Realistic simulations of quantum materials:
Combining density function theory and dynamical mean-field theory

TRIQS Summer School 2025

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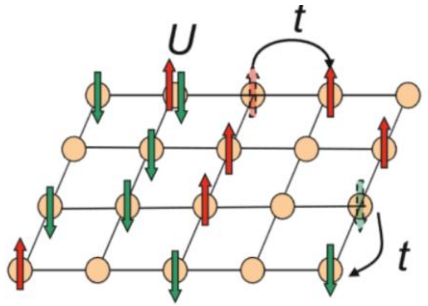
Objective: Simulating correlated materials

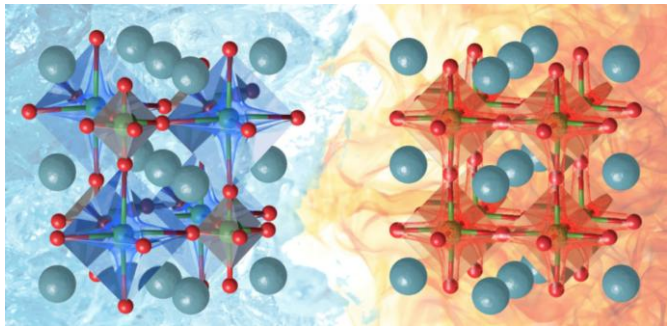
- So far solving model Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

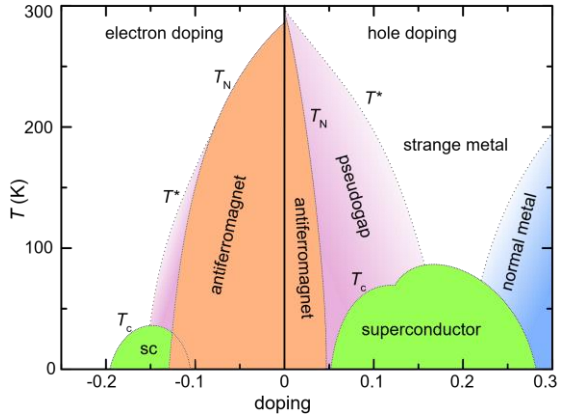


Yamada, Imamura & Machida, *SCFA* 2018

- We want to understand and predict **material specific properties**

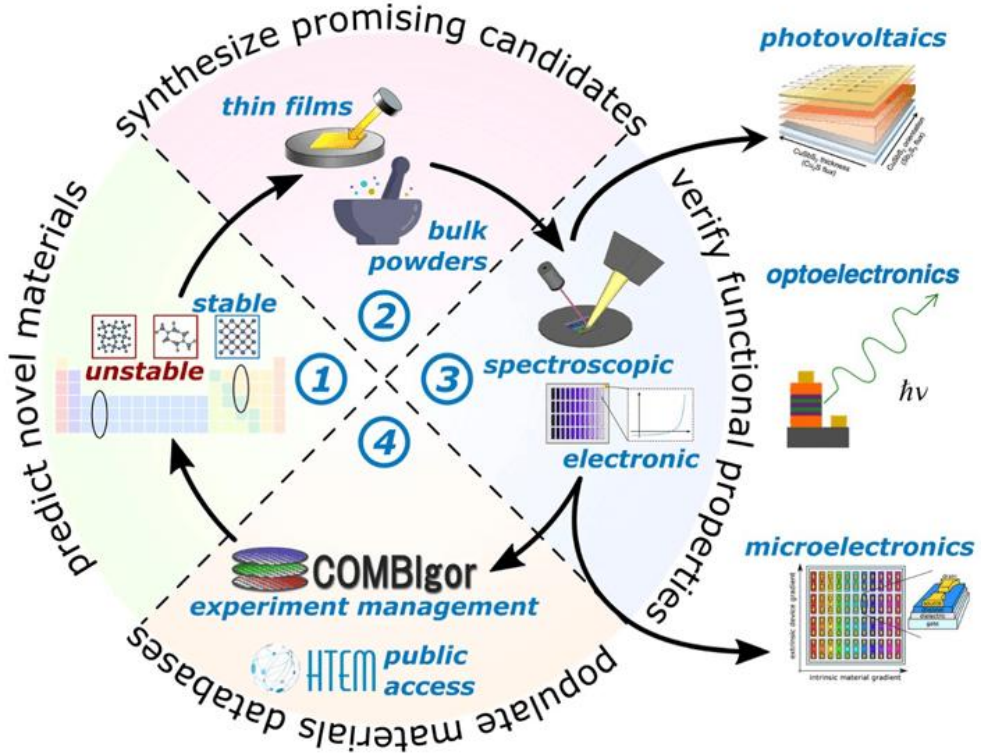


Mercy *et al.*, *Nat. Comm.* **8**, 1677 (2017)



Motzkau, Wikimedia Commons

Optimized search for technological applications

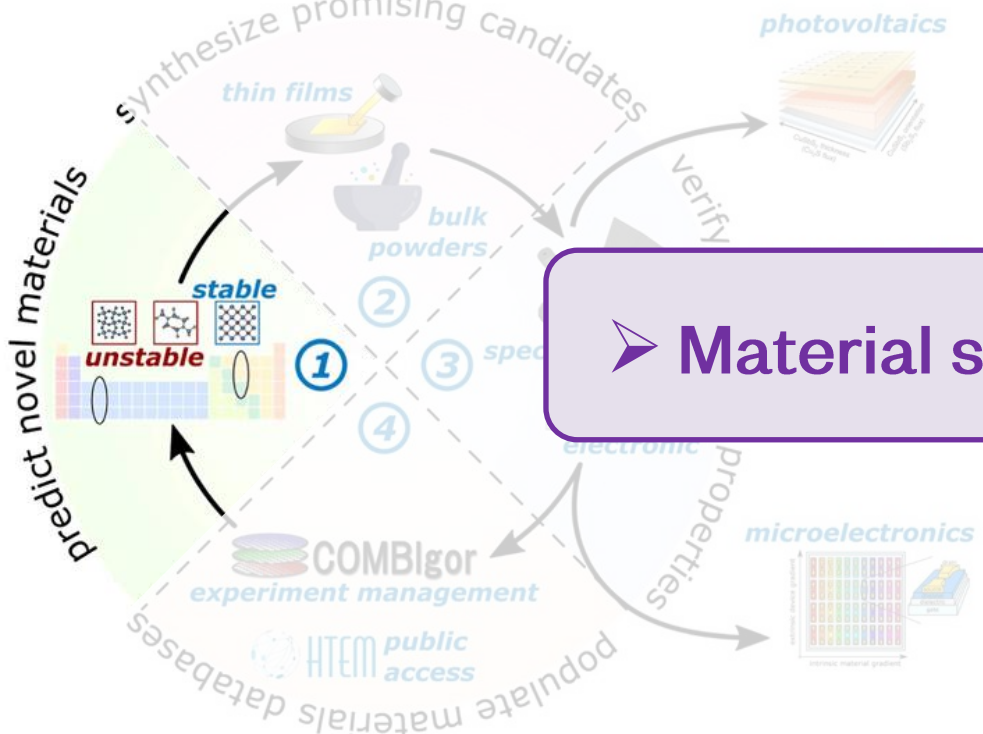


https://www.nrel.gov/materials-science/materials-discovery

Correlated electrons	Mott switches, neuromorphic devices
High-Tc superconductors	Power, magnet tech, quantum coherence
Topological insulators/semimetals	Spintronics, quantum computing
Quantum spin liquids	Topological qubits, error correction
Multiferroics	Cross-coupled memory and sensors
Topological superconductors	Majorana qubits
2D materials	Flexible electronics, optoelectronics
Heavy fermions	Quantum criticality, theoretical models
Quantum Hall systems	Quantum metrology, anyons
Spin-orbit materials	Spintronics, skyrmions
CDW materials	Ultrafast devices, THz tech
Twisted materials	Tunable quantum states, flat-band physics

ChatGPT (GPT-4), OpenAI

Optimized search for technological applications



https://www.nrel.gov/materials-science/materials-discovery

➢ **Material specific simulations**

Correlated electrons	Mott switches, neuromorphic devices
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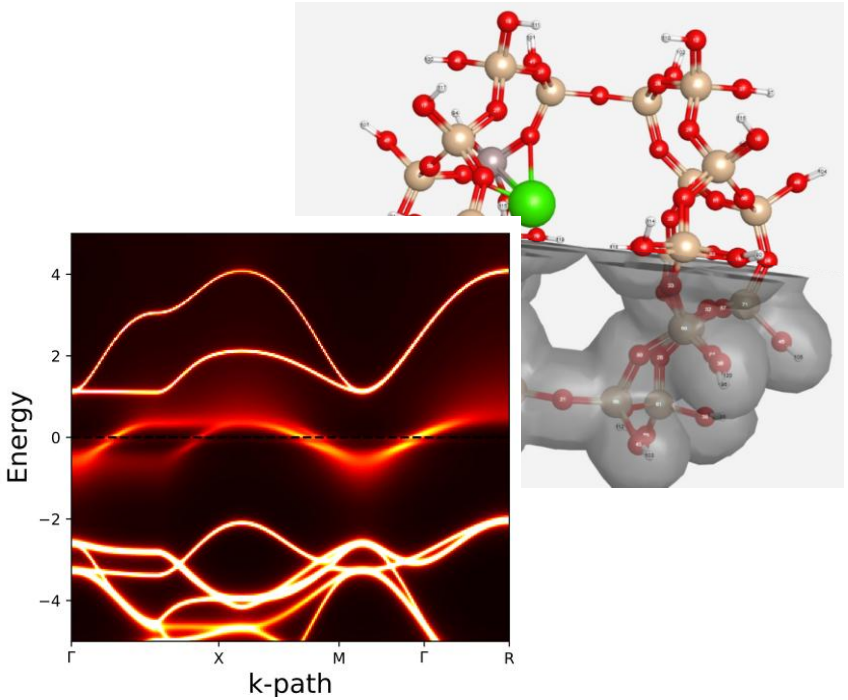
Electronic structure with correlations

➢ Electronic structure

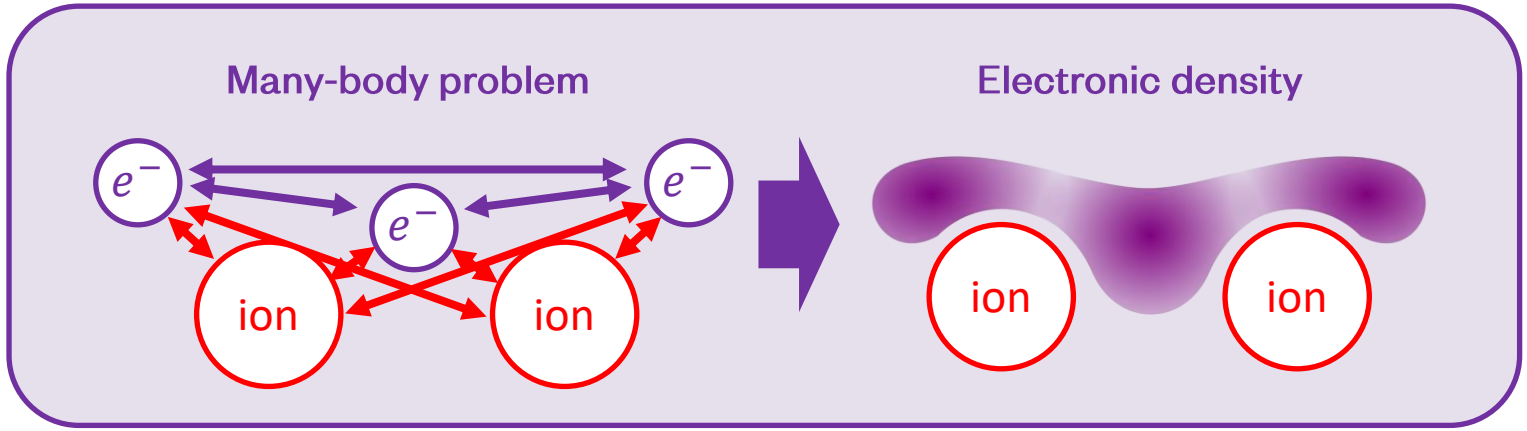


Electronic states

$$H|\Psi_\nu\rangle = [H_{ae}+H_{ee}]|\Psi_\nu\rangle = E_\nu|\Psi_\nu\rangle$$

Many interacting electrons = Many-body problem

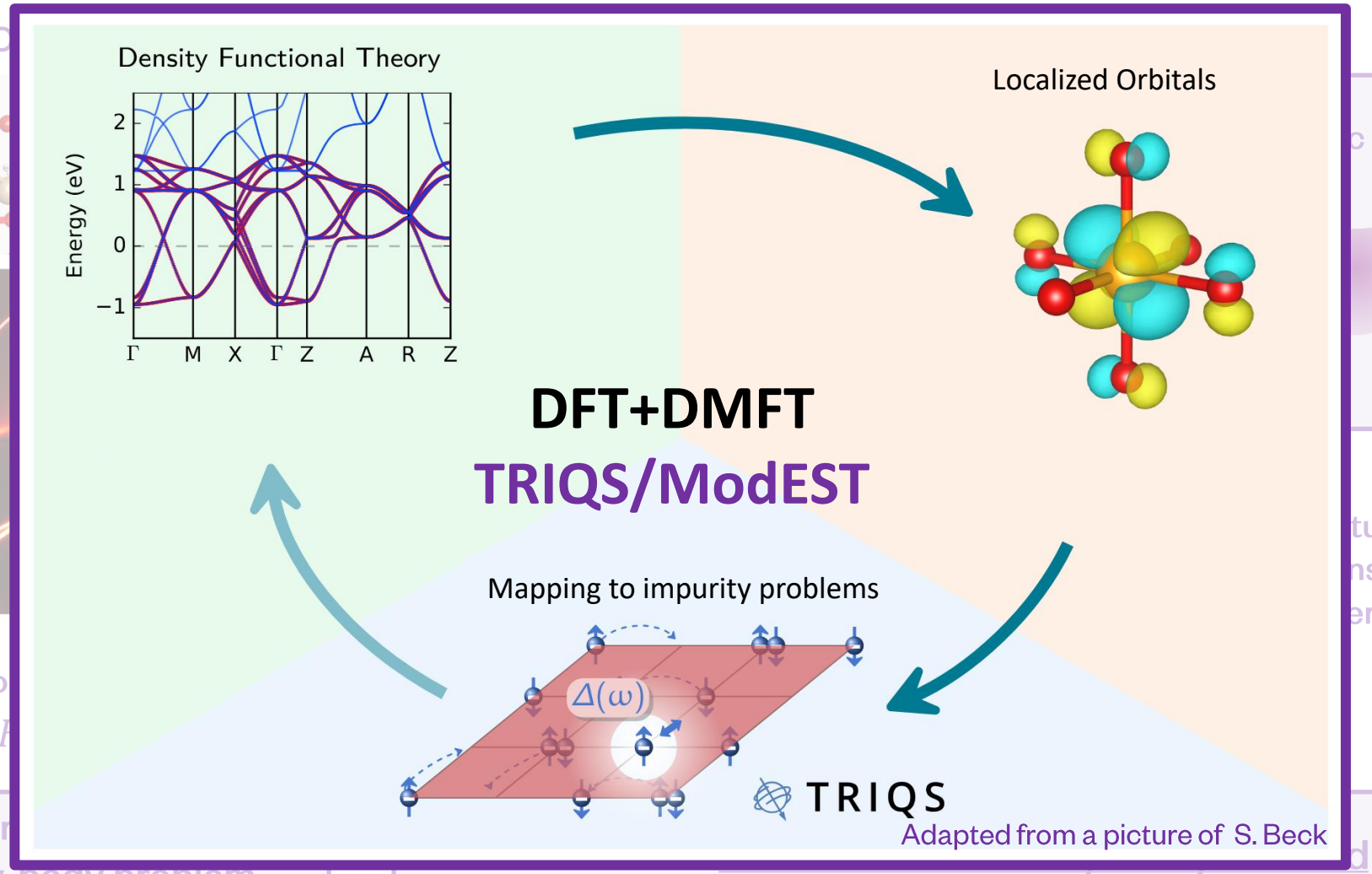
Density functional theory (DFT)



- Can treat large systems efficiently
- Predicts most often the right crystal structure
- Helps to estimate the screened interactions
- Misses most of the correlations we are interested in

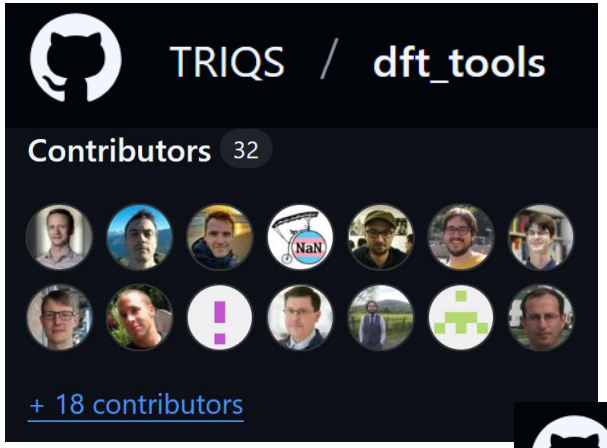
Correct with a many-body method

Electronic structure with correlations

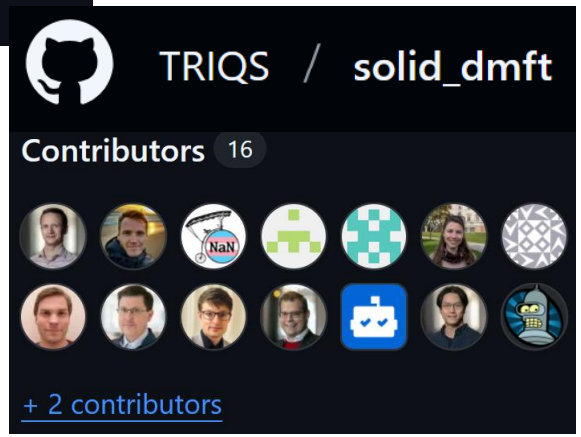


TRIQS/ModEST

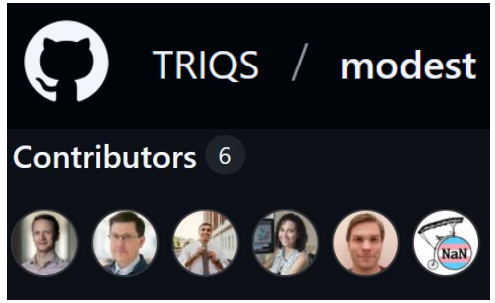
- New implementation standing « on the shoulders of giants »



First release in 2019



First release in 2021



Not released yet

O. Parcollet

H. Labolita J. Coulter

Outline

- Density functional theory
- Localized orbitals
- Mapping to impurity problems
- Post-processing

Density functional theory

Overview of DFT

- **Energy for electrons** in a solid:

$$E[v_{\text{ext}}] = \langle \Psi | \mathcal{H}[v_{\text{ext}}] | \Psi \rangle = T + V_{\text{el-el}} + \int d\mathbf{r} \rho(\mathbf{r}) v_{\text{ext}}(\mathbf{r}) \quad \text{with} \quad \rho(\mathbf{r}) = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})$$

- **Solving** this Hamiltonian:

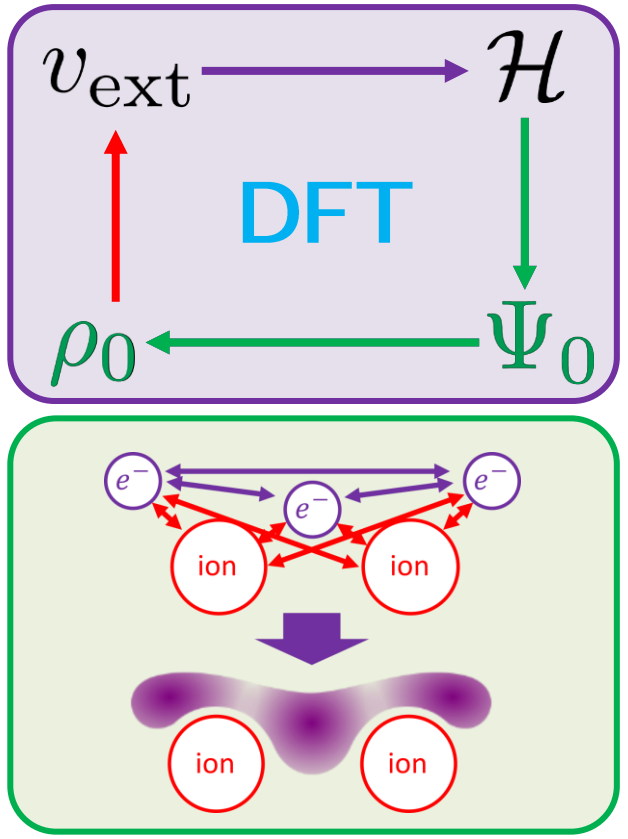
$$v_{\text{ext}} \rightarrow \mathcal{H}[v_{\text{ext}}] \rightarrow E_0 = \langle \Psi_0 | \mathcal{H}[v_{\text{ext}}] | \Psi_0 \rangle \rightarrow \rho_0(\mathbf{r}) = |\langle \mathbf{r} | \Psi_0 \rangle|^2$$

- **Hohenberg-Kohn theorems** in the 1960s:

1. Given $\rho_0(\mathbf{r}) \Leftrightarrow v_{\text{ext}}(\mathbf{r})$
2. Ground-state energy $E_0[\rho]$

- **Kohn-Sham equations** in 1965:

Mapping to a non-interacting system



Outline

- Density functional theory
  - Legendre transformation
  - Kohn-Sham equations
  - Self-consistency loop
  - Advantages & limitations
- Localized orbitals
- Mapping to impurity problems
- Post-processing

Legendre transformation

- Add a source that couples through field $J(\mathbf{r})$ to a physical quantity: **the density** $\rho(\mathbf{r})$

$$E'[J] = T + V_{\text{el-el}} + \int d\mathbf{r}\rho(\mathbf{r})v_{\text{ext}}(\mathbf{r}) + \int d\mathbf{r}\rho(\mathbf{r})J(\mathbf{r}) \quad \text{and} \quad \frac{\delta E'[J]}{\delta J(\mathbf{r})} = \rho(\mathbf{r})$$

- Can perform the **Legendre transformation** which eliminates $J(\mathbf{r})$ in favor of the dual $\rho(\mathbf{r})$

$$\Gamma_{\text{DFT}}[\rho] = E'[J] - \int d\mathbf{r}\rho(\mathbf{r})J(\mathbf{r}) \quad \text{and} \quad J[\rho](\mathbf{r}) = \frac{\delta\Gamma_{\text{DFT}}[\rho]}{\delta\rho(\mathbf{r})} \text{, thus } E'[J[\rho]]$$

- Physical system recovered at **stationarity**:

$$\frac{\delta\Gamma_{\text{DFT}}[\rho]}{\delta\rho(\mathbf{r})} = J(\mathbf{r}) = 0\,, \quad \Gamma_{\text{DFT}}[\rho]\Big|_{J=0} = E'[J[\rho] = 0] = E[\rho] = \underbrace{[T + V_{\text{el-el}}]\,[\rho]}_{F[\rho]} + \int d\mathbf{r}\rho(\mathbf{r})v_{\text{ext}}(\mathbf{r})$$

Convexity of the Legendre transform ⇨ Ground-state

Legendre transformation

- Add… $J(\mathbf{r})$ … $\rho(\mathbf{r})$

Hohenberg-Kohn theorem #2:

There exists a universal functional $F[\rho]$ such that the total energy functional

$$E[\rho] = F[\rho] + \int d\mathbf{r}\; v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r})$$

achieves its minimum at the true ground-state density $\rho_0(\mathbf{r})$ where $E_0 \equiv E[\rho_0] \leq E[\rho]$.

- Can… …ual $\rho(\mathbf{r})$

- Physical system recovered at **stationarity**:

$$\frac{\delta\Gamma_{\text{DFT}}[\rho]}{\delta\rho(\mathbf{r})} = J(\mathbf{r}) = 0\,, \quad \Gamma_{\text{DFT}}[\rho]\Big|_{J=0} = E'[J[\rho]=0] = E[\rho] = \underbrace{[T + V_{\text{el-el}}]\,[\rho]}_{F[\rho]} + \int d\mathbf{r}\rho(\mathbf{r})v_{\text{ext}}(\mathbf{r})$$

Convexity of the Legendre transform ⇨ Ground-state

Hohenberg-Kohn theorems

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- The potential $v_{\text{ext}}(\mathbf{r})$ already acts as a source for the physical quantity $\rho(\mathbf{r})$

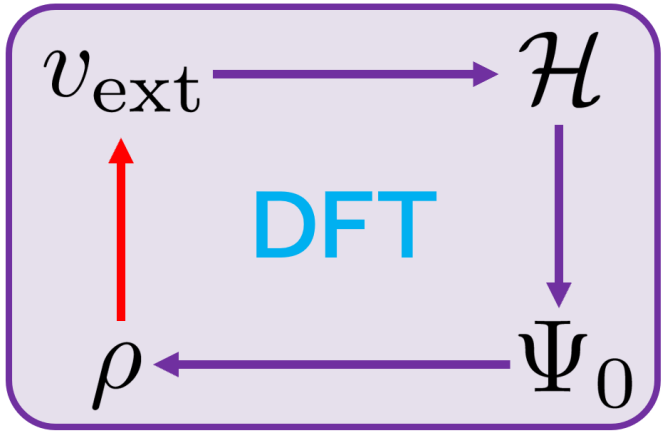
$$E[v_{\text{ext}}] = F[\rho] + \int d\mathbf{r}\rho(\mathbf{r})v_{\text{ext}}(\mathbf{r}) \quad \text{is a Legendre transform:} \quad \frac{\delta E[v_{\text{ext}}]}{\delta v_{\text{ext}}(\mathbf{r})} = \rho(\mathbf{r}), \text{ and } \frac{\delta F[\rho]}{\delta \rho(\mathbf{r})} = -v_{\text{ext}}(\mathbf{r})$$

$\Rightarrow$ Uniqueness of $v_{\text{ext}}[\rho]$

Hohenberg-Kohn theorem #1:

For any system of interacting particles in an external potential $v_{\text{ext}}(\mathbf{r})$, this potential is uniquely determined by the ground-state electron density $\rho_0(\mathbf{r})$. Consequently, all ground-state properties of the system are uniquely determined by $\rho_0(\mathbf{r})$.

Hohenberg-Kohn theorem #2



Kohn-Sham equation

- **Key insight:** Expand the DFT functional around a non-interacting reference

$$[T + V_{ee}][\rho] = T_s[\rho] + V_H[\rho] + V_{xc}[\rho] \quad \text{with} \quad V_H[\rho] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

Kinetic of non-interacting particles — Rest — Hartree

- The DFT functional becomes

$$\Gamma_{\mathrm{DFT}}[\rho] = \underbrace{T_s[\rho] + V_{\mathrm{ext}}[\rho]}_{\Gamma_0[\rho]} + \underbrace{V_H[\rho] + V_{xc}[\rho]}_{\Delta\Gamma[\rho]} \quad \text{and} \quad 0 = \frac{\delta\Gamma_0[\rho]}{\delta\rho} + \frac{\delta\Delta\Gamma[p]}{\delta\rho} = -J_0 + \frac{\delta\Delta\Gamma[p]}{\delta\rho}$$

- Working in the non-interacting system $\Gamma_0[\rho]$ with a **constraining field** $J_0 = \frac{\delta\Delta\Gamma[p]}{\delta\rho} = v_{\mathrm{int}}$ yields the same density as the original system

Non-interacting KS orbitals with $\rho_{\mathrm{KS}}(\mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2$ living in the effective potential $v_{\mathrm{KS}} = v_{\mathrm{ext}} + v_{\mathrm{int}}$

Kohn-Sham equation

- **Key insight:** Expand the DFT functional around a non-interacting reference

$$[T + V_{ee}][\dots] + \frac{1}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

- The DFT functional

$$\Gamma_{\mathrm{DFT}}[\rho] = \underbrace{T_s[\rho]}_{\Gamma} + \dots = -J_0 + \frac{\delta\Delta\Gamma[p]}{\delta\rho}$$

- Working in the non-i… eld $J_0 = \frac{\delta\Delta\Gamma[p]}{\delta\rho} = v_{\mathrm{int}}$ yields the same density as the original system

Non-interacting KS orbitals with $\rho_{\mathrm{KS}}(\mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2$ living in the effective potential $v_{\mathrm{KS}} = v_{\mathrm{ext}} + v_{\mathrm{int}}$

Same approach in other methods

Method	Physical quantity	Constraining field
Baym-Kadanoff	$G_{\alpha\beta}(i\omega, \mathbf{k})$	$\Sigma_{\alpha\beta}(i\omega, \mathbf{k})$
DMFT	$G^{\mathrm{loc}}_{\alpha\beta}(i\omega)$	$\Sigma^{\mathrm{imp}}_{\alpha\beta}(i\omega)$
LDA	$\rho(\mathbf{r})$	$v_{\mathrm{int}}(\mathbf{r})$
LDA+DMFT	$\rho(\mathbf{r})$, $G^{\mathrm{loc}}_{\alpha\beta}(i\omega)$	$v_{\mathrm{int}}(\mathbf{r})$, $\Sigma^{\mathrm{imp}}_{\alpha\beta}(i\omega)$

Self-consistency loop

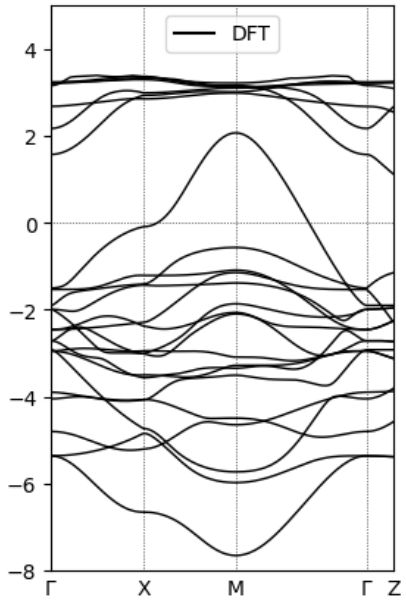
- Minimization of energy with Lagrange multiplier:

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2 \qquad \frac{\delta E[\rho]}{\delta \phi_i^*(\mathbf{r})} - \sum_j \epsilon_j \frac{\delta}{\delta \phi_i^*(\mathbf{r})} \left[\int d\mathbf{r}' |\phi_j(\mathbf{r}')|^2 \right] = 0$$

- Kohn-Sham Schrodinger-like equation and Green's function:

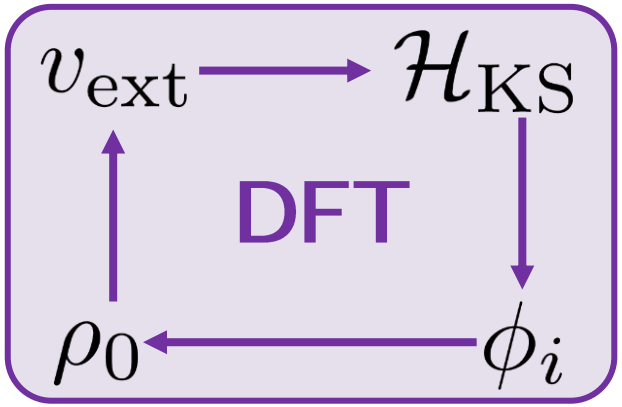
$$\left[-\frac{1}{2}\nabla^2 + v_{\mathrm{KS}}(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}) \qquad G(\mathbf{r}, \mathbf{r}'; i\omega) = \sum_i \frac{\phi_i(\mathbf{r}) \phi_i^*(\mathbf{r}')}{i\omega - \epsilon_i + \mu}$$

$$v_{\mathrm{KS}} = v_{\mathrm{ext}} + v_H + v_{xc}$$



- **Variational method:** convergence with energy minimization

- Easy to interpolate, from a given density



Advantages and limitations

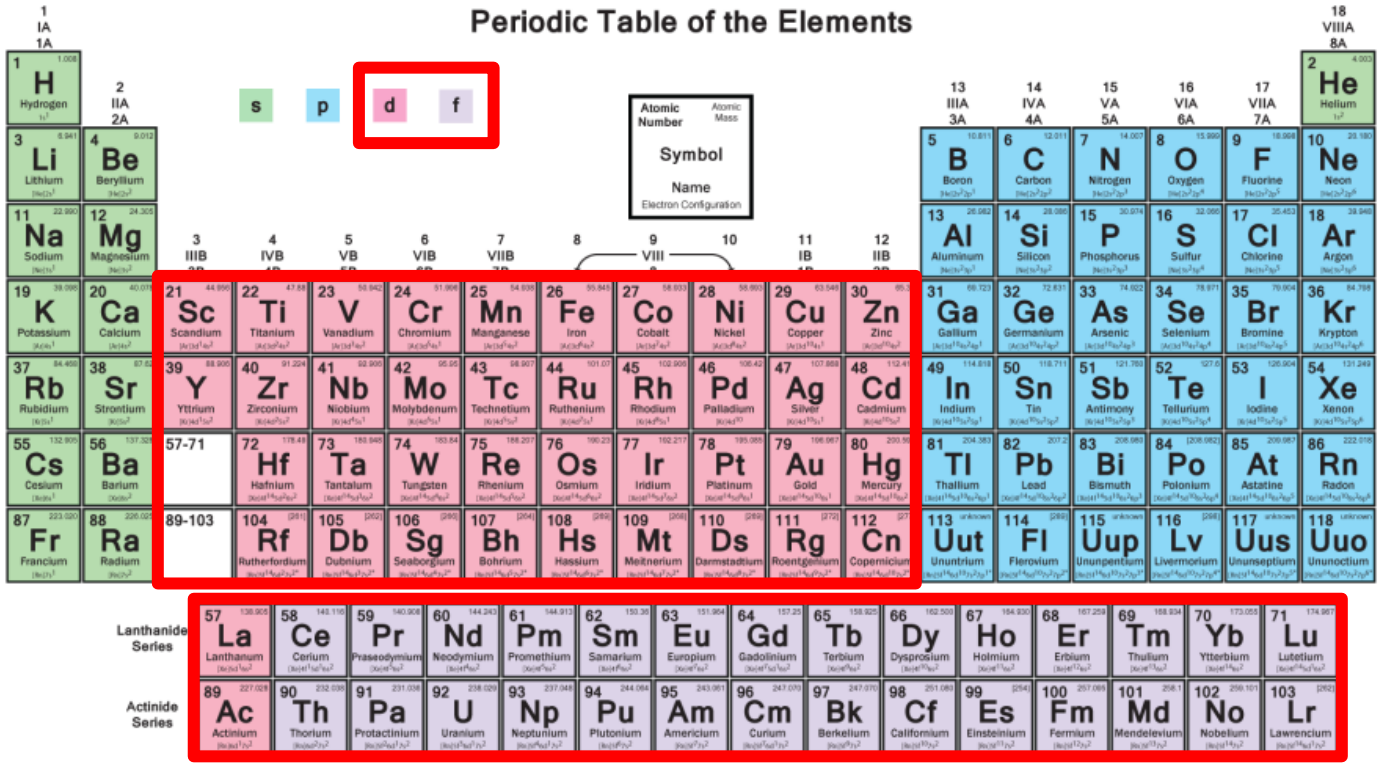
✅ Advantages

1. Computational efficiency
2. Reasonably accurate for many materials
3. Versatile and widely implemented
4. Conceptual simplicity
5. Good starting point for corrections

❌ Limitations

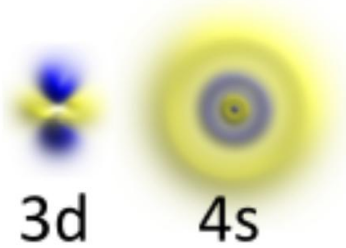
1. Failure to capture strong correlation
2. Lack of systematic improvement
3. Exchange-correlation functional ambiguity
4. Poor description of excited states
5. Static mean-field nature

Strongly correlated electrons



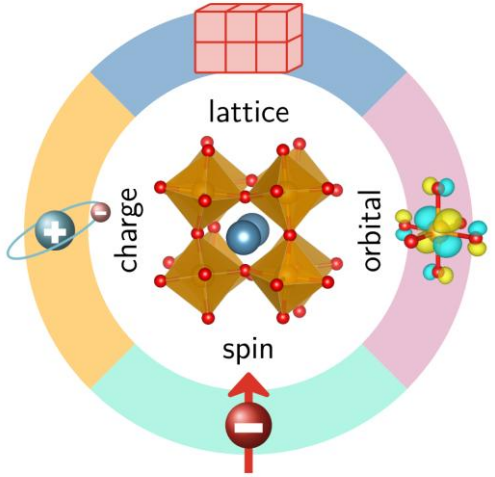
Todd Helmenstine, sciencenotes.org

Localized close to the nucleus



Wikimedia Commons – Atomic orbitals

Interplay of degrees of freedom



Picture of S. Beck

Density functional theory: Summary

- The **Hohenberg-Kohn theorems** demonstrate:
  1. The electronic density $\rho_0(\mathbf{r})$ uniquely determines the ground-state properties
  2. The existence of variational principle for $E_0[\rho]$, with a universal functional

- The **Kohn-Sham equations** leverage an auxiliary system of non-interacting electrons that reproduces the same ground-state $\rho_0(\mathbf{r})$ as for the interacting system

- These can be shown using the **Legendre transformation**

- Converging the **self-consistency loop** yields a charge density for the ground-state

- In practice, **strong correlations** are poorly accounted for

Localized orbitals

Momentum versus position

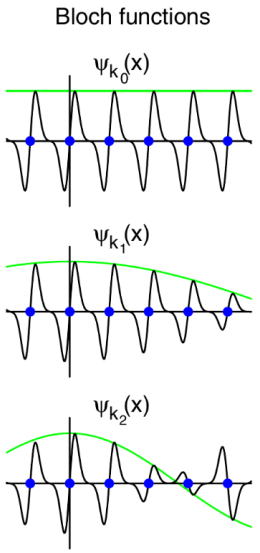
Bloch basis for DFT

Bloch theorem:

For electrons in a periodic potential, the solutions to the Schrödinger equation are Bloch functions:

$$\mathcal{H}|\psi_\nu(\mathbf{k})\rangle = \epsilon_\nu(\mathbf{k})|\psi_\nu(\mathbf{k})\rangle$$

where $\langle \mathbf{r}|\psi_\nu(\mathbf{k})\rangle = u_{\nu\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ with $u_{\nu\mathbf{k}}(\mathbf{r}) = u_{\nu\mathbf{k}}(\mathbf{r}+\mathbf{T})$



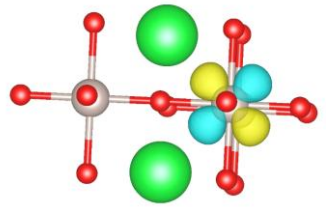
Remarks:

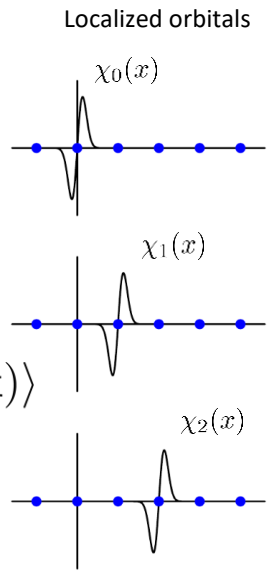
- Band $\nu \in \mathbb{Z}$ and momentum $\mathbf{k} \in \mathrm{BZ}$
- Eigenfunctions $|\psi_\nu(\mathbf{k})\rangle$ are orthonormal
- Have a gauge freedom $|\psi_\nu(\mathbf{k})\rangle \to e^{i\phi(\mathbf{k})}|\psi_\nu(\mathbf{k})\rangle$
- Can be smooth functions of $\mathbf{k}$

Localized orbitals

Interactions are typically localized:

- Localized space





Option: Maximally localized Wannier functions

$$|\chi_m^{\mathbf{R}}\rangle = V\int \frac{d\mathbf{k}}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_\nu U_{m\nu}(\mathbf{k})|\psi_\nu(\mathbf{k})\rangle$$

$$\langle \mathbf{r}|\chi_m^{\mathbf{R}}\rangle = \langle \mathbf{r}+\mathbf{R}|\chi_m^0\rangle$$

Projectors: $P_{m\nu}(\mathbf{k}) \equiv \langle \chi_m^{\mathbf{R}}|\psi_\nu(\mathbf{k})\rangle$

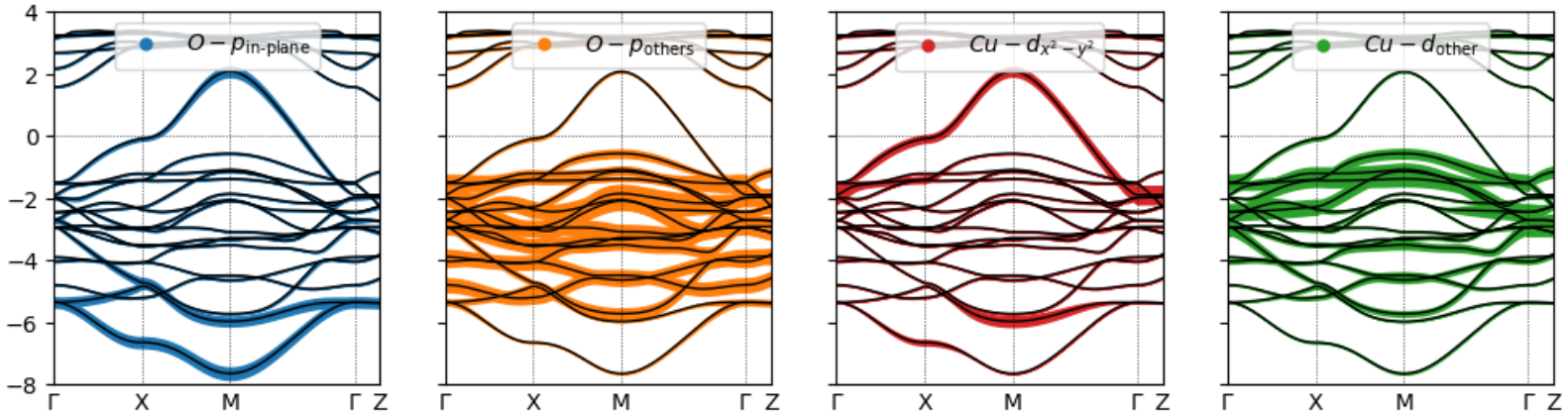
Bloch basis ↔ Localized orbitals

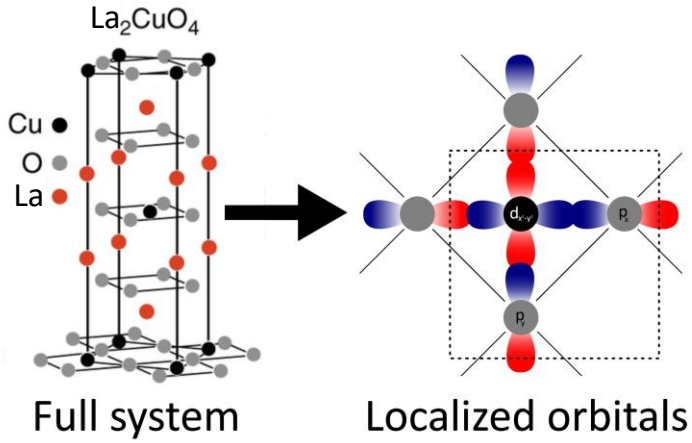
Outline

- Density functional theory
- Localized orbitals
  - Choosing the orbital subspace
  - Maximally localized Wannier functions
  - Projectors
  - One-body elements @ ModEST
- Mapping to impurity problems
- Post-processing

Choosing the orbital subspace

Orbital character: $|\langle \tilde{\chi}^{\mathbf{R}}_m | \psi_\nu(\mathbf{k}) \rangle|^2$ **with** $|\tilde{\chi}^{\mathbf{R}}_m\rangle$ **some hydrogen-like real spherical harmonic**





Potential subsets:

- Single-band Cu-$d_{x^2-y^2}$ model
- Three-band dp-model
- Single-site full Cu-d-shell model
- All Cu and O orbitals

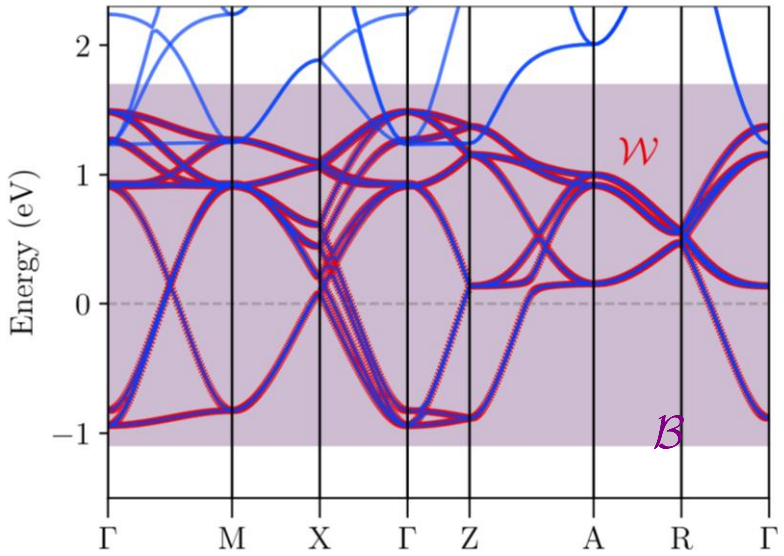
Depends on the physics targeted and the computational resources

Maximally localized Wannier functions

Wannier functions: $|w_m^{\mathbf{R}}\rangle = V \int \frac{d\mathbf{k}}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{\nu\in\mathcal{B}(\mathbf{k})} U_{m\nu}(\mathbf{k})|\psi_\nu(\mathbf{k})\rangle$

- **Orthonormal:** $\langle w_m^{\mathbf{R}}|w_{m'}^{\mathbf{R}'}\rangle = \delta_{mm'}\delta(\mathbf{R}-\mathbf{R}')$
- **Gauge freedom of the unitary transform $U(\mathbf{k})$ can be used to minimize the spread**

$$U = \arg\min_U \left\{ \sum_m \left[\langle w_n^{\mathbf{0}}|\mathbf{r}\cdot\mathbf{r}|w_n^{\mathbf{0}}\rangle - |\langle w_n^{\mathbf{0}}|\mathbf{r}^2|w_n^{\mathbf{0}}\rangle|^2 \right] \right\}$$ **, can be recasted in terms of** $M_{\nu\nu'}^{(\mathbf{k},\mathbf{b})} \equiv \langle u_\nu(\mathbf{k})|u_{\nu'}(\mathbf{k}+\mathbf{b})\rangle$



In practice, in WANNIER90 **:**

- **Start with trial localized orbitals** $|g_m\rangle$**:** $|\phi_n(\mathbf{k})\rangle \equiv \sum_{\nu\in\mathcal{B}(\mathbf{k})} \underbrace{\langle\psi_\nu(\mathbf{k})|g_m\rangle}_{A_{\nu m}(\mathbf{k})} |\psi_\nu(\mathbf{k})\rangle$
- **Orthonormalize:** $|\tilde{\psi}_\nu(\mathbf{k})\rangle = \sum_{\nu'\in\mathcal{B}(\mathbf{k})} S_{\nu\nu'}^{-1/2}(\mathbf{k})|\phi_{\nu'}(\mathbf{k})\rangle$ with $S_{\nu\nu'}(\mathbf{k}) = [A^\dagger A(\mathbf{k})]_{\nu\nu'}$
- **Minimize the spread**

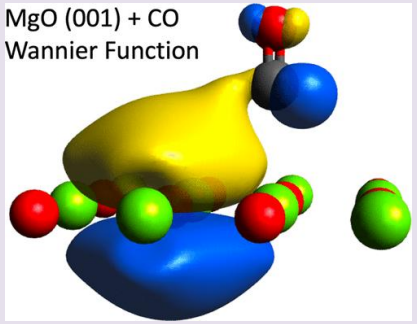
Applications

- **Effective low-energy tight-biding models**
  - Compact and flexible for modeling large complex systems

$$[t_{ij}]_{mm'} = \langle w_m^{\mathbf{R}_i} | \hat{H}_{\mathrm{KS}} | w_{m'}^{\mathbf{R}_j} \rangle$$

$$\mathcal{H}_0 = \sum_{ij} \sum_{mm'\sigma} [t_{ij}]\, c_{im\sigma}^{\dagger} c_{jm'\sigma}$$

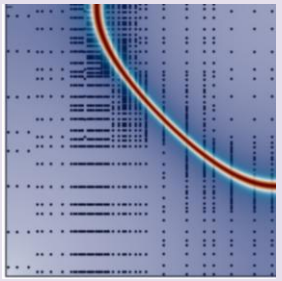
- **Visualization of low-energy effective orbitals**
  - Identify relevant orbitals and understand chemical bonding



Zhu *et al.*, *J. of Phys. Chem. A* **128**, 8570 (2024)

- **Interpolation of Hamiltonian and orbitals**
  - Accurate Fermi surface, density of states, quantum geometry evaluations & optical and transport properties

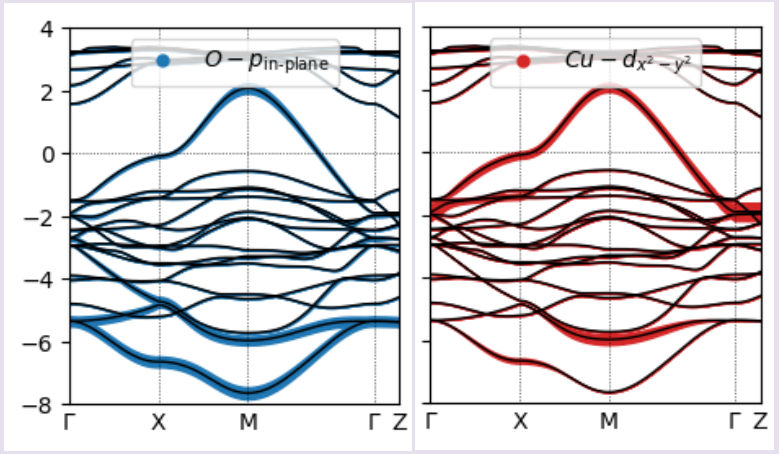
Adaptative integration



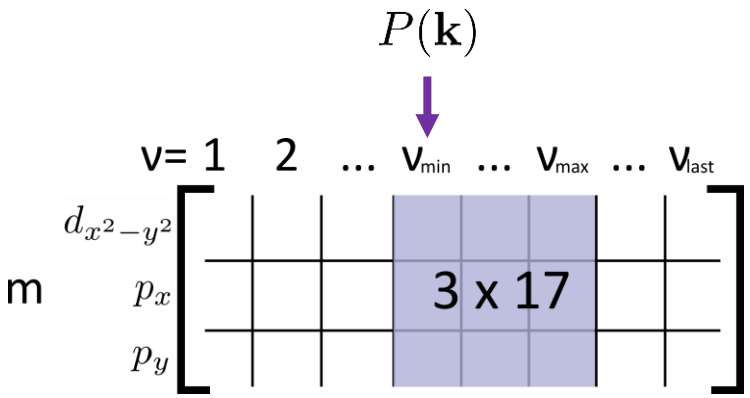
Kaye *et al.*, *SciPost Phys.* **15**, 062 (2023)

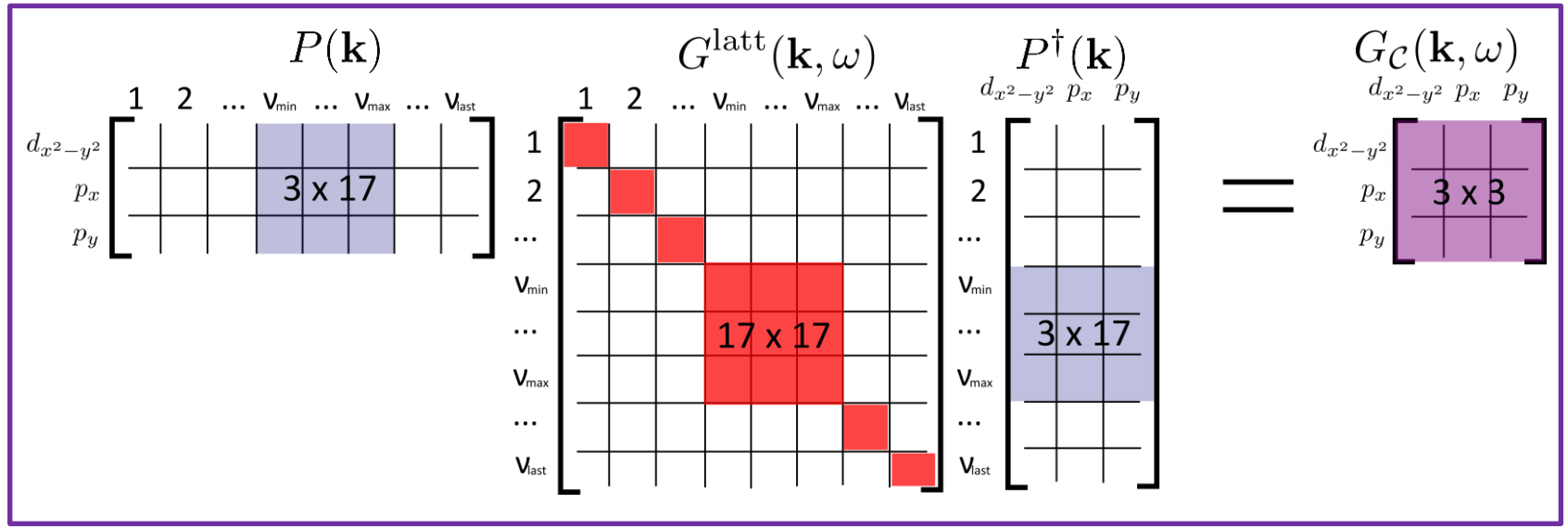
Projectors: From bands to orbitals

- **Example**: 3-orbital model of La_2CuO_4
  - Total of 5 Cu-$3d$ and 12 O-$2p$ orbitals: 17
  - Only interested in Cu-$3d_{x^2-y^2}$ and 2 of the O-$2p$
  - We selected all the bands



$$\Rightarrow P_{m\nu}(\mathbf{k}) \equiv \langle \chi_m^{\mathbf{R}} | \psi_\nu(\mathbf{k}) \rangle$$





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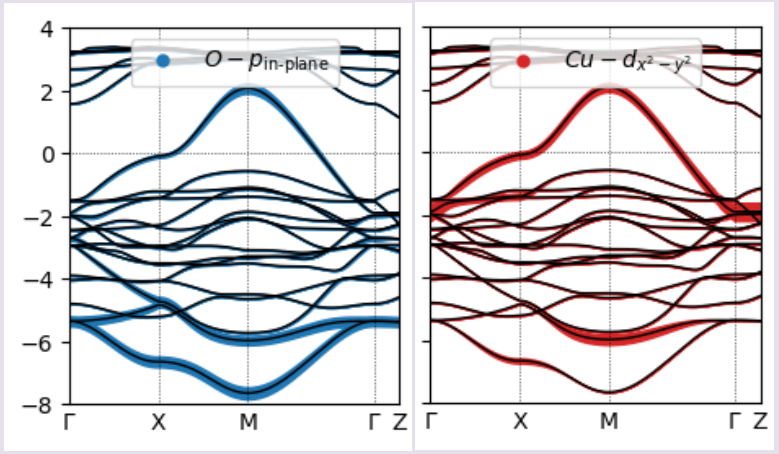

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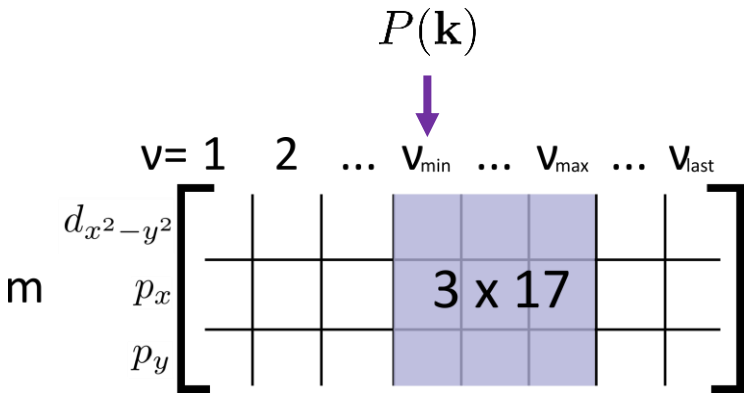
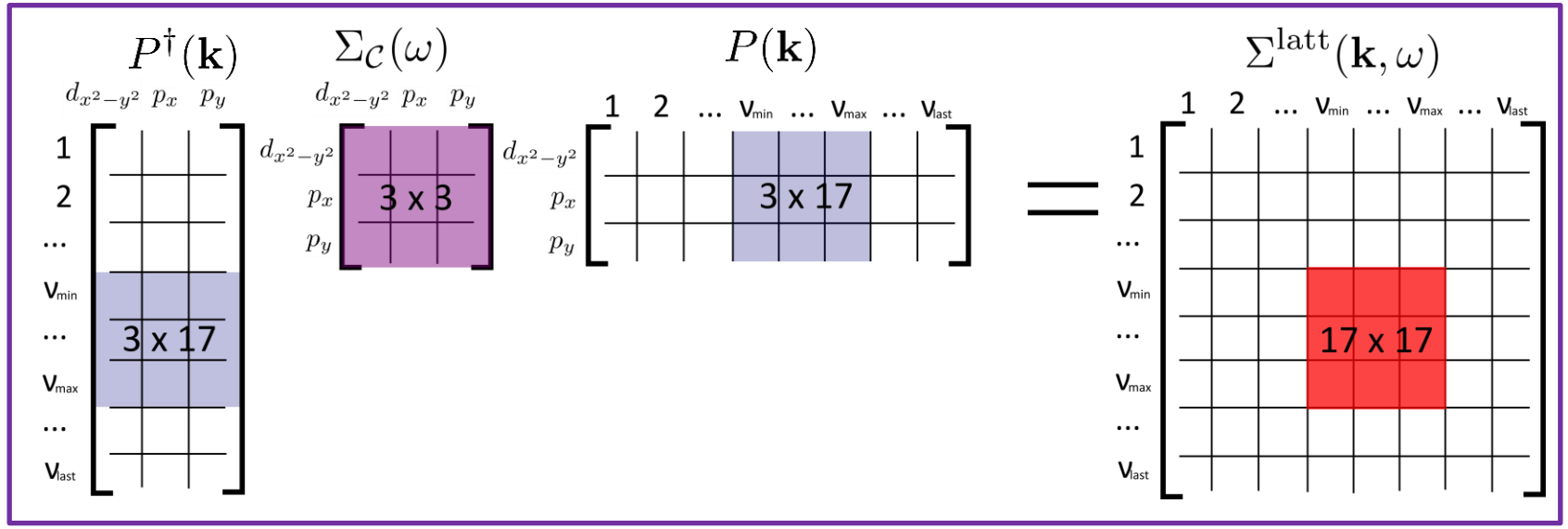
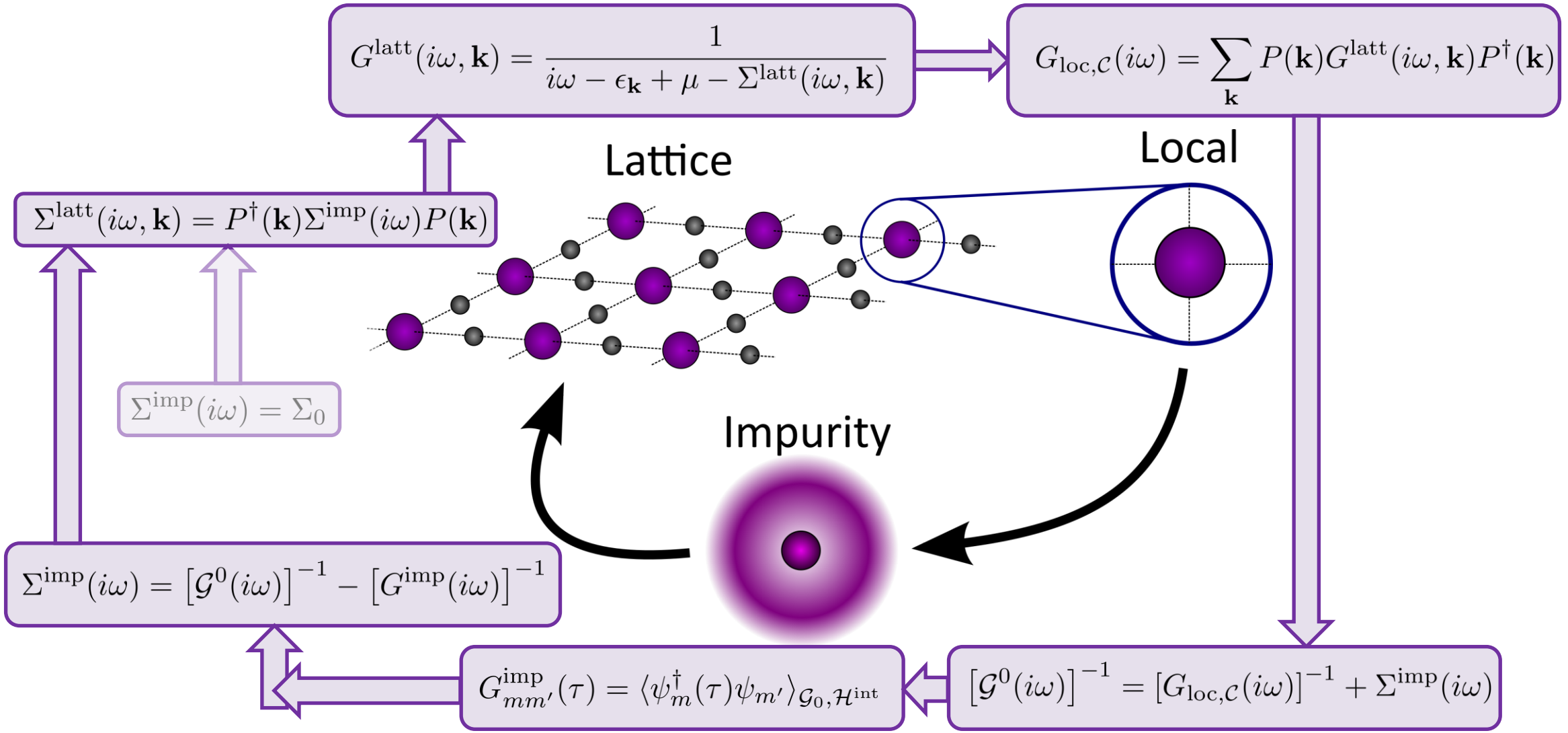
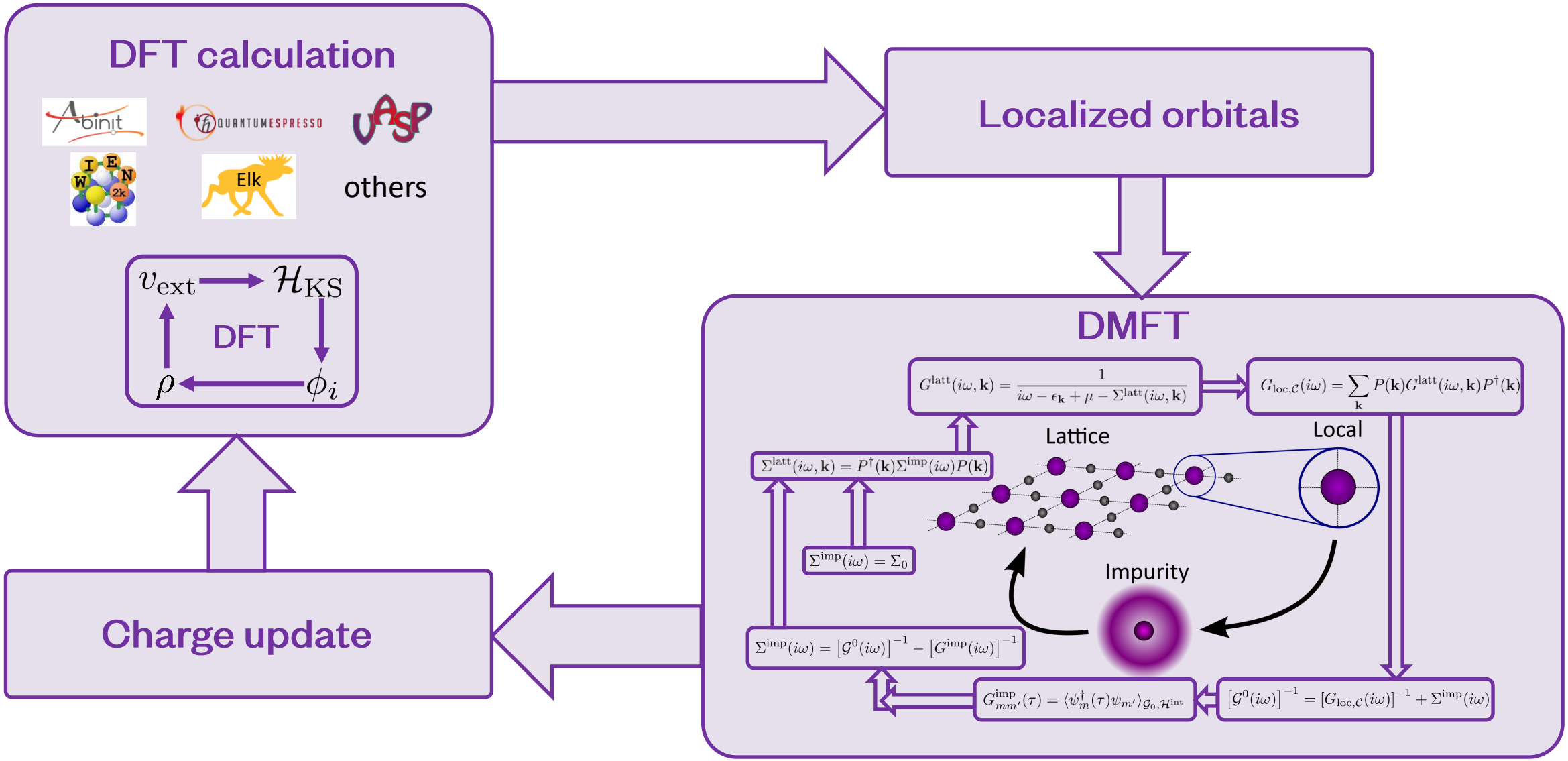




Dynamical mean-field theory



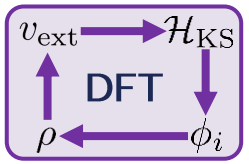
Charge self-consistent DFT+DMFT



Two options for the lattice

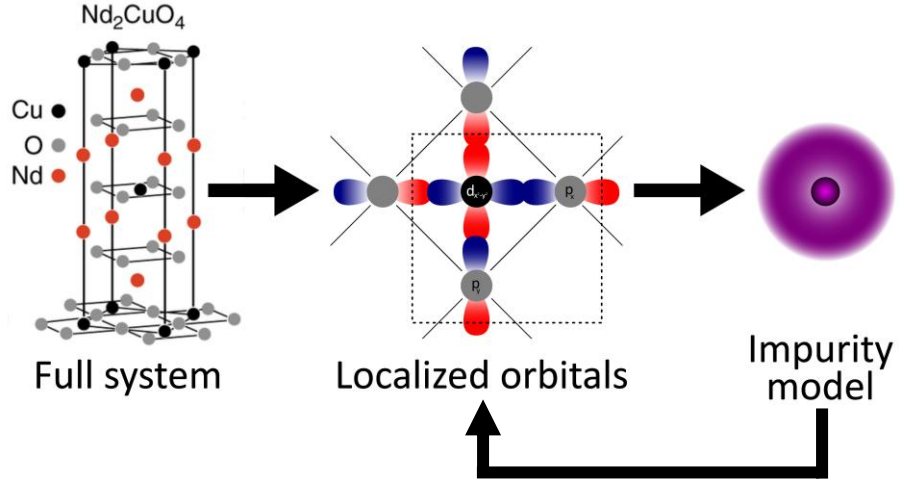
Two ways to perform DFT+DMFT:

➢ DMFT on DFT model

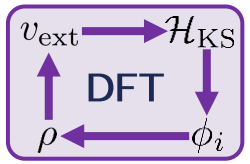


WANNIER90

$$\mathcal{H}_0 = \sum_{ii'\sigma\sigma'mm'} [t_{ii'}^{\sigma\sigma'}]_{mm'} c_{im\sigma}^{\dagger} c_{i'm'\sigma'}$$



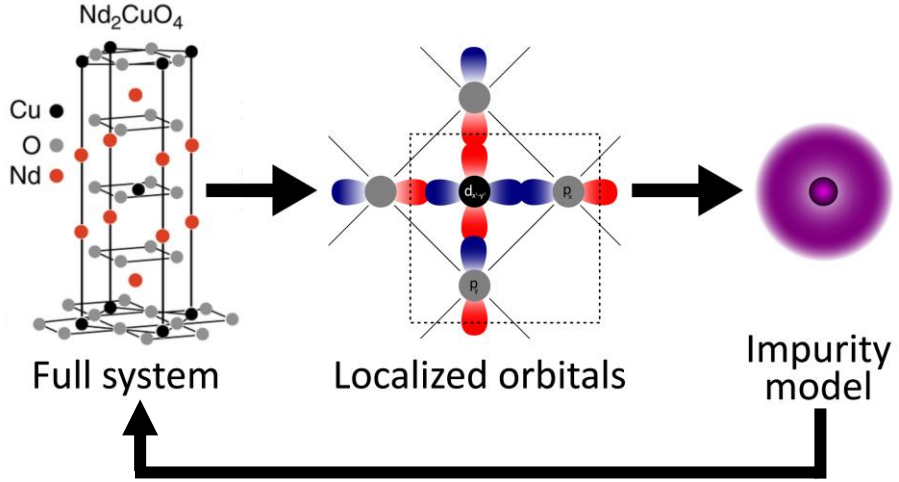
➢ DFT+DMFT



WANNIER90

$\epsilon_\nu(\mathbf{k})$

$P_{m\nu}(\mathbf{k})$



One-body elements @ ModEST

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➢ In tutorial 5b: multiorbital $SrVO_3$

```
One body elements representing a downfolding from (restricted) Bloch 𝓑 to Correlated space 𝓒 from DFT code [one_body_elements_on_grid]
  H:
    Band dispersion ε^σ(k) on a grid [band_dispersion]:
      Number of bands (max): 21
      Represented on a fixed grid of 35 points.
      Shape of H[k_idx, σ, ν, ν'] = [35, 1, 21, 21]
      ε^σ(k) is matrix valued? = false
  C_space:
    Local space [orbital_set]:
      Total dimension [M]: 3
      Number of correlated atoms: 1
      Number of inequivalent correlated atoms = 1
      Atomic decomposition:
         dim_a:   3
             a:   0
        irreps: [1, 1, 1]
  P:
    Downfolding projector P^σ_mν(k) on a grid [downfolding_projector]:
      Shape of P[k_idx, σ, m, ν]  = [35, 1, 3, 21]
  IBZ = true
    [I]rreduicible [B]rillouin [Z]one symmetry operations from the DFT code [ibz_symmetry_ops]
      Number of symmetry ops: 48
      Number of rotations per op: 1
```

$[\epsilon_{\mathrm{KS}}(\mathbf{k})]^{\sigma}_{\nu\nu'}$

$\{|\chi^{\mathbf{R}}_{m}\rangle\}$

$[P(\mathbf{k})]^{\sigma}_{m\nu}$

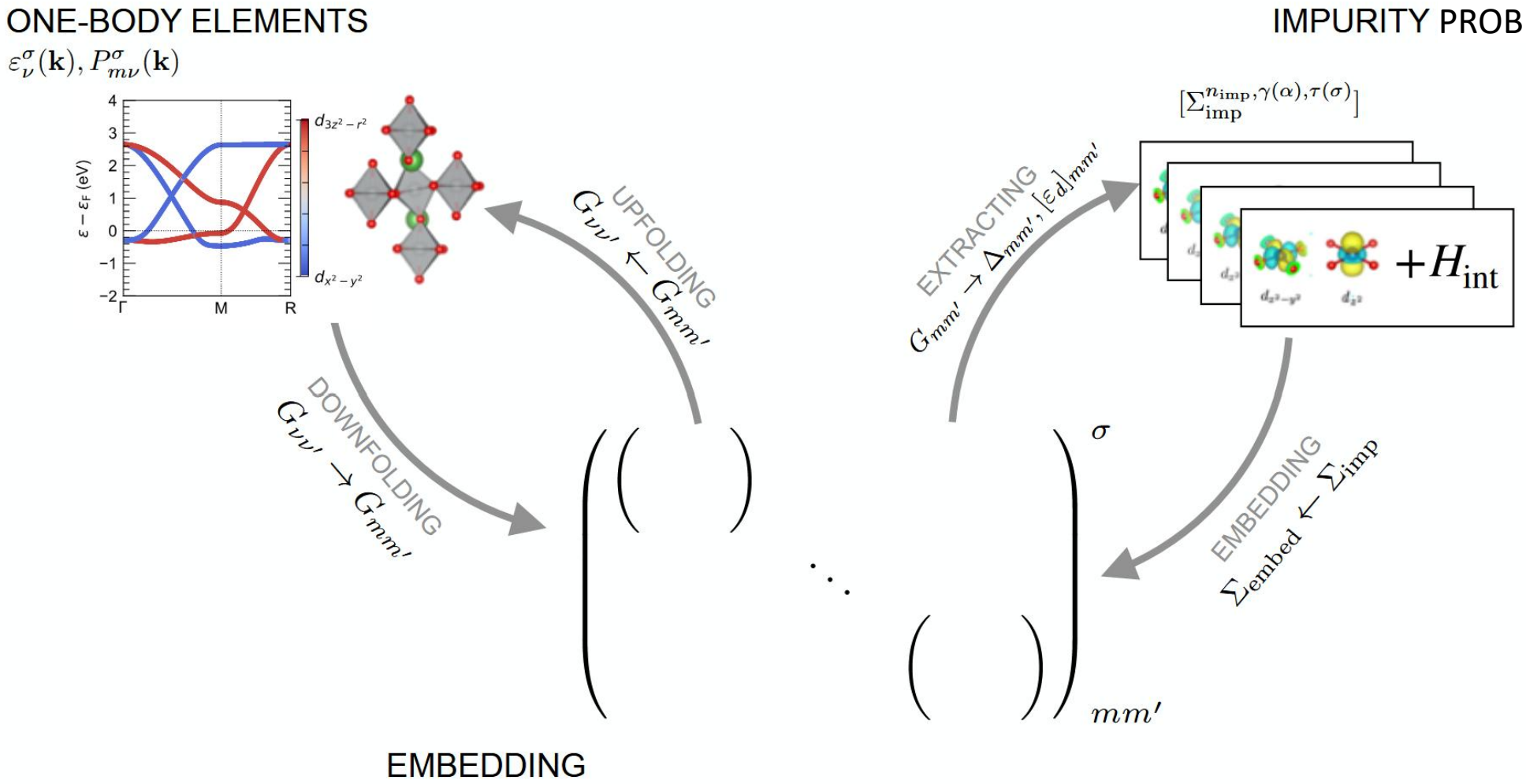
Information about symmetries

Localized orbitals: Summary

- Localized orbitals offer a **much better basis** to treat strong local interactions
- The **choice of orbitals** depends on the system and the physics targeted
  - Plotting the **orbital character** is a great tool at the DFT level
- **Maximally localized Wannier functions** are a common choice of construction
  - **Wannier90** is often used
- Once the orbitals constructed, there are **two types of DFT+DMFT:**
  - **Model-like calculations** with an extracted tight-binding model
  - **Whole-solid calculations** with projectors
- **Obe @ ModEST**: all needed to move between the KS bands and the localized orbitals

Mapping to impurity problems

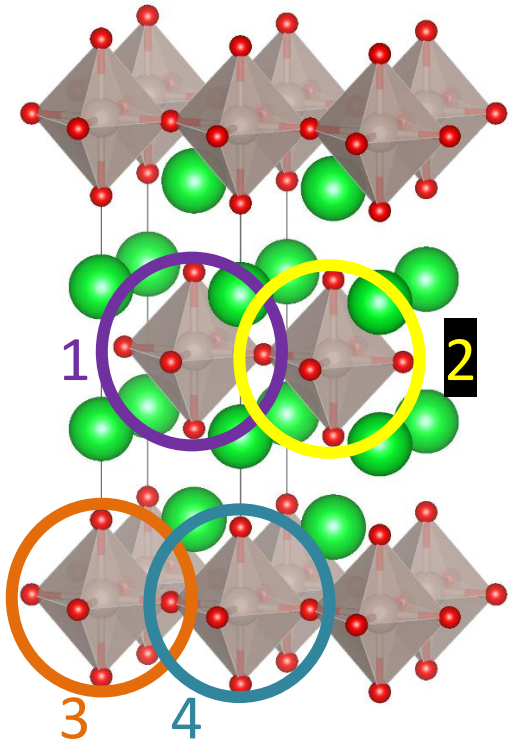
Embedding @ ModEST



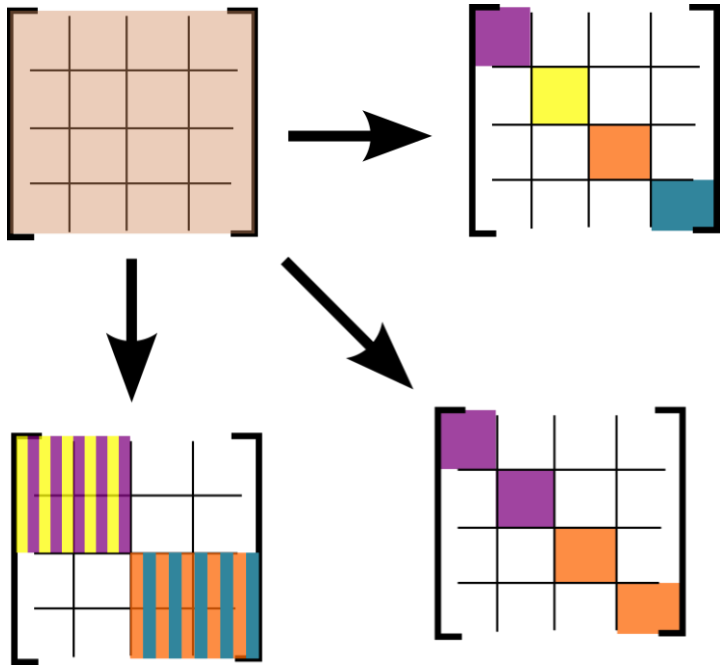
Outline

- Density functional theory
- Localized orbitals
- Mapping to impurity problems
  - Embeddings
  - Impurity problems
  - Impurity parameters
- Post-processing

The many possibilities of embeddings



- Localized orbital sets: $\{\mathrm{Ni}_1, \mathrm{Ni}_2, \mathrm{Ni}_3, \mathrm{N4}\}$

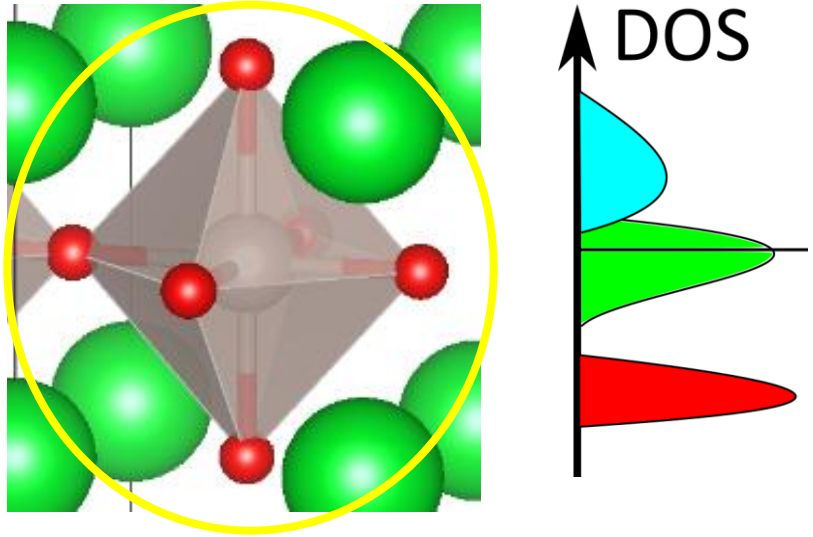


Multi-site DMFT
(inhomogeneous)
With inequivalent sites

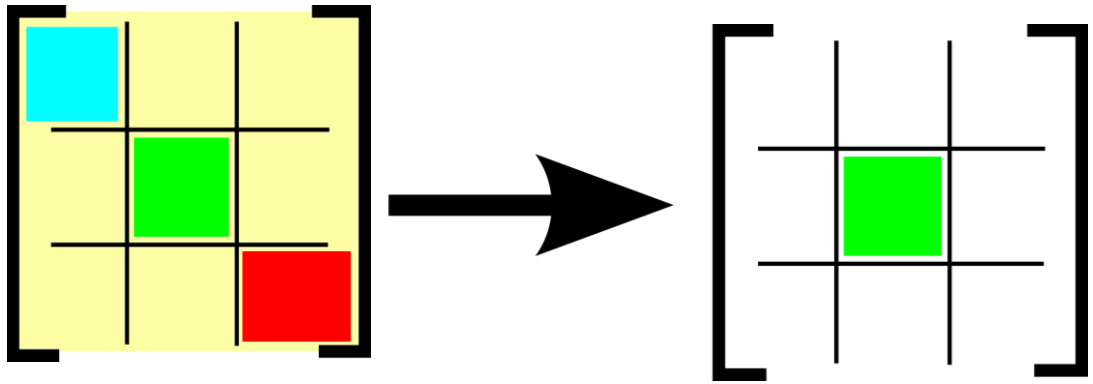
Multi-site DMFT
(inhomogeneous)
With equivalent sites

Multi-cluster DMFT

The many possibilities of embeddings



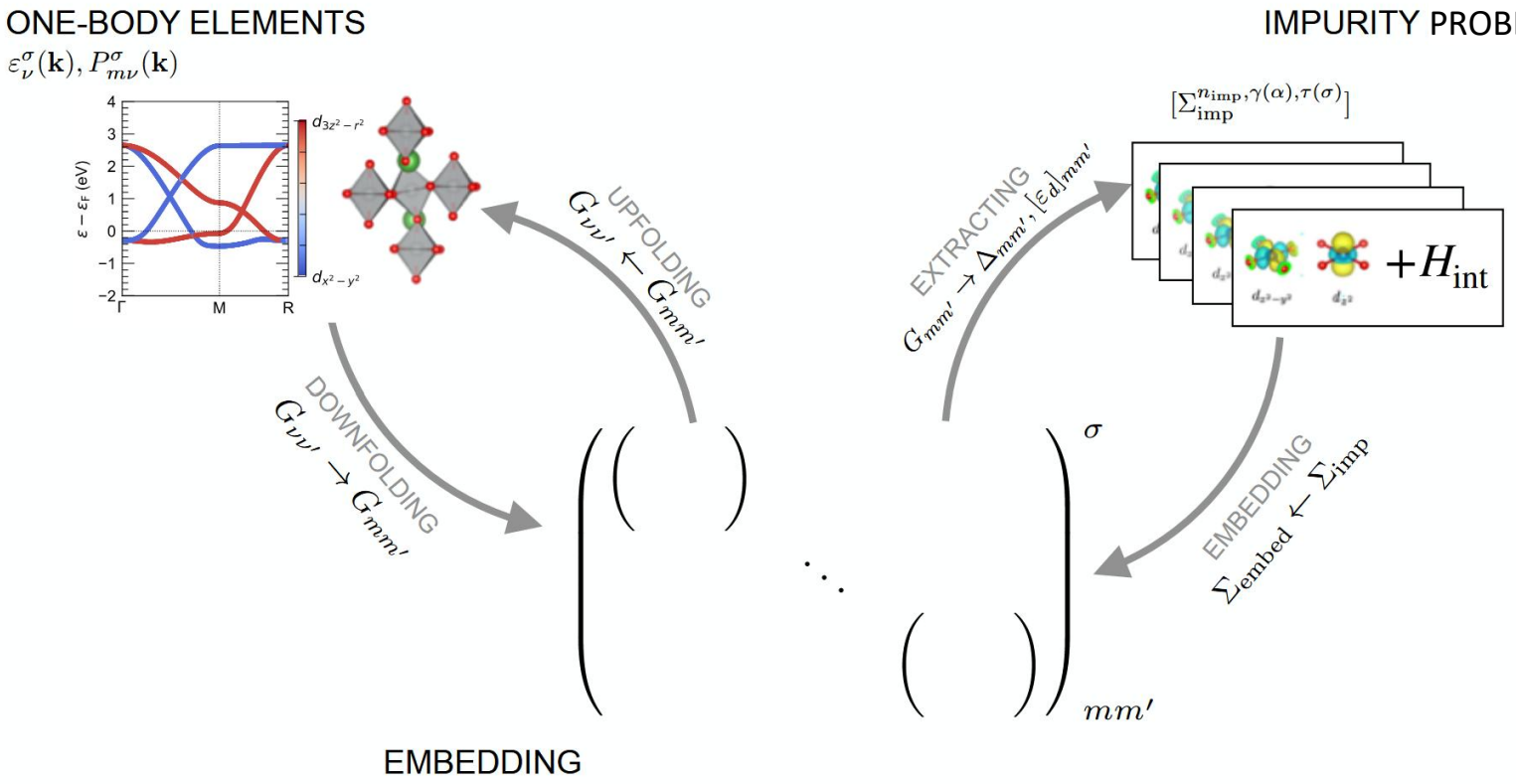
Dropping degrees of freedom



Other options:

- Use the block symmetries
- Finding those block symmetries
- None-trivial mapping in spins

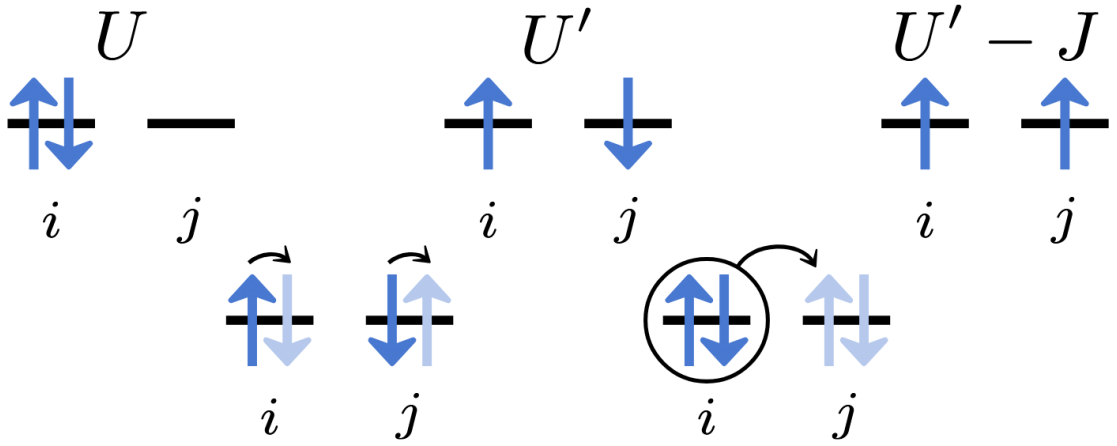
Impurity problems



- **Embedding maps** the right orbitals to the right impurity problem
- Each **impurity problem is solved individually**
- Embedding brings back all the self-energies, **ready to upfold**

Interactions parameters

Interacting Hamiltonians:



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

Values of U/J:

- Correspond to screened values
- Often treated as parameters
- Can be approximated using
  - cRPA
  - cDFT
  - Linear response
- Hear more in GW+EDMFT

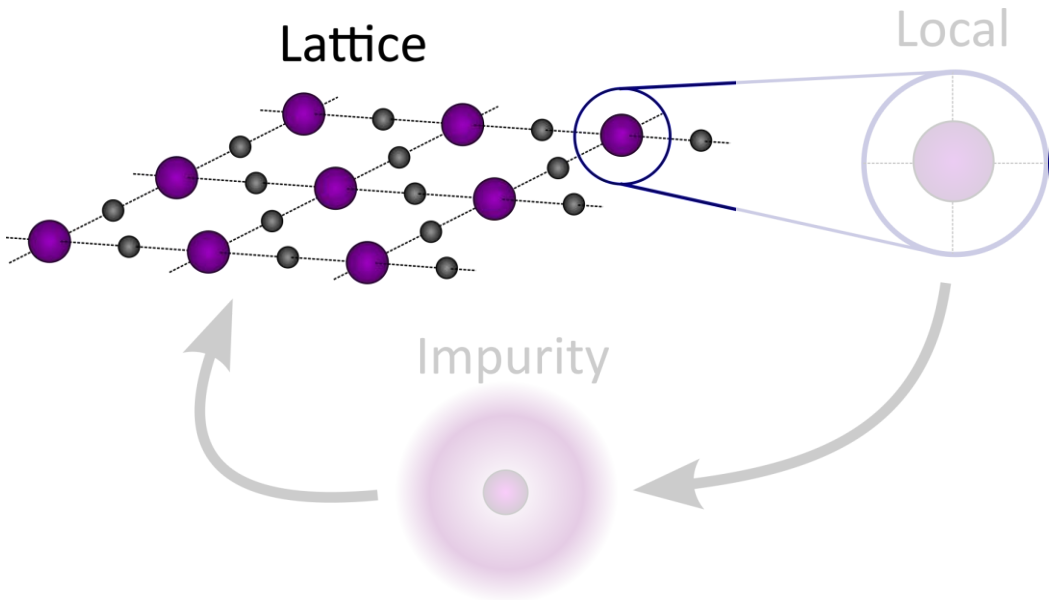
Mapping to impurity problems: Summary

- There are **many possibilities of embedding** depending on the numerical resources available and type of physics that is wanted
  - Multi-site DMFT in equivalent/inequivalent atoms
  - Clustering of atoms
  - Block diagonalization and drop of orbitals
  - Non-trivial spin mappings

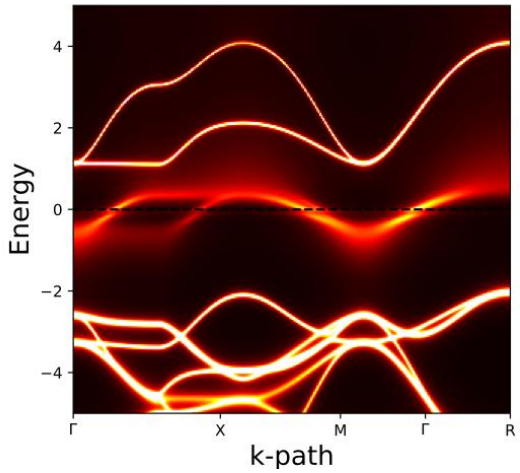
- **Impurities** are **treated separately** and **reassembled** at the embedding level

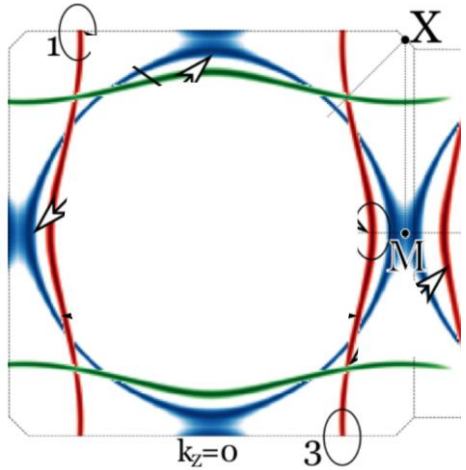
Post-processing

Spectral function



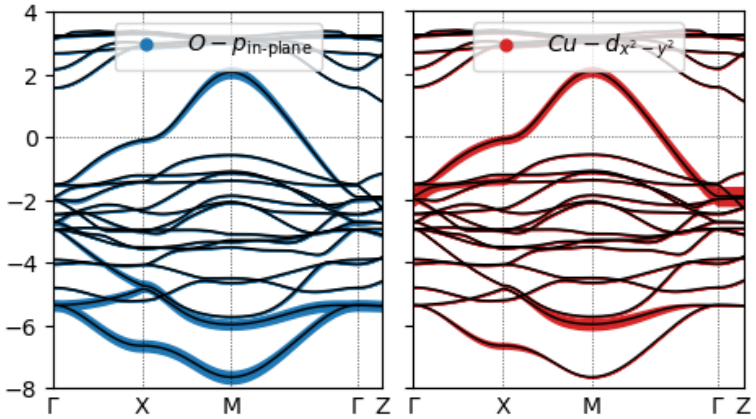
$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Tr}\mathrm{Im}G^{\mathrm{latt}}(\mathbf{k},\omega)$$

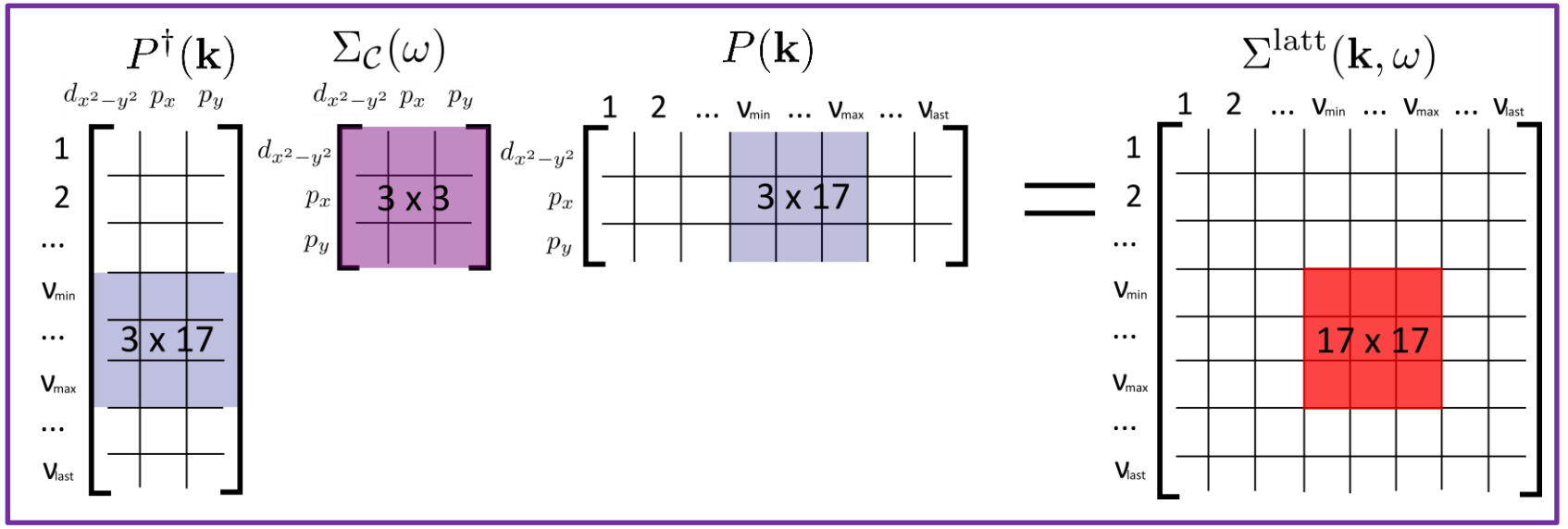


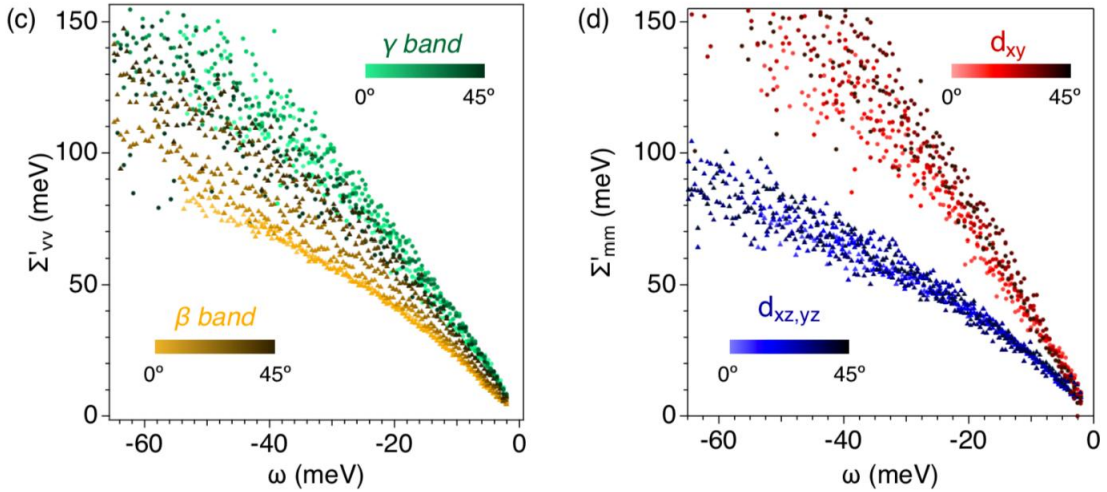


- Analytical continuation of the self-energy
- Embedding to the lattice gives **k**-dependence

Momentum dependence of Σ







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

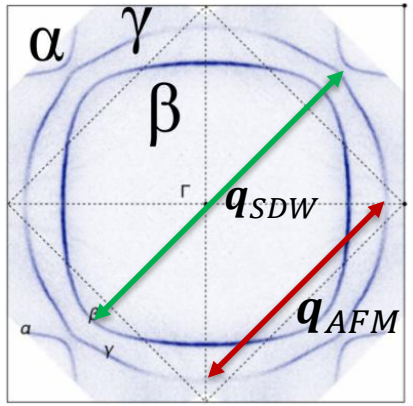
- Self-energy extracted from ARPS for Sr_2RuO_4
  - Non-local in band basis
  - Local in orbital basis

Accessible observables

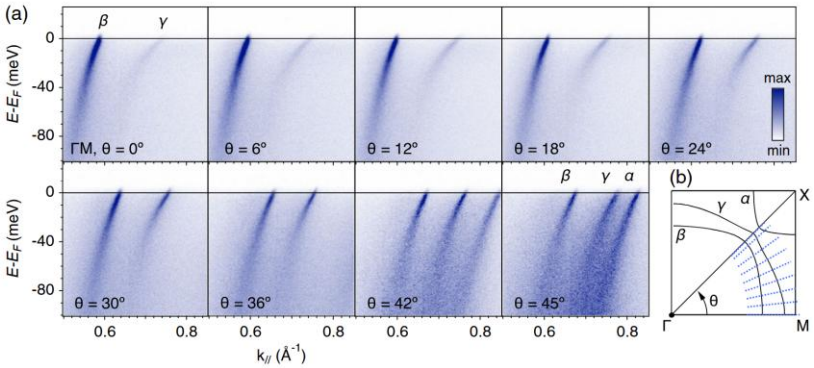
Spectral function

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega)$$

- Fermi surface & Electronic dispersion



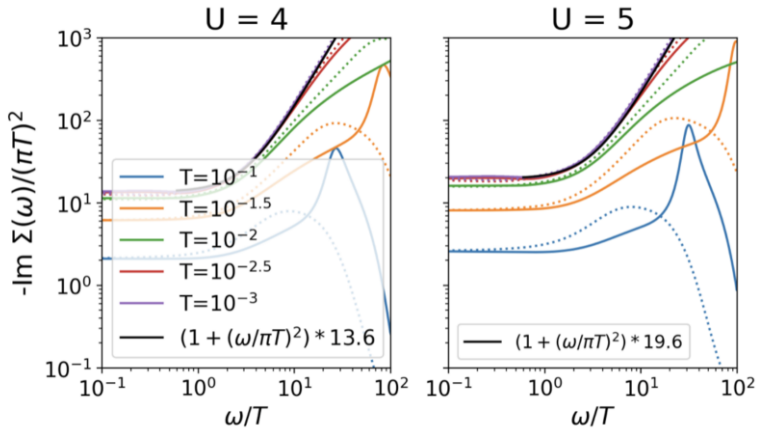
Tamai *et al.*, *Phys. Rev. X* **9**, 021048 (2019)



Transport

- Resistivity

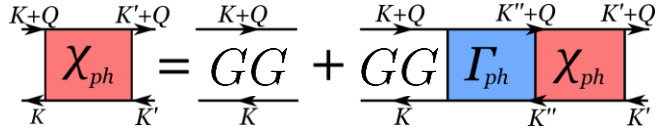
$$\rho(T) = \left[\Phi(\epsilon_F)\int_{-\infty}^{+\infty} d\omega \left(-\frac{df}{d\omega}\right)\frac{1}{2|\mathrm{Im}\Sigma(\omega,T)|}\right]^{-1}$$



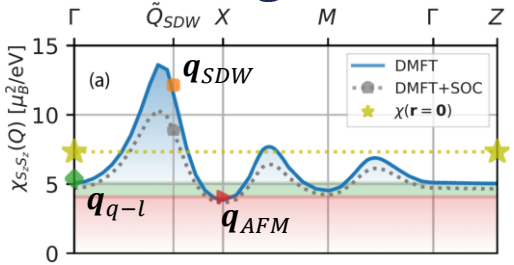
Kazemi *et al.*, *in preparation*

- Seebeck
- Thermal conductivity
- Optical conductivity

Other susceptibilities

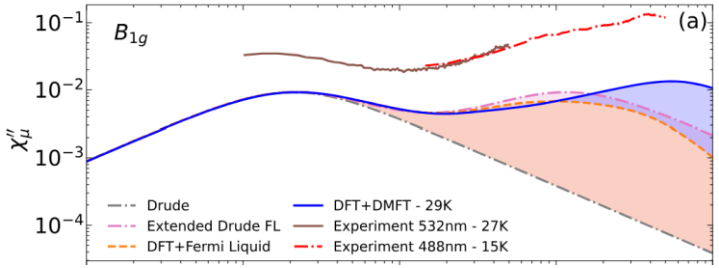


- Magnetic



Steffens *et al.*, *Phys. Rev. Lett.* **122**, 047004 (2019)
Strand *et al.*, *Phys. Rev. B* **100**, 125120 (2019)

- Raman scattering



Blesio *et al.*, *Phys. Rev. Res.* **6**, 023124 (2024)

Conclusion

Conclusion

- **Density functional theory** serves a great starting point for the simulations of materials but needs to be corrected to account for strong correlations
- While it is naturally expressed in the Bloch basis, the treatment of interactions in naturally performed for a set of **localized orbitals**, which defines **projectors**
- There are many possible mappings from the localized orbitals to a set of distinct impurity problems taken care of by the concept of **Embeddings**, which also allow reembedding the resulting self-energies onto the original lattice
- Performing these steps is supported by the **TRIQS @ ModEST** software which you will now try!

Thank you.

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