{G^R(\mathbf{r},t)}$$




A. Damascelli, Z. Hussain, and Z.-X. Shen, Rev. Mod. Phys. 75, 473 (2003)

# Spectral function $A(\mathbf{k},\omega)$ - non-interacting

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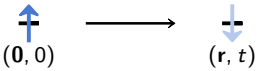


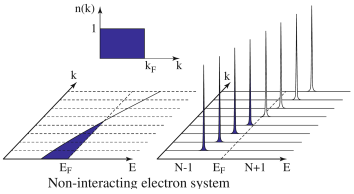

Non-interacting electron system

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + \mathrm{i}\eta}$$

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\delta(\omega - \epsilon_{\mathbf{k}})$$

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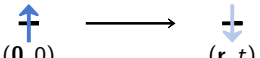


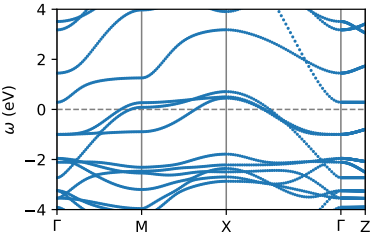


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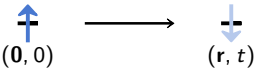


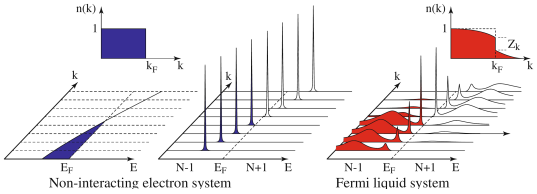


$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\omega)}$$

$$\Sigma(\omega) = \Sigma'(\omega) + \mathrm{i}\Sigma''(\omega)$$

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\frac{\Sigma''(\omega)}{(\omega - \epsilon_{\mathbf{k}} - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$

A. Damascelli, Z. Hussain, and Z.-X. Shen, Rev. Mod. Phys. 75, 473 (2003)

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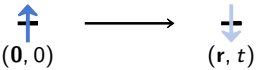


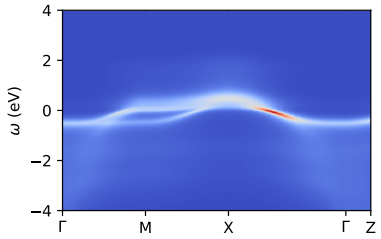


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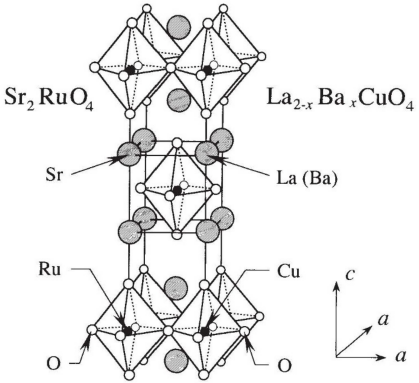
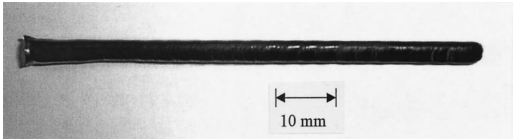
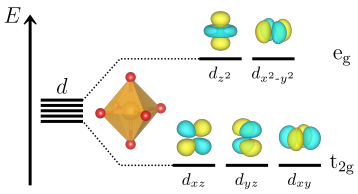
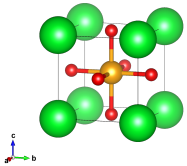
# Case study: Fermi surface of $Sr_2RuO_4$



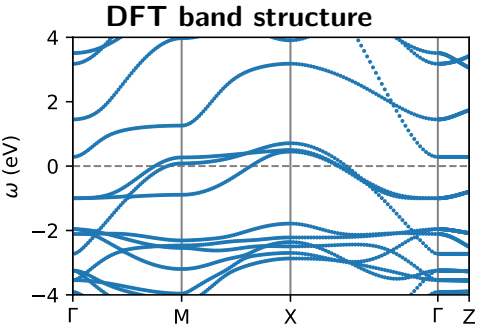



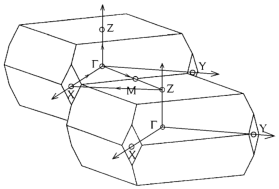



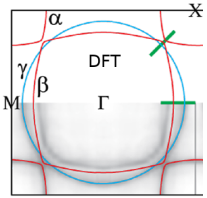
- octahedral crystal field
- key action in $t_{2g}$ subspace

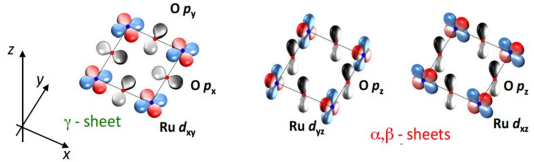
Y. Maeno *et al.*, Nature 372, 532 (1994)

# Low-energy physics dominated by $t_{2g}$ orbitals



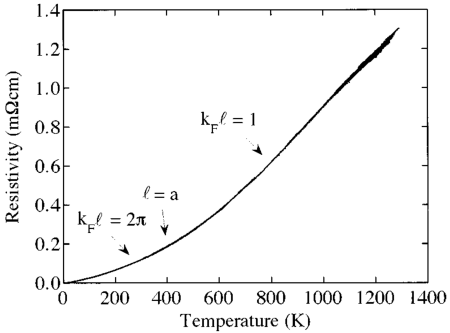




M. W. Haverkort *et al.*, Phys. Rev. Lett. 101, 026406 (2008)

# The electronic structure of $Sr_2RuO_4$

- correlated metal ($U = 2.3$ eV)




A. W. Tyler *et al.*, Phys. Rev. B 58, R10107 (1998)

# The electronic structure of $Sr_2RuO_4$

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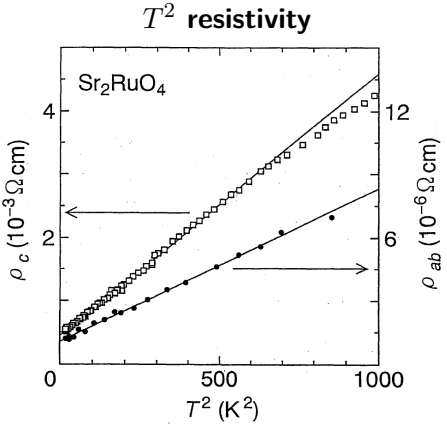


Y. Maeno *et al.*, J. Phys. Soc. Jpn. 66, 1405 (1997)

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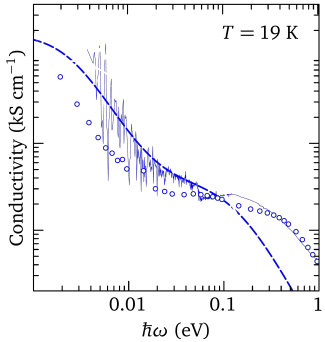
**shoulder in optics**

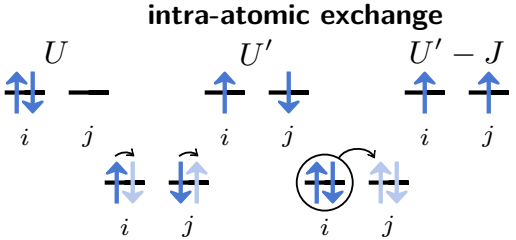



D. Stricker *et al.*, Phys. Rev. Lett. 113, 087404 (2014)

- self-energy $\Sigma''(\omega, T) \sim \omega^2 + (\pi T)^2$

# The electronic structure of $Sr_2RuO_4$

- correlated metal ($U = 2.3$ eV)
- Fermi liquid ($T_{\mathrm{FL}} \approx 25$ K)
- Hund physics ($J = 0.4$ eV)



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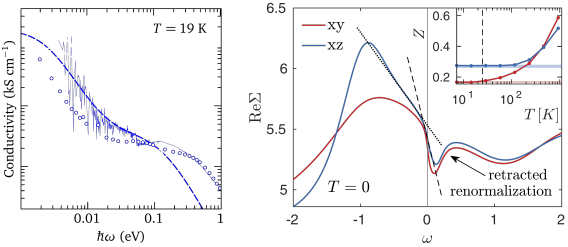
**two-stage coherence, orbital differentiation**




F. Kugler *et al.*, Phys. Rev. Lett. 124, 016401 (2020)

- non-FL excess of spectral weight
- e.g. quantum oscillation, NMR spectroscopy, ...

# The electronic structure of $Sr_2RuO_4$

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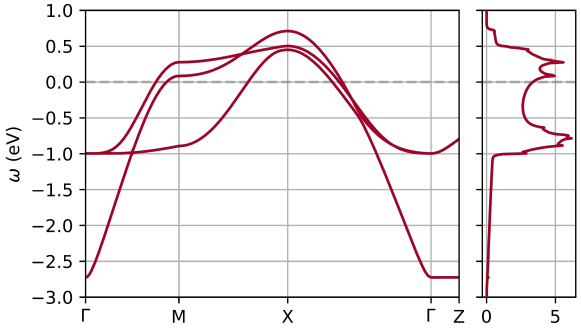


- drives orbital differentiation

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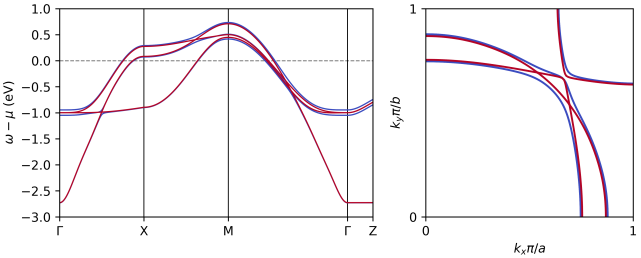
- spin-orbit coupling ($\lambda \approx 0.2$ eV)




- strong effect of SOC on Fermi surface

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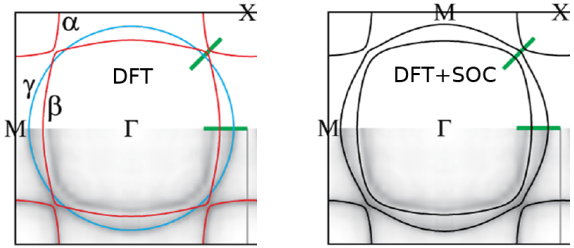


M. W. Haverkort *et al.*, Phys. Rev. Lett. 101, 026406 (2008)

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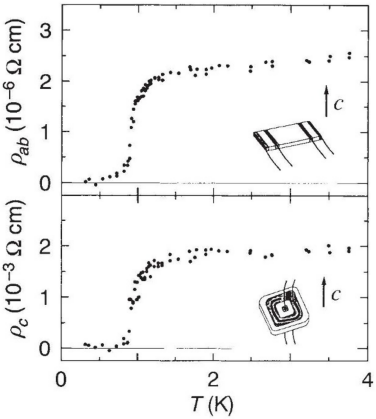
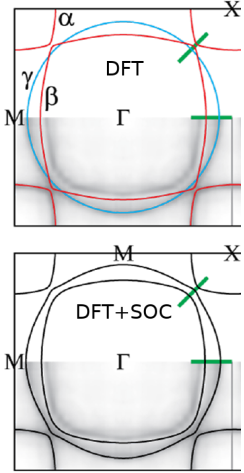
- spin-orbit coupling ($\lambda \approx 0.2$ eV)
- superconductivity ($T_{\mathsf{C}} \approx 1.5$ K)




Y. Maeno *et al.*, Nature 372, 532 (1994)

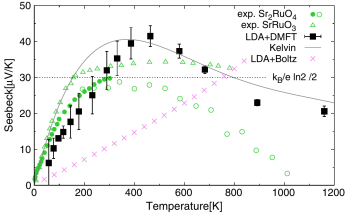
# Where DFT may be insufficient

**Fermi surface**




M. W. Haverkort *et al.*, Phys. Rev. Lett. 101, 026406 (2008)

**Seebeck**




- also: mass enhancement, orbital occupations, optics, SOC, ...
- **more obvious**: local-moment paramagnet (**Mott insulator**) versus (anti-)ferromagnet or non-magnetic metal in DFT

J. Mravlje, A. Georges, Phys. Rev. Lett. 117, 036401 (2016)

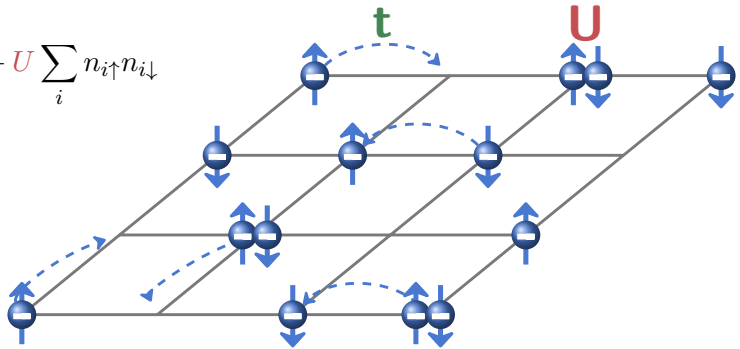
# DFT+DMFT

FLATIRON INSTITUTE

- **situation:** complex physics arising from strong local Coulomb interaction in partially filled orbitals in strongly correlated materials
- **goal:** ab-initio, material-realistic description
- **challenge:** combining localized, atomic-like and itinerant electronic behavior
- **ansatz:** DFT+DMFT, downfolding & embedding
- **example:** Fermi surface of $Sr_2RuO_4$

# recap: the Hubbard model

$$H = -\sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



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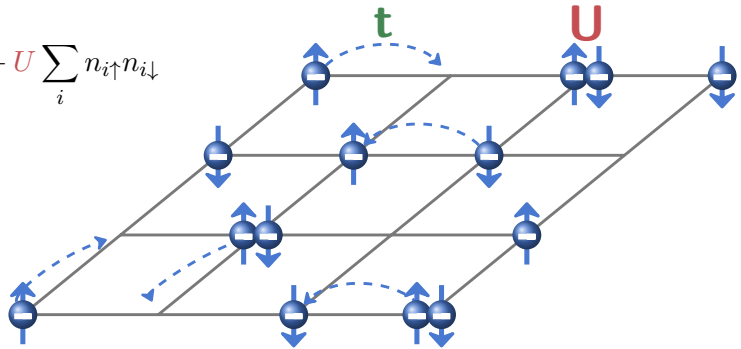
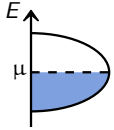



In the limits:

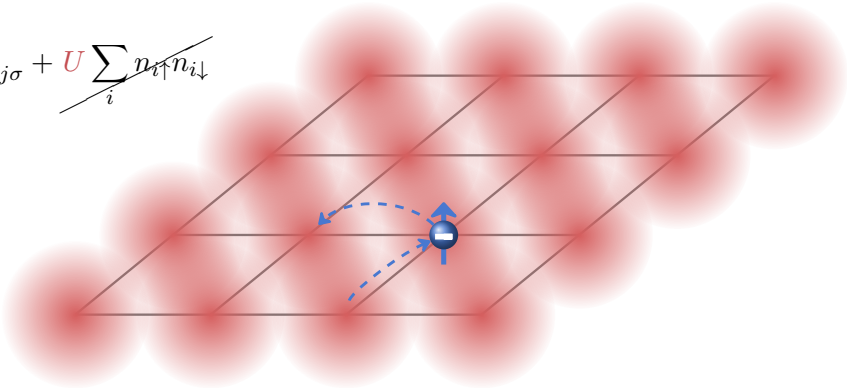
$t \gg U$:



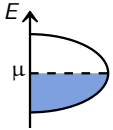

metallic

# recap: the Hubbard model

$$H = -\sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



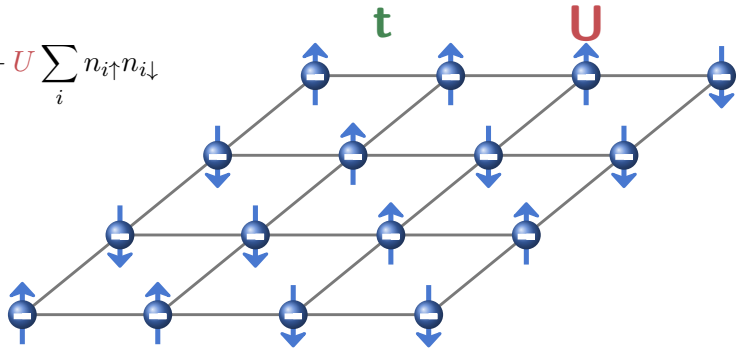
In the limits:

$t \gg U$: 

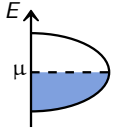
metallic

# recap: the Hubbard model

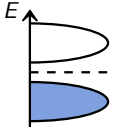
$$H = -\sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$




In the limits:

$t \gg U$: 

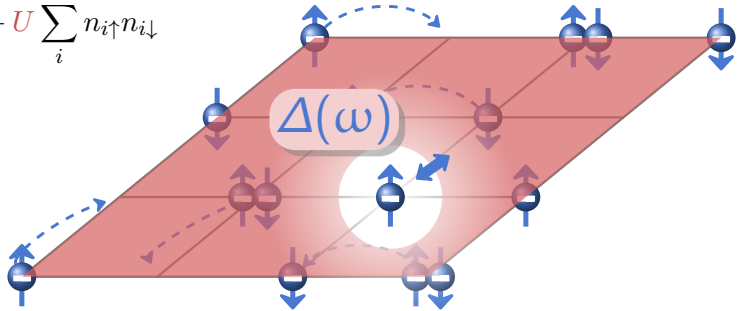
metallic

$t \ll U$: 

insulating

# recap: Dynamical Mean Field Theory

$$H = -\sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



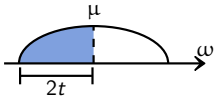

- map lattice to effective impurity model (AIM) embedded in bath
- impurity-bath coupling $\Delta(\omega)$ determined self-consistently
- basic ingredients: $t$, $U$

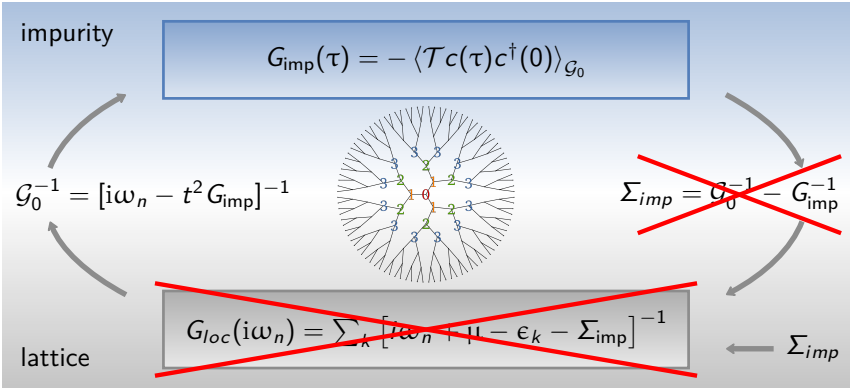

W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 3 (1989)

A. Georges and G. Kotliar, Phys. Rev. B 45, 12 (1992)

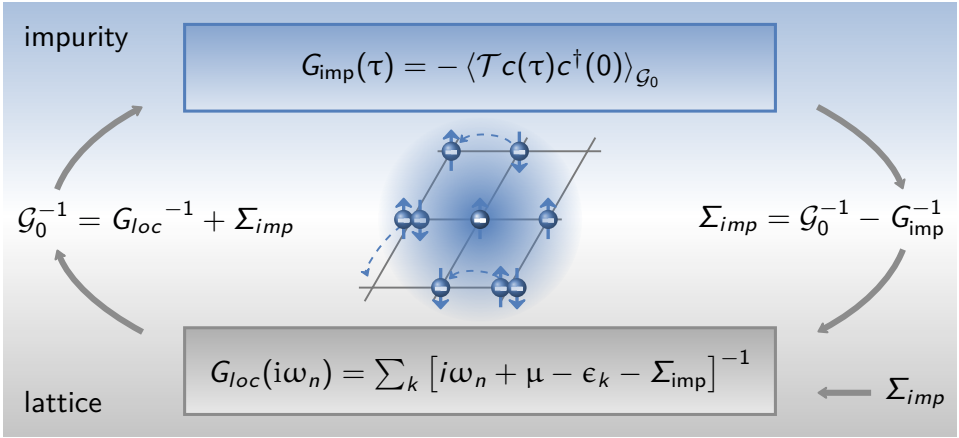
# DMFT self-consistency - example: Bethe lattice

$z \to \infty$: $\quad \rho(\omega) = \frac{1}{2\pi t^2}\sqrt{4t^2 - \omega^2}$



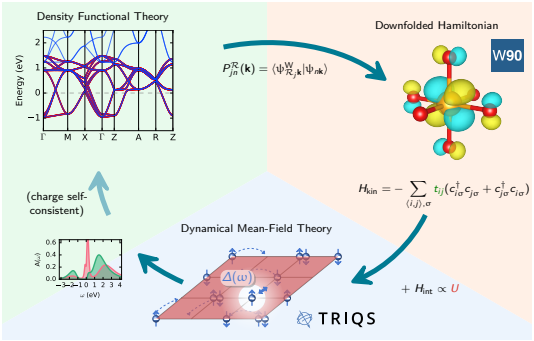



# DMFT self-consistency - *ab initio* electronic structure




- basic ingredients: $t$, $U$, and $P$

# DMFT from first principles




DFT+DMFT ingredients:

- target bands $t$
- projector functions $P$
- interaction Hamiltonian $H_{\mathrm{int}}$
- (energy window, double counting, how to determine $H_{\mathrm{int}}$, ...)
- impurity solver
- charge self-consistency
- ...

# DFT+DMFT ingredients: target bands $t$

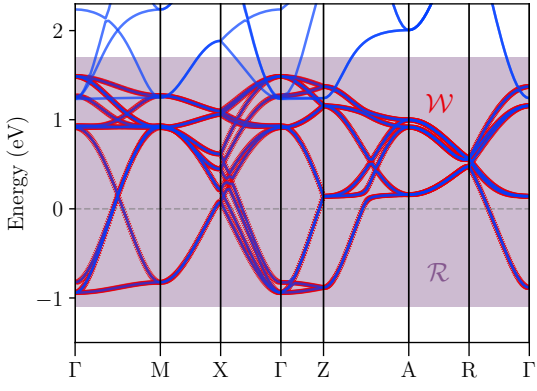
- partitioning of the system
- maximally localized Wannier functions $|\mathbf{R}j\rangle$ from Kohn-Sham states $|\psi_{n\mathbf{k}}\rangle$:

$$|\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle = \sum_n V_{\mathbf{k},nj}|\psi_{n\mathbf{k}}\rangle$$

$$|\mathbf{R}j\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{R}}|\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle$$

- hopping elements:

$$H^{\mathrm{W}}_{\mathbf{k},ij} = \langle\psi^{\mathrm{W}}_{i\mathbf{k}}|\hat{H}|\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle \;\rightarrow\; t_{ij}(\mathbf{R}) = \langle\mathbf{0}i|\hat{H}|\mathbf{R}j\rangle$$




N. Marzari, and D. Vanderbilt, Phys. Rev. B 56, 20 (1997)

# DFT+DMFT ingredients: projector functions $P$

lattice Green's function:

$$\hat{G}(\mathbf{k}, \mathrm{i}\omega_n) = \left[(\mathrm{i}\omega_n + \mu)\mathbb{1} - \hat{H}_{\mathbf{k}} - \Delta\hat{\Sigma}(\mathbf{k}, \mathrm{i}\omega_n)\right]^{-1}$$

downfolding:

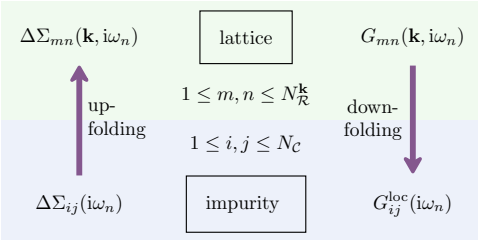
$$G^{\mathrm{loc}}_{ij,\mathcal{R}}(\mathrm{i}\omega_n) = \sum_{\mathbf{k},mn} P^{\mathcal{R}}_{im}(\mathbf{k}) G_{mn}(\mathbf{k}, \mathrm{i}\omega_n) P^{\mathcal{R}*}_{nj}(\mathbf{k})$$

with projector onto orbital $j$ at atomic site $\mathcal{R}$:

$$P^{\mathcal{R}}_{jn}(\mathbf{k}) = \langle \psi^{\mathrm{W}}_{\mathcal{R}_j\mathbf{k}} | \psi_{n\mathbf{k}} \rangle$$

upfolding:

$$\Delta\Sigma_{mn}(\mathbf{k}, \mathrm{i}\omega_n) = \sum_{\mathcal{R},ij} P^{\mathcal{R}*}_{mi}(\mathbf{k}) \Delta\Sigma^{\mathcal{R}}_{ij}(\mathrm{i}\omega_n) P^{\mathcal{R}}_{jn}(\mathbf{k})$$




- basis transformation
- entanglement
- local symmetries

# Double counting

- $E_U$ is a functional of the orbital occupations, but $E_{\mathrm{XC}}$ is a non-linear functional of the total electron density
- ill-posed problem due to the formally incompatible footing: diagrammatic vs. non-perturbative
- different analytic, *phenomenological* expressions have been proposed: FLL, AMF, ANI, Kunes, nominal...
- remedy: $GW$+DMFT

$$\Delta\Sigma_{ij}^{\mathcal{R}}(\mathrm{i}\omega_n) = \Sigma_{ij}^{\mathcal{R}}(\mathrm{i}\omega_n) - \Sigma_{\mathrm{DC}}$$

$$E_{\mathrm{DFT}+U}[\rho] = E_{\mathrm{DFT}}[\rho] + E_U[n_{ij}^{\sigma}] - E_{\mathrm{DC}}$$

$$E_{\mathrm{XC}} \approx E_{\mathrm{XC}}^{\mathrm{LDA}}[\rho] = \int \mathrm{d}\mathbf{r}\, \epsilon_{\mathrm{XC}}^{\mathrm{hom}}[\rho(\mathbf{r})]\rho(\mathbf{r})$$

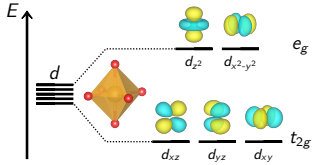
$$E_{\mathrm{XC}}[n_{ij}^{\sigma}]\,?$$

# DFT+DMFT ingredients: interaction Hamiltonian $U$

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{ijkl}^{\text{at } \mathcal{R}} U_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

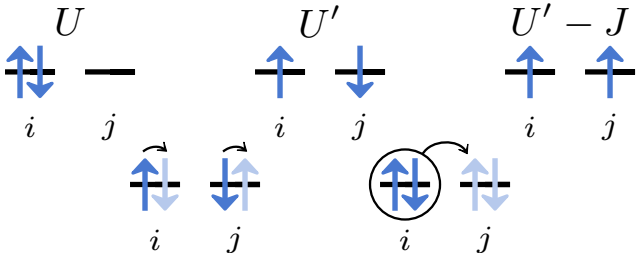
$$V_{ijkl} = \int \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}' w_{i\mathbf{0}}^*(\mathbf{r}) w_{j\mathbf{0}}^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} w_{l\mathbf{0}}(\mathbf{r}') w_{k\mathbf{0}}(\mathbf{r})$$

- complicated 4-rank tensor
- use symmetries to reduce complexity
- for cubic systems: Hubbard-Kanamori parametrization
- for spherical systems: Slater parametrization




J. Kanamori, Prog. Theor. Exp. Phys. 30 (1963)

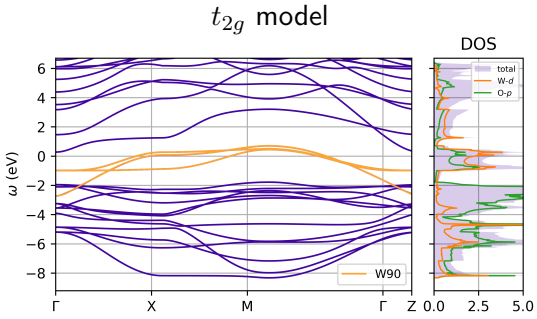
# DFT+DMFT ingredients: interaction Hamiltonian $U$




$$\hat{H}_U = U \sum_i n_{i\uparrow} n_{i\downarrow} + U' \sum_{i \neq j} n_{i\uparrow} n_{j\downarrow} + (U' - J) \sum_{i<j,\sigma} n_{i\sigma} n_{j\sigma}$$
$$- J \sum_{i \neq j} c^\dagger_{i\uparrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\uparrow} + J \sum_{i \neq j} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow}$$

J. Kanamori, Prog. Theor. Exp. Phys. 30 (1963)

# DFT+DMFT ingredients: energy window



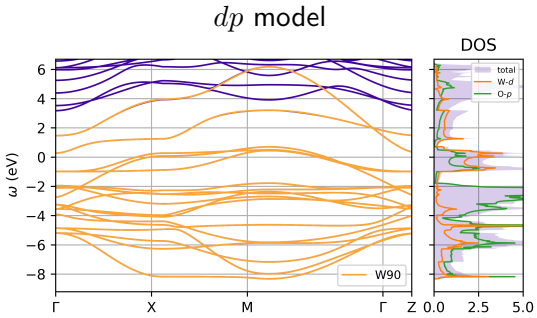

pros:

- no DC
- nominal occupations
- less work for impurity solver

cons:

- smaller $U$, more frequency-dependent
- larger spread $\Omega$, oxygen tails $\rightarrow$ less localized
- no information on $e_g$ states...

# DFT+DMFT ingredients: energy window




pros:

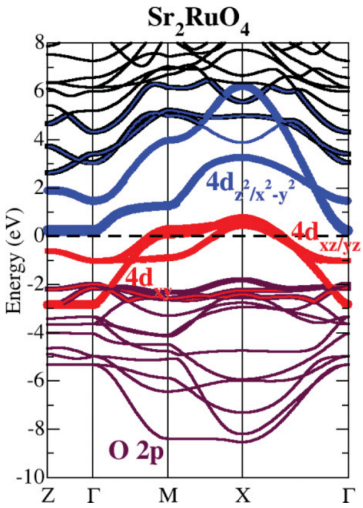
- more localized, DMFT more valid
- larger $U$ and more atomic-like, less frequency-dependent
- renormalizes all states

cons:

- DC, in principle $U_{dp}$, $U_p$
- fractional occupations
- heavy for impurity solver

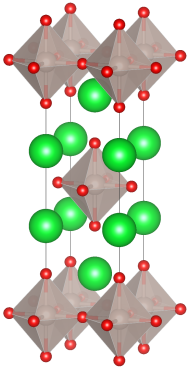
# How to determine Coulomb interaction

- $V$ of the order of 11 eV for $t_{2g}$, i.e. $\gg$ bandwidth $\approx 3.4$ eV
- effective Coulomb interaction screened by surrounding electrons
- screened interaction $U(\mathbf{r}, \mathbf{r}')$ in practice:
  - cRPA: screening channels, frequency dependence, Hund $J$
  - cLDA: only full $d$ shell, static, no Hund $J$
- $d - dp$: $F^0 = 3.23$ eV, $\bar{U}_{mm} = 4.1$ eV, $t_{2g} - t_{2g}$: $\mathcal{U} = 2.56$ eV



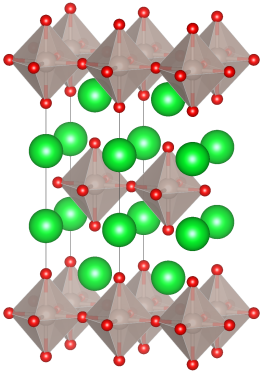

L. Vaugier, H. Jiang, S. Biermann, Phys. Rev. B 86, 165105 (2012)

# Multi-site DMFT



$$\Sigma = \left( \Sigma_{\mathrm{imp}} \right)$$

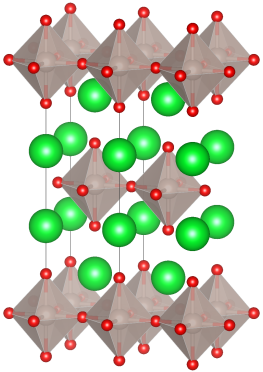
# Multi-site DMFT



$$\Sigma = \begin{pmatrix} \Sigma^1_{\text{imp}} & & & \\ & \Sigma^2_{\text{imp}} & & \\ & & \Sigma^3_{\text{imp}} & \\ & & & \Sigma^4_{\text{imp}} \end{pmatrix}$$

- self-energy approximated as block-diagonal in orbital basis

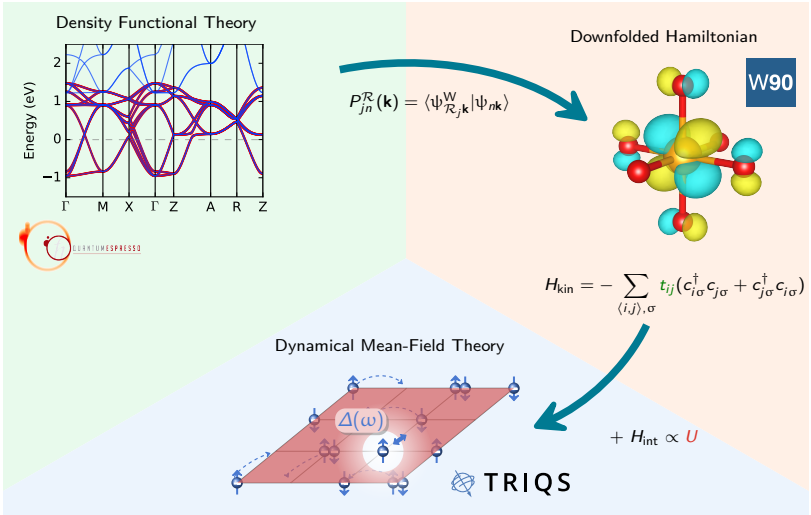
# Multi-site DMFT



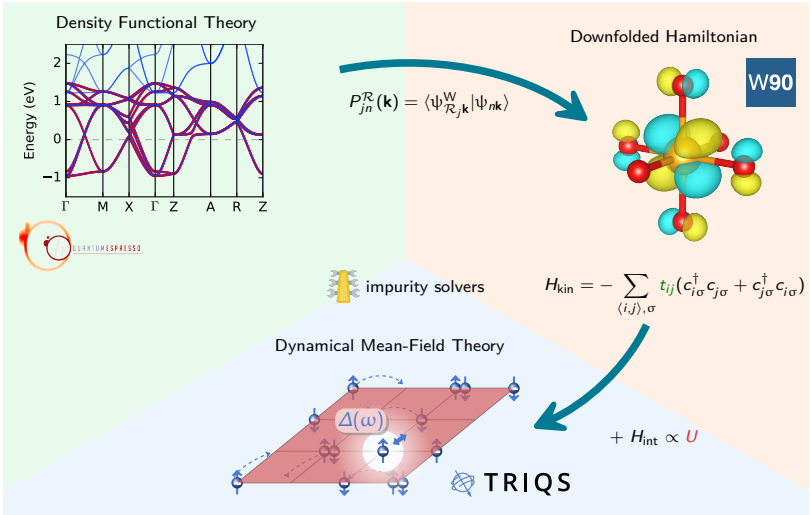
$$\Sigma = \begin{pmatrix} \Sigma^1_{\mathrm{imp}} & & & \\ & & & \\ & & & \\ & & & \end{pmatrix}$$

- self-energy approximated as block-diagonal in orbital basis
- map self-energy to symmetry-equivalent sites
- use spin channel for AFM solutions

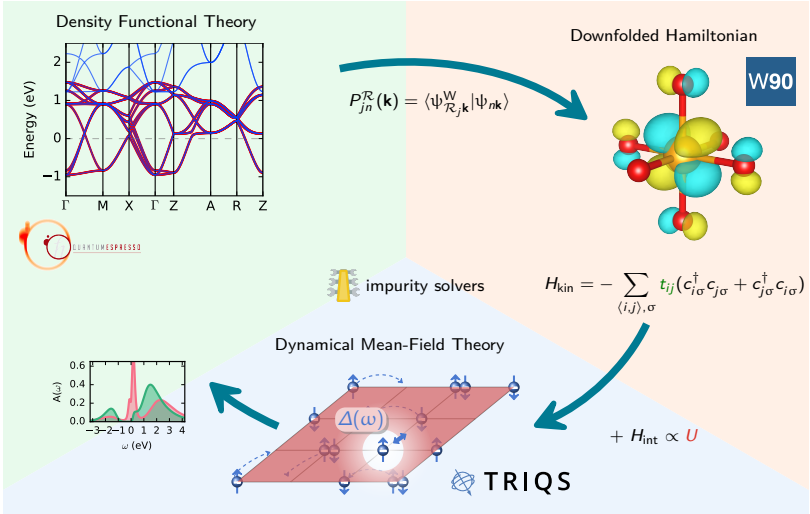
# DFT+DMFT workflow



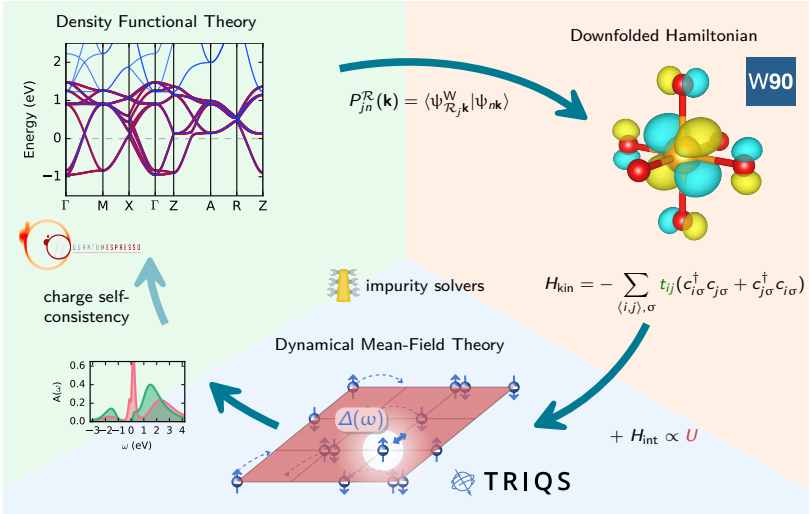
# DFT+DMFT workflow



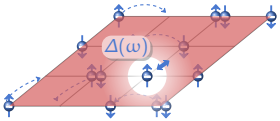
# DFT+DMFT workflow



# DFT+DMFT workflow



# Impurity solvers




$$G_\sigma^{\text{imp}}(\tau) = \left\langle \mathcal{T} c_\sigma(\tau) c_\sigma^\dagger(0) \right\rangle_{\mathcal{G}_0}$$

approximate solvers:

- Hartree(-Fock)
- Hubbard-I
- Iterated perturbation theory (IPT)
- Slave boson technique
- ...

numerically exact solvers:

- Quantum Monte Carlo (QMC)
- exact diagonalization (ED)
- numerical renormalization group (NRG)
- density matrix renormalization group (DMRG)
- tensor-network based approaches (MPS/TTN)

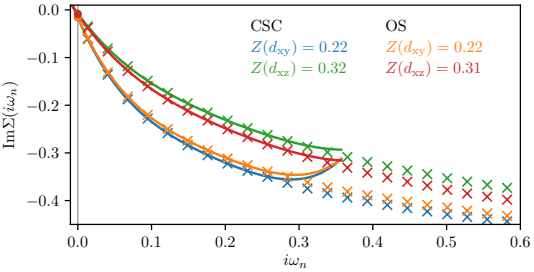
→ see other lectures in this school

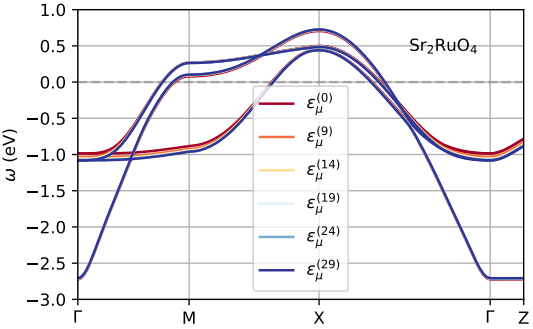
# Charge self-consistency: spectral density-functional approach

| Method | Physical quantity | Constraining field |
|---|---|---|
| Baym-Kadanoff | $G_{\alpha\beta}(\mathbf{k}, i\omega)$ | $\Sigma_{\mathrm{int},\alpha\beta}(\mathbf{k}, i\omega)$ |
| DMFT (BL) | $G_{\mathrm{loc},\alpha\beta}(i\omega)$ | $\mathcal{M}_{\mathrm{int},\alpha\beta}(i\omega)$ |
| DMFT (AL) | $G_{\mathrm{loc},\alpha\beta}(i\omega)$ | $\Delta_{\alpha\beta}(i\omega)$ |
| LDA+DMFT (BL) | $\rho(r),\ G_{\mathrm{loc},ab}(i\omega)$ | $V_{\mathrm{int}}(r),\ \mathcal{M}_{\mathrm{int},ab}(i\omega)$ |
| LDA+DMFT (AL) | $\rho(r),\ G_{\mathrm{loc},ab}(i\omega)$ | $V_{\mathrm{int}}(r),\ \Delta_{ab}(i\omega)$ |
| LDA+$U$ | $\rho(r),\ n_{ab}$ | $V_{\mathrm{int}}(r),\ \lambda_{ab}$ |
| LDA | $\rho(r)$ | $V_{\mathrm{int}}(r)$ |

G. Kotliar *et al.*, Rev. Mod. Phys. 78, 865 (2006)

# Quasiparticle mass renormalization in $Sr_2RuO_4$

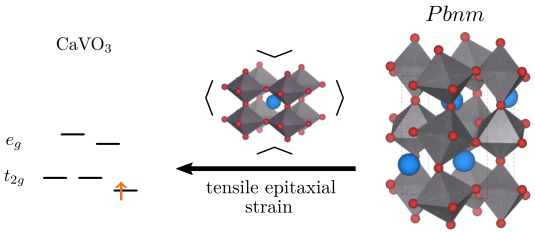


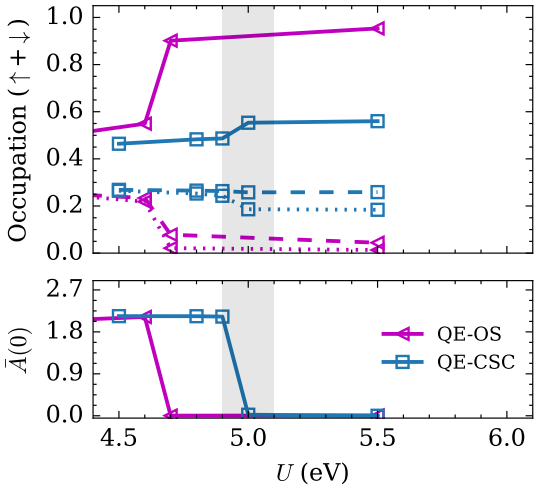

- CT-HYB solver, $\beta = 232$ eV$^{-1}$
- minimal effect of charge self-consistency

A. Hampel, SB, and C. Ederer, Phys. Rev. Res. 2, 033088 (2020)

# Orbital polarization in $CaVO_3$ (tensile strain)




- CT-HYB solver, $\beta = 40$ eV$^{-1}$
- charge self-consistency strongly reduces the orbital polarization found in one-shot calculations

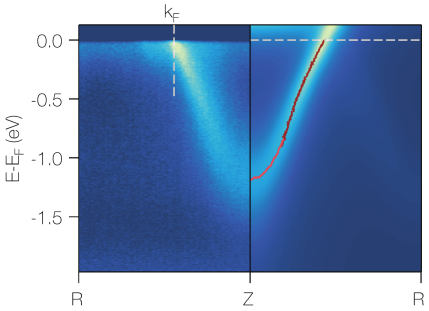



A. Hampel, SB, and C. Ederer, Phys. Rev. Res. 2, 033088 (2020)

# Post-processing

What we can compute:

- spectral properties





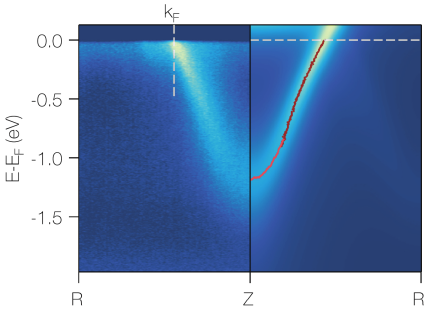
E. Cappelli *et al.*, Phys. Rev. Mater. 6, 075002 (2022)

A. Marrazzo, SB *et al.*, arxiv:2312.10769 (2023)

# Post-processing

What we can compute:

- spectral properties

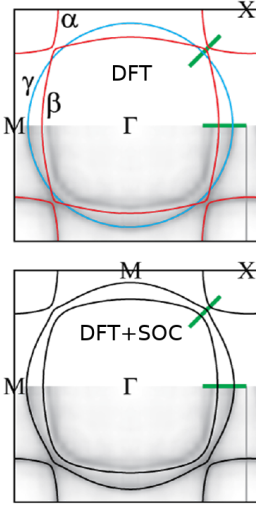



- optical and thermal conductivity
- Hall and Seebeck coefficient
- two-particle correlation function (susceptibilities)
- x-ray photoemission and absorption spectroscopy
- resonant inelastic x-ray scattering
- phonon spectra
- electronic Raman spectroscopy
- ...

E. Cappelli *et al.*, Phys. Rev. Mater. 6, 075002 (2022)

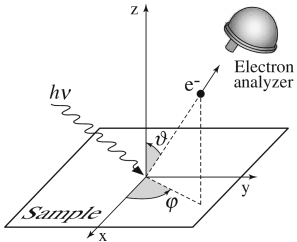
A. Marrazzo, SB *et al.*, arxiv:2312.10769 (2023)

# Back to the experiment

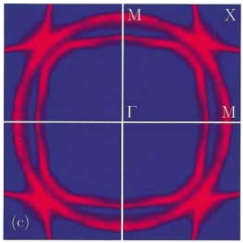



$$E_{\mathrm{kin}} = h\nu - \phi - |E_{\mathrm{B}}|$$

$$\hbar\mathbf{k}_{\parallel} = \sqrt{2mE_{\mathrm{kin}}} \cdot \sin\theta$$




Photoemission geometry



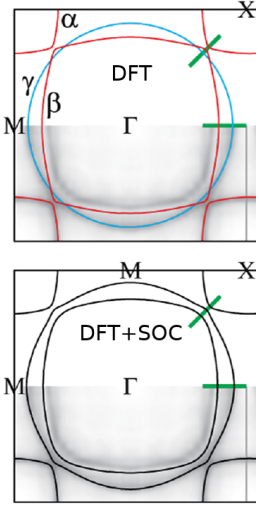

M. W. Haverkort *et al.*, Phys. Rev. Lett. 101, 026406 (2008)

A. Damascelli *et al.*, Rev. Mod. Phys. 75, 473 (2003)

A. Damascelli *et al.*, Phys. Rev. Lett. 85, 5194 (2000)

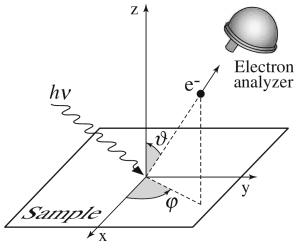
A. Tamai *et al.*, Phys. Rev. X 9, 021048 (2019)

# Back to the experiment

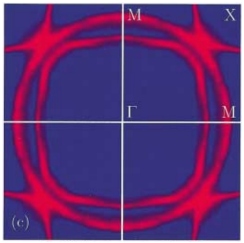


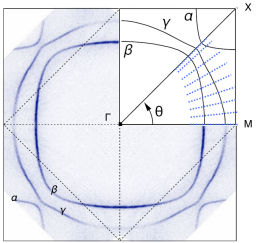

$$E_{\mathrm{kin}} = h\nu - \phi - |E_{\mathrm{B}}|$$

$$\hbar\mathbf{k}_{\parallel} = \sqrt{2mE_{\mathrm{kin}}} \cdot \sin\theta$$




Photoemission geometry




M. W. Haverkort *et al.*, Phys. Rev. Lett. 101, 026406 (2008)

A. Damascelli *et al.*, Rev. Mod. Phys. 75, 473 (2003)

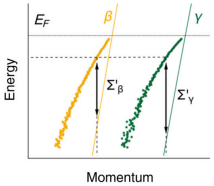
A. Damascelli *et al.*, Phys. Rev. Lett. 85, 5194 (2000)

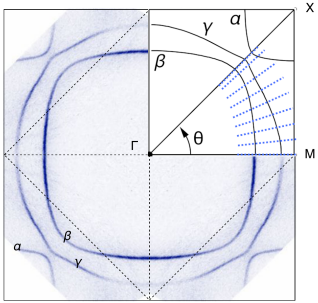
A. Tamai *et al.*, Phys. Rev. X 9, 021048 (2019)

# Is DMFT a good method for this application?

- QP equation:

$$\omega - \epsilon_\nu(\mathbf{k}^\nu_{\max}(\omega)) - \Sigma'_{\nu\nu'}(\omega, \mathbf{k}^\nu_{\max}(\omega)) = 0$$

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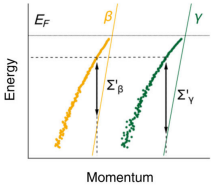


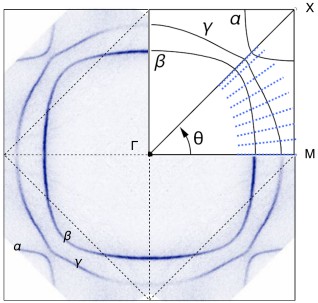


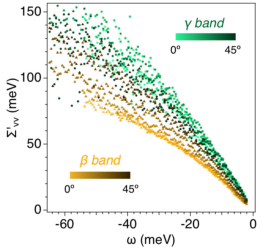


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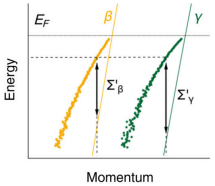


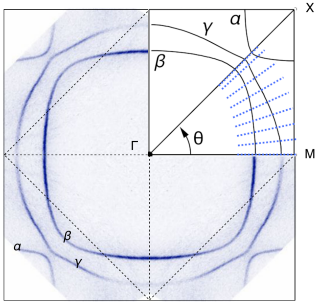


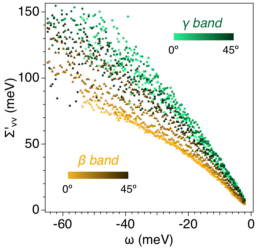


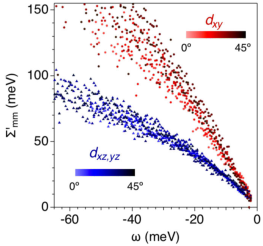


➔ self-energy is local *in the orbital basis*!

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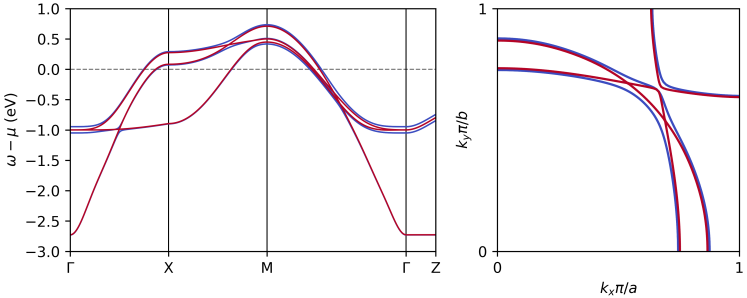
# Spin-orbit coupling in $Sr_2RuO_4$

spin-orbit coupling $\lambda$

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{xy} & 0 & 0 & 0 & \frac{\lambda_{xy}}{2} & \frac{i\lambda_{xy}}{2} \\ 0 & \varepsilon_{yz} & -\frac{i\lambda_z}{2} & -\frac{\lambda_{xy}}{2} & 0 & 0 \\ 0 & \frac{i\lambda_z}{2} & \varepsilon_{xz} & -\frac{i\lambda_{xy}}{2} & 0 & 0 \\ 0 & -\frac{\lambda_{xy}}{2} & \frac{i\lambda_{xy}}{2} & \varepsilon_{xy} & 0 & 0 \\ \frac{\lambda_{xy}}{2} & 0 & 0 & 0 & \varepsilon_{yz} & \frac{i\lambda_z}{2} \\ -\frac{i\lambda_{xy}}{2} & 0 & 0 & 0 & -\frac{i\lambda_z}{2} & \varepsilon_{xz} \end{pmatrix}$$

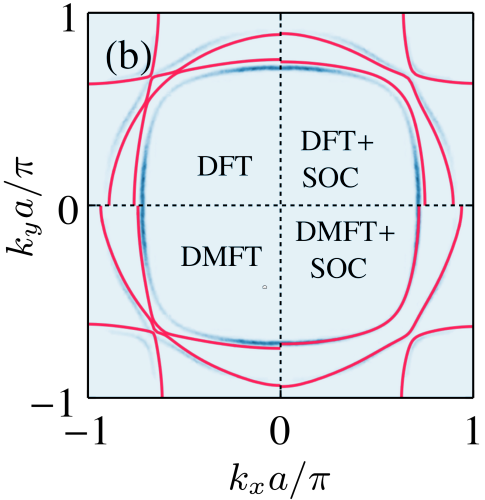



$$\hat{H}_\lambda^{\mathrm{SOC}} = \frac{\lambda}{2} \sum_{ij} \sum_{\sigma\sigma'} c_{i\sigma}^\dagger (\mathbf{l}_{ij} \cdot \boldsymbol{\sigma}_{\sigma\sigma'}) c_{j\sigma'}$$

- correlation-induced enhancement of crystal-field splitting
- correlation-induced enhancement of effective spin-orbit coupling

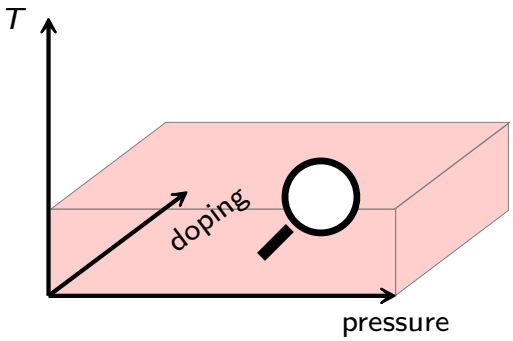
# Back to the experiment

- novel tree tensor-network impurity solver:
  - real-time/frequency axis
  - $T = 0$ K
  - energy-independent resolution
  - including spin-orbit coupling for the first time
- other quantities: mass enhancement, orbital occupations, optics, thermopower, Hall coefficient, magnetic susceptibility, RIXS, Raman scattering, ...




X. Cao *et al.*, Phys. Rev. B 104, 115119 (2021)

# More problems - more literature




- double counting
- more orbitals, more complex systems
- screening
- (real-frequency) impurity solvers and analytic continuation
- superconductivity
- out of equilibrium
- low-$T$, exotic states