# Intro to Wannierization

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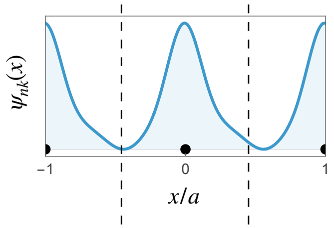
## Crystal lattice imposes translation symmetry

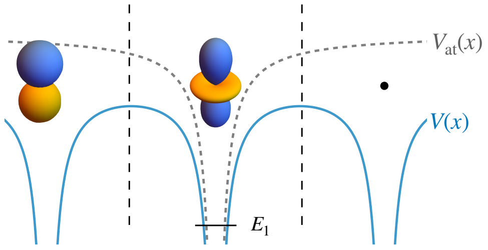
Bloch's theorem $\psi_{nk}(x+a) = c \cdot \psi_{nk}(x)$



$H = H_{\text{at}} + \Delta U$

Atomic-like description survives?

Localized, decay as $|r - r_0| \to \infty$



*Tight-binding* $V(x)$

e.g. Muffin-tin orbitals, APW, …

**Wannier functions**

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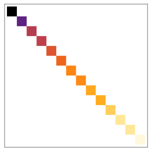
## Best basis to represent a Kohn-Sham Hamiltonian?

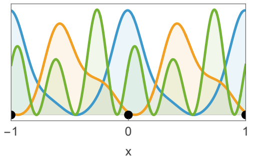
**Bloch** $|\psi_{n\mathbf{k}}\rangle$

DFT

$H_k$



**Periodic orbitals** $|\psi_{n\mathbf{k}}(\mathbf{r})\rangle$

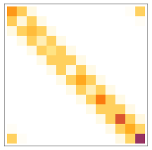


Natural eigenbasis for $H_\mathbf{k}$ — $\mathbf{k}$ space

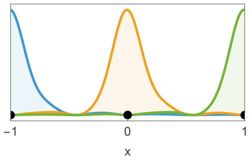
Overlaps for all $|\psi_{n\mathbf{k}}(\mathbf{r})\rangle$ — $\mathbf{r}$ space

**Wannier** $|W_{nR}\rangle$

$H_k^W$



**Localized orbitals** $|W_{n\mathbf{R}}(\mathbf{r})\rangle$



Not an Eigenbasis for $H_\mathbf{k}$ — $\mathbf{k}$ space

**Nearest neighbors** overlap — $\mathbf{r}$ space

Still a description
of electronic states

Small overlaps → tight binding

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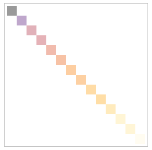
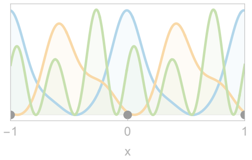
## Best basis to represent a Kohn-Sham Hamiltonian?

**Bloch** $|\psi_{n\mathbf{k}}\rangle$

$H_k$

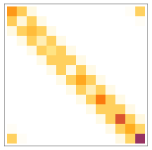


**Periodic orbitals** $|\psi_{n\mathbf{k}}(\mathbf{r})\rangle$

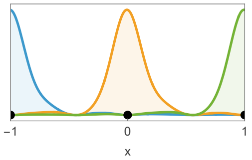


**Wannier** $|W_{nR}\rangle$

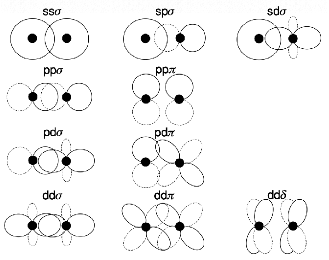
$H_k^W$



**Localized orbitals** $|W_{n\mathbf{R}}(\mathbf{r})\rangle$

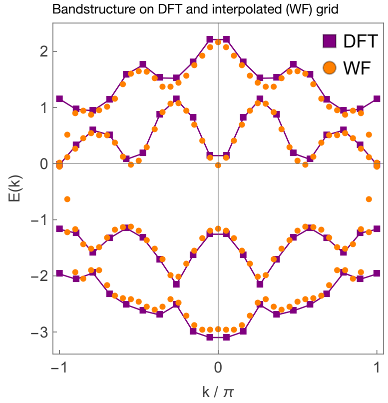


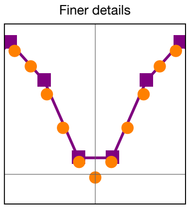
14.2 Matrix elements with atomic orbitals



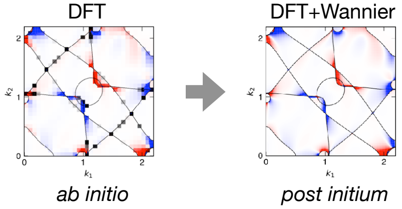
Localized orbitals are intuitive

## You can *interpolate* the DFT band-structure with Wannier





Running DFT on a fine grid
is more expensive than
DFT on coarse grid + Wannier



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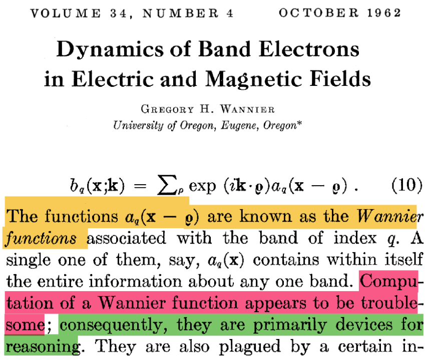

VOLUME 34, NUMBER 4 OCTOBER 1962

### Dynamics of Band Electrons in Electric and Magnetic Fields

Gregory H. Wannier
*University of Oregon, Eugene, Oregon**

$$b_q(\mathbf{x};\mathbf{k}) = \sum\nolimits_\rho \exp\,(i\mathbf{k}\cdot\boldsymbol{\varrho})a_q(\mathbf{x}-\boldsymbol{\varrho})\,. \qquad (10)$$

The functions $a_q(\mathbf{x}-\boldsymbol{\varrho})$ are known as the *Wannier functions* associated with the band of index $q$. A single one of them, say, $a_q(\mathbf{x})$ contains within itself the entire information about any one band. Computation of a Wannier function appears to be troublesome; consequently, they are primarily devices for reasoning. They are also plagued by a certain in-

Definition

Problem

Importance?

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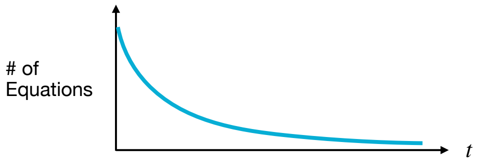
## In this talk…

1. What is a Wannier Function (WF)?
2. How to build WFs?
3. Applications of WFs
4. VASP tutorial (& state of the art if we have time)



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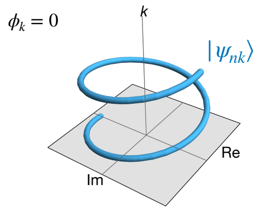
## **Phases** in Bloch functions $|\psi_{nk}\rangle$

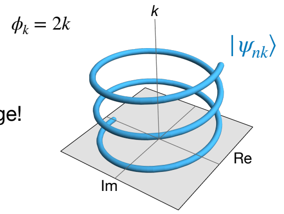
$U(1)$ **gauge** invariance

$$H_k|\psi_{nk}\rangle = \varepsilon_{nk}|\psi_{nk}\rangle$$
$$\langle\psi_{nk}|H_k|\psi_{nk}\rangle = \varepsilon_{nk}$$

$$H_k\, e^{-i\phi_k}|\psi_{nk}\rangle = \varepsilon_{nk}\, e^{-i\phi_k}|\psi_{nk}\rangle$$
$$\langle\psi_{nk}|e^{+i\phi_k}\, H_k\, e^{-i\phi_k}|\psi_{nk}\rangle = \varepsilon_{nk}$$
$$\langle\psi_{nk}|H_k|\psi_{nk}\rangle = \varepsilon_{nk}$$



Physical observables don't depend on gauge!



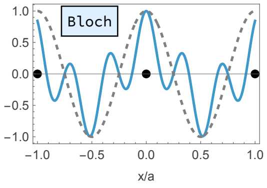
## Wannier Functions as Fourier Transformed $|\psi_{n\mathbf{k}}\rangle$

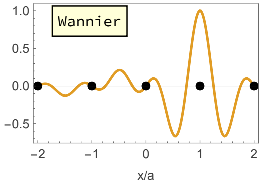
Sampling over $\mathbf{k}$

$$|\psi_{n\mathbf{k}}(\mathbf{r})\rangle$$

from DFT

$$|W_{n\mathbf{R}}(\mathbf{r})\rangle = \frac{1}{N}\sum_{\mathbf{k}\in\mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}}|\psi_{n\mathbf{k}}(\mathbf{r})\rangle$$





$U(1)$ gauge invariance

**Invariant?**

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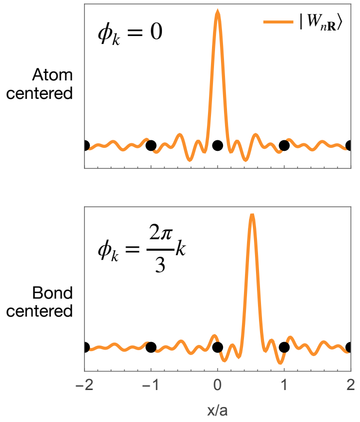
## WFs are **non-unique** localized orbitals



$|W_{n\mathbf{R}}\rangle$ **does** change with the phase $e^{-i\phi_k}$

**Gauge freedom**

$e^{-i\phi_{\mathbf{k}}}$, or $U_{mn\mathbf{k}}$

DFT calculates at individual $\mathbf{k}$-points
(can't get rid of $\phi_k$)

Task: fix and **smooth** the gauge $U_{mn\mathbf{k}}$

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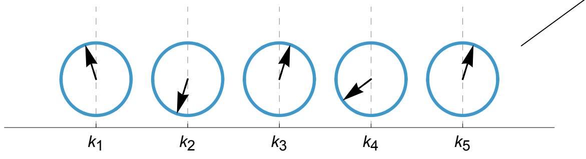
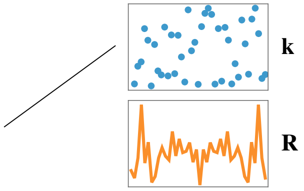
## DFT has non-smooth phases

Phase from DFT

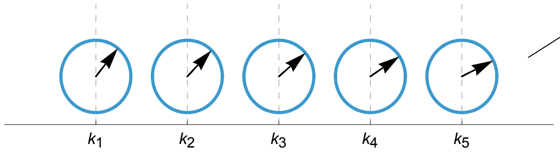
WAVECAR



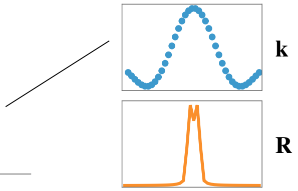
Non-smooth gauge



Fixed phase (smoothened $U_{mn\mathbf{k}}$, our task )



Smooth gauge



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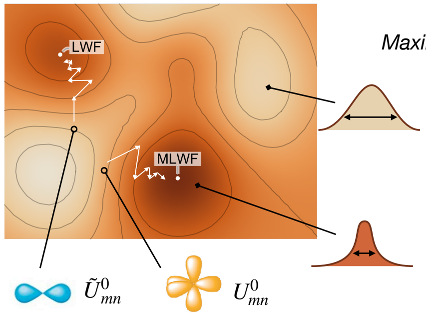
## **Smoothening** $U_{mn\mathbf{k}}$ via projections (LOCPROJ)

Marzari, N. & Vanderbilt, D. Maximally localized generalized Wannier functions for composite energy bands. PRB 56, 12847 **(1997)**

$$\Omega = \sum_n \left[\langle r^2\rangle_n - \langle \vec{r}_n\rangle^2\right]$$

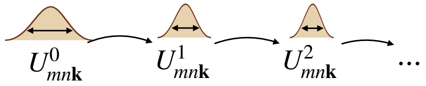


Extremely non-convex space

Initial gauge: $U^0_{mn\mathbf{k}} = A_{mn\mathbf{k}} \equiv \langle\psi_{m\mathbf{k}}|g_n\rangle$ guess

*Maximally Localized WF* (MLWF) minimizes $\Omega$

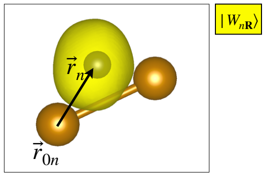
WANNIER90



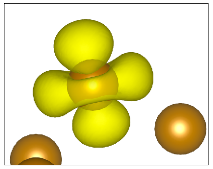
Iterate through steepest descent

**1)** how to choose $g_n$?

## Smoothening $U_{mn\mathbf{k}}$ via projections (LOCPROJ)



Not atom-centered



Atom centered

*Maximally Localized WF* (MLWF) minimizes

$$\Omega = \sum_n \left[ \langle r^2 \rangle_n - \langle \vec{r}_n \rangle^2 \right] = \textbf{Variance}$$

Marzari, N. & Vanderbilt, D. Maximally localized generalized Wannier functions for composite energy bands. PRB 56, 12847 **(1997)**

Only needs $|u_{n,\mathbf{k}}\rangle$ from DFT !

WANNIER90

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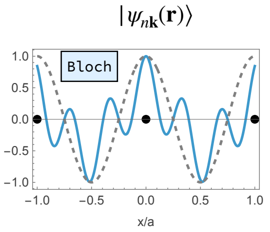

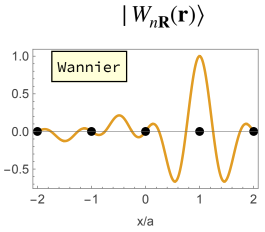

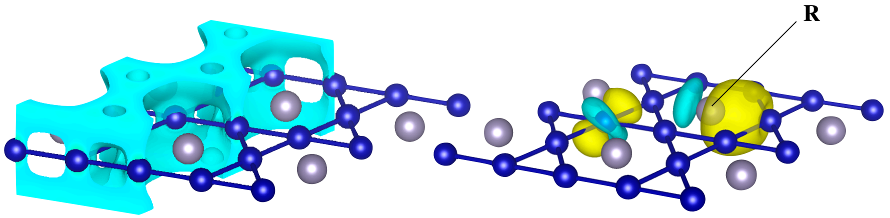

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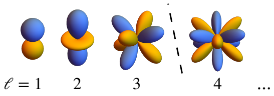
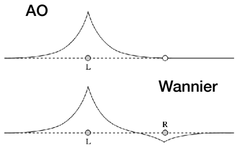
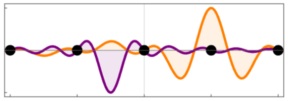
| LCAO | Wannier |
|---|---|
| Fixed basis set | A "representation" |
| Not orthogonal in periodic potential | Fourier transform of $|\psi_{n\mathbf{k}}\rangle$,<br>keeps orthogonality |
| $|\psi_{m\mathbf{k}}\rangle = \sum_{n\ell m} c_{m,\,n\ell m} \underbrace{|R_{n\ell} Y_\ell^m\rangle}_{\text{AO}}$ | $|\psi_{m\mathbf{k}}\rangle = \sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j} |W_{m\mathbf{R}_j}\rangle$ |
| Computational tool,<br>Need to truncate -> errors | True electronic wavefunction,<br>Tails overlap with neighboring atoms |



Same shape in any system





Not transferable, system-dependent

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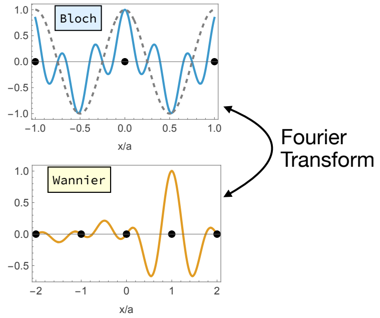
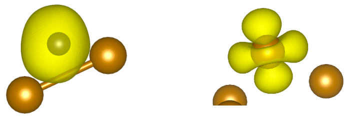
## Summary pt.1

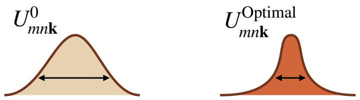
Wannier functions are like localized orbitals built from Bloch functions

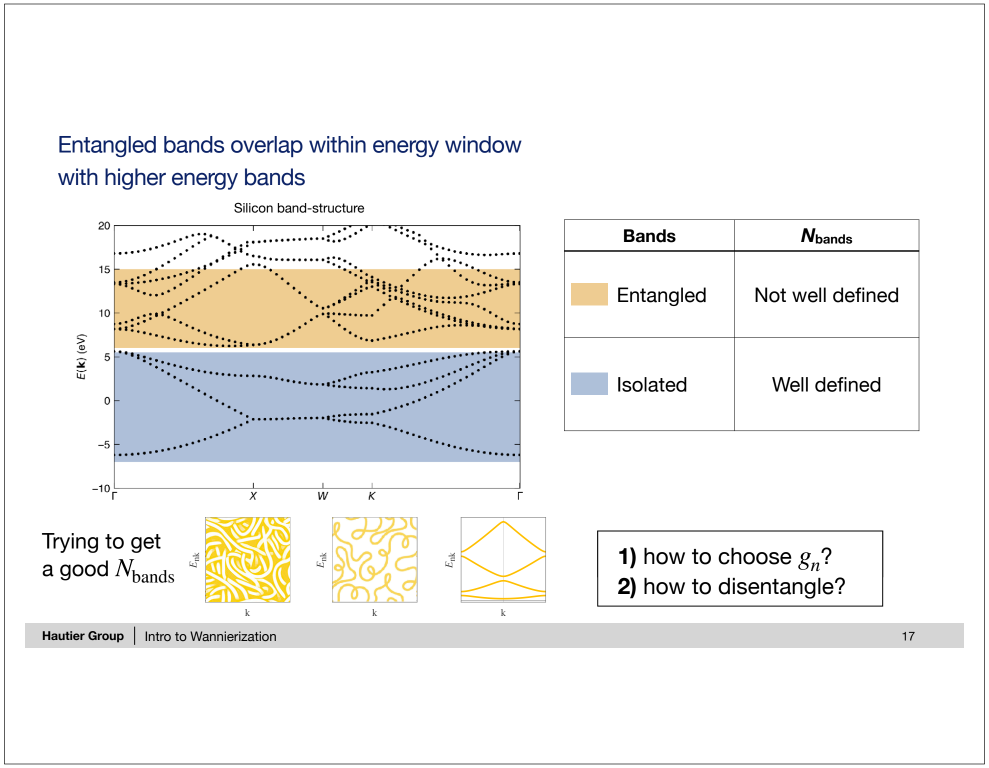


Wannier functions have different shapes depending on which matrix $U_{mn\mathbf{k}}$ we use



We can guess a matrix $U_{mn\mathbf{k}}$ via atomic orbitals and refine our guess in $\mathbf{k}$ space





## Entangled bands overlap within energy window with higher energy bands

| Bands | $N_{\text{bands}}$ |
|---|---|
| 🟧 Entangled | Not well defined |
| 🟦 Isolated | Well defined |

Trying to get a good $N_{\text{bands}}$

**1)** how to choose $g_n$?
**2)** how to disentangle?

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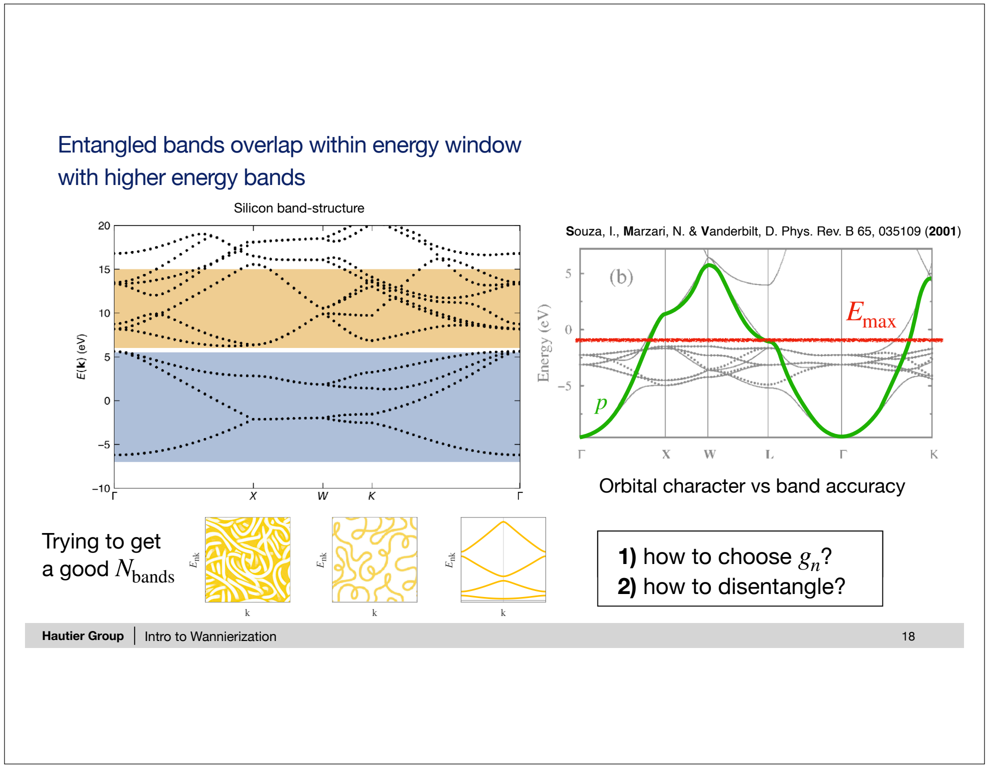

## Entangled bands overlap within energy window with higher energy bands

**S**ouza, I., **M**arzari, N. & **V**anderbilt, D. Phys. Rev. B 65, 035109 (**2001**)

Orbital character vs band accuracy

Trying to get a good $N_{\text{bands}}$

**1)** how to choose $g_n$?
**2)** how to disentangle?

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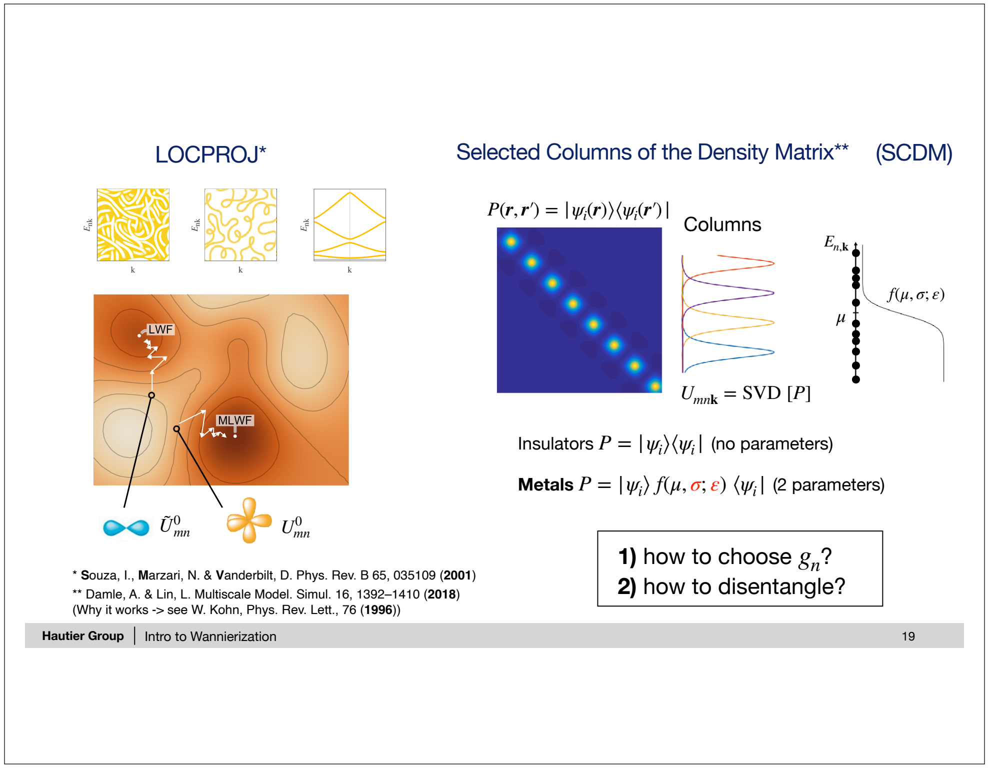

## LOCPROJ*

## Selected Columns of the Density Matrix** (SCDM)

$P(\mathbf{r}, \mathbf{r}') = |\psi_i(\mathbf{r})\rangle\langle\psi_i(\mathbf{r}')|$

Columns

$U_{mn\mathbf{k}} = \text{SVD}\ [P]$

Insulators $P = |\psi_i\rangle\langle\psi_i|$ (no parameters)

**Metals** $P = |\psi_i\rangle\ f(\mu, \sigma; \varepsilon)\ \langle\psi_i|$ (2 parameters)

**1)** how to choose $g_n$?
**2)** how to disentangle?

* **S**ouza, I., **M**arzari, N. & **V**anderbilt, D. Phys. Rev. B 65, 035109 (**2001**)
** Damle, A. & Lin, L. Multiscale Model. Simul. 16, 1392–1410 (**2018**)
(Why it works -> see W. Kohn, Phys. Rev. Lett., 76 (**1996**))

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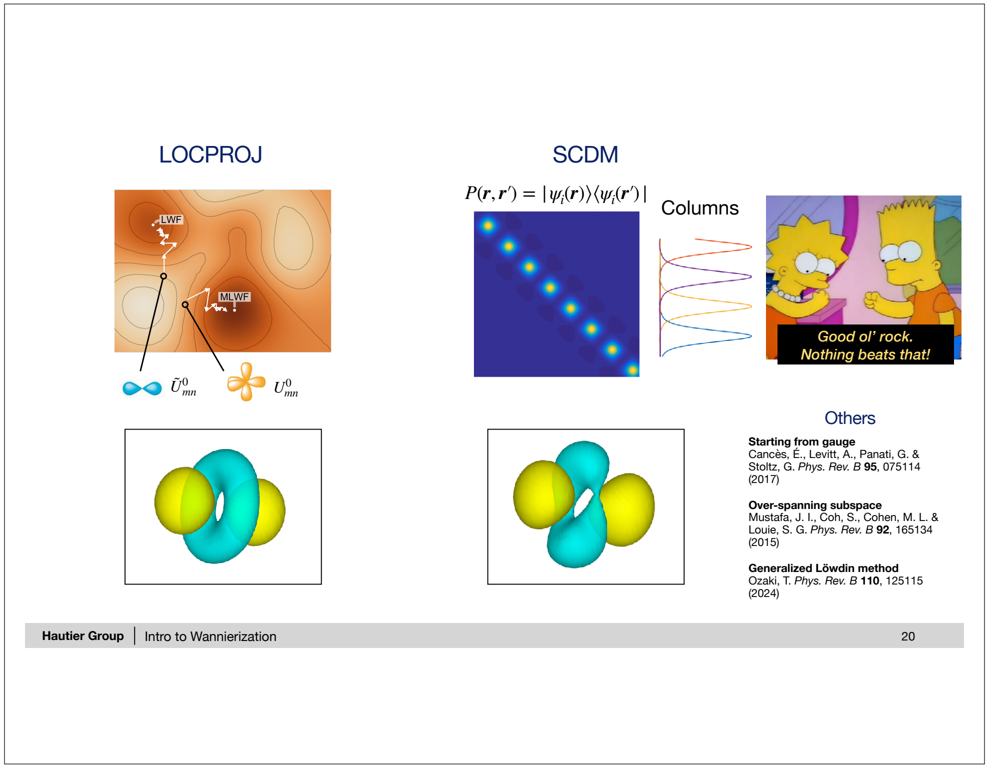


## LOCPROJ

## SCDM

$P(\mathbf{r}, \mathbf{r}') = |\psi_i(\mathbf{r})\rangle\langle\psi_i(\mathbf{r}')|$

Columns

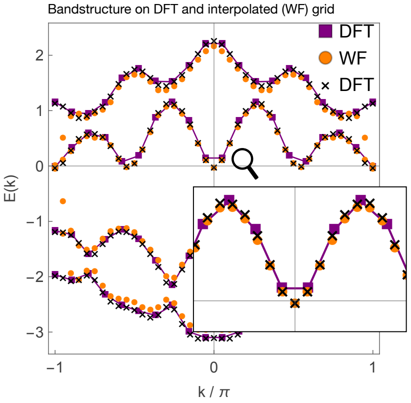
### Others

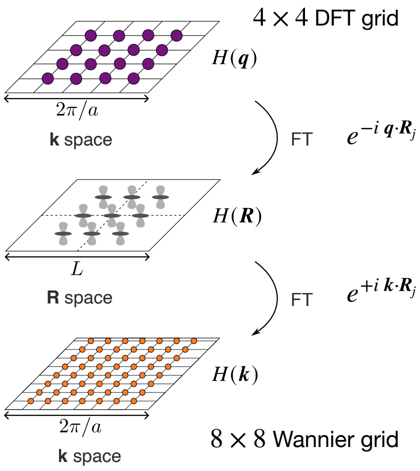
**Starting from gauge**
Cancès, É., Levitt, A., Panati, G. & Stoltz, G. *Phys. Rev. B* **95**, 075114 (2017)

**Over-spanning subspace**
Mustafa, J. I., Coh, S., Cohen, M. L. & Louie, S. G. *Phys. Rev. B* **92**, 165134 (2015)

**Generalized Löwdin method**
Ozaki, T. *Phys. Rev. B* **110**, 125115 (2024)

## Applications: **Band interpolation**


Bandstructure on DFT and interpolated (WF) grid



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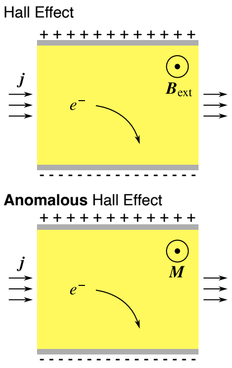
## Applications: **Anomalous Hall Effect**



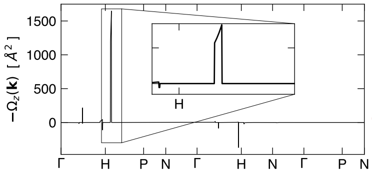
Driven by a magnetization $\boldsymbol{M}$ rather than an external $\boldsymbol{B}$ field

Full expression is tedious (Kubo formula)

$$\Omega^{\alpha}_{xy}(\boldsymbol{k}) \propto \text{Im} \sum_{m\neq n} \langle n | \partial_{k_x} | m\rangle\langle m | \partial_{k_y} | n\rangle \qquad |n\rangle \equiv |\psi_{nk}\rangle$$

Berry curvature

Can use $\langle u_{m,\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n,\mathbf{k+b}}\rangle \equiv \langle \mathbf{r}_{mn}\rangle / i$



Needs dense **k**-points

Berry Curvature calculation for Fe BCC (using Wannier interpolation)

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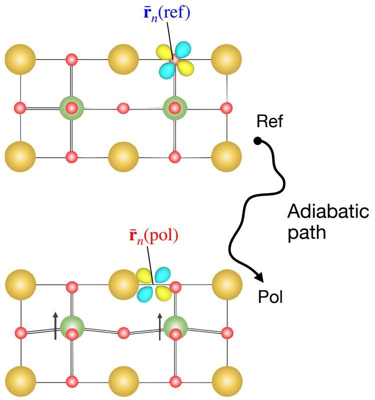
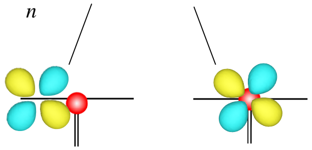
## Applications: **Electric polarization**



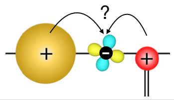
Only needs endpoints*

$$\boxed{\Delta\mathbf{P}_{\text{elec}}} = \mathbf{P}(\text{pol}) - \mathbf{P}(\text{ref})$$

$$= e\sum_{n}^{N_{\text{occ}}} \bar{\mathbf{r}}_n(\text{pol}) - \bar{\mathbf{r}}_n(\text{ref})$$



*Uncertainty regarding center $\cancel{\rightarrow}$ adiabatic path

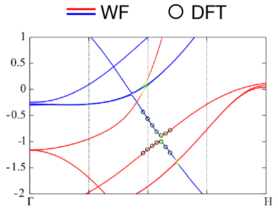


**Resta, Vanderbilt. Theory of Polarization, 2007**

Alaerts, L., Schimpf, J., Li, X., Zheng, J., Banyas, E., Neaton, J. B., ... & Hautier, G. (2026). Discovery of a new weberite-type antiferroelectric: La3NbO7. arXiv preprint arXiv:2601.04916.

---

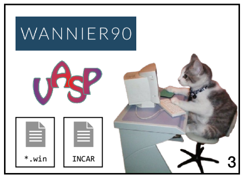
Can interpolate any operator from DFT



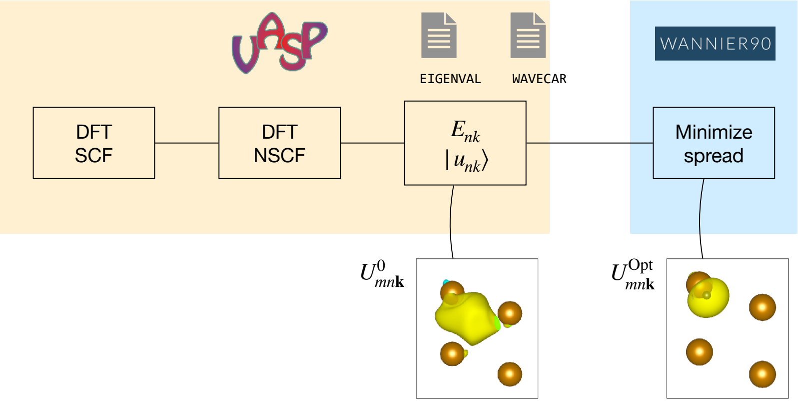
Yates, J. R., X. Wang, D. Vanderbilt, and I. Souza, 2007, Phys. Rev. B 75, 195121.

Not trivial to optimize the spread **and** subspace (mainly in metals and entangled regions)

Up next…



## Standard workflow



DFT SCF

DFT NSCF

$E_{nk}$ $|u_{nk}\rangle$

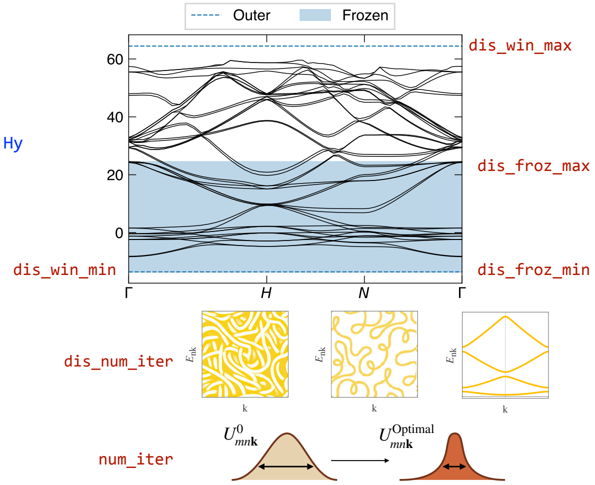
Minimize spread

---

```
INCAR

ALGO = Normal
LORBIT = 11
...

LWANNIER90 = TRUE
LOCPROJ    = 1 : p : Hy
NBANDS     = 20
```

WANNIER90

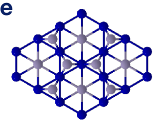
```
*.win

num_wann: 20
dis_froz_max: 30.0d0
dis_froz_min: 5.0d0
dis_num_iter: 500
num_iter: 400
```

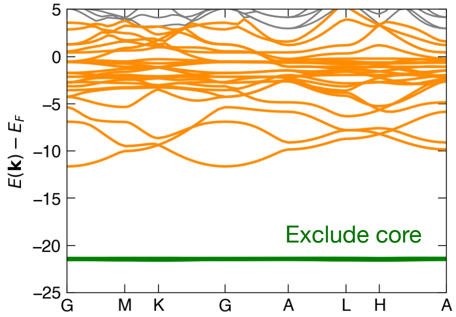


---

## Wannierizing in practice

**CoSn**
mp-20536





num_bands = $N_{\mathrm{KS}}$ − exclude_bands

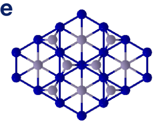
num_wann = 20

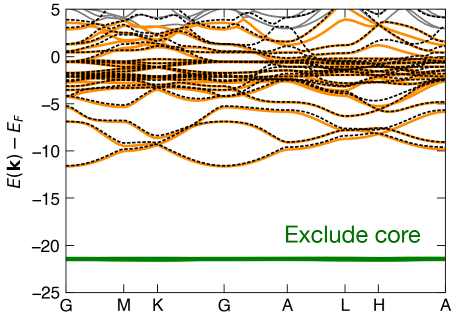
num_wann $< N_{\mathrm{KS}}$ disentanglement!

---

## Wannierizing in practice

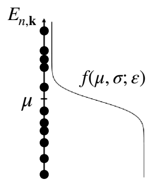
**CoSn**
mp-20536





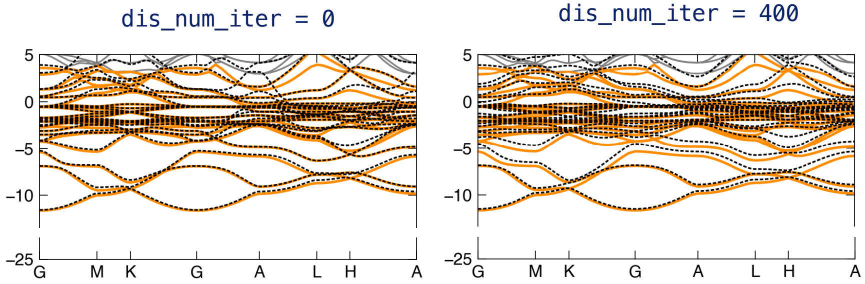
num_bands = $N_{\mathrm{KS}}$ − exclude_bands

num_wann = 20



num_wann $< N_{\mathrm{KS}}$ disentanglement!

## Don't run SCDM with `dis_num_iter > 0` !

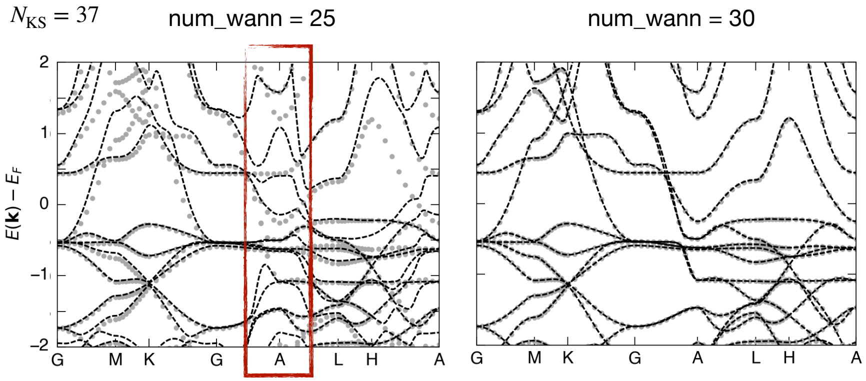

`dis_num_iter = 0`

`dis_num_iter = 400`

SCDM Subspace is already disentangled!

---

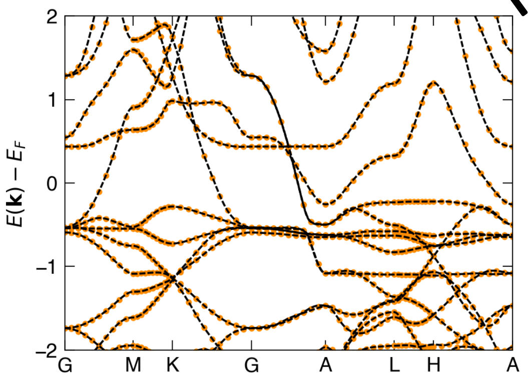
## Having more basis elements will match the bands easier

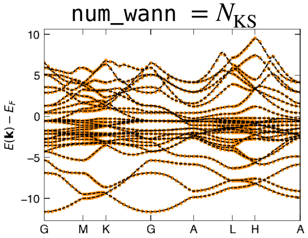

$N_{\mathrm{KS}} = 37$ num_wann = 25

num_wann = 30

---

## Solution to disentanglement: **don't disentangle**



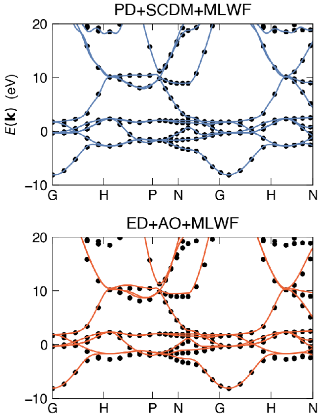

`num_wann` $= N_{\mathrm{KS}}$

**Pro:**
No subspace smoothening needed, less automation

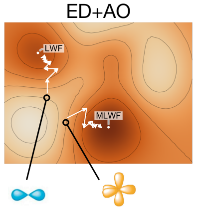
**Con:**
bigger matrices or subspace, might need a lot of projections

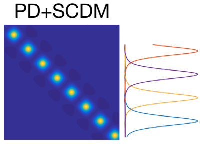
---

## Best bands does not mean best WFs

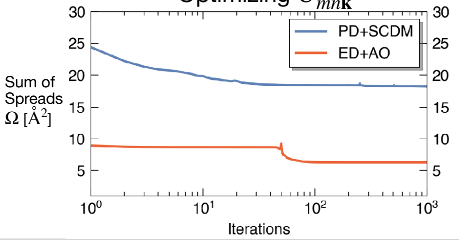

PD+SCDM+MLWF

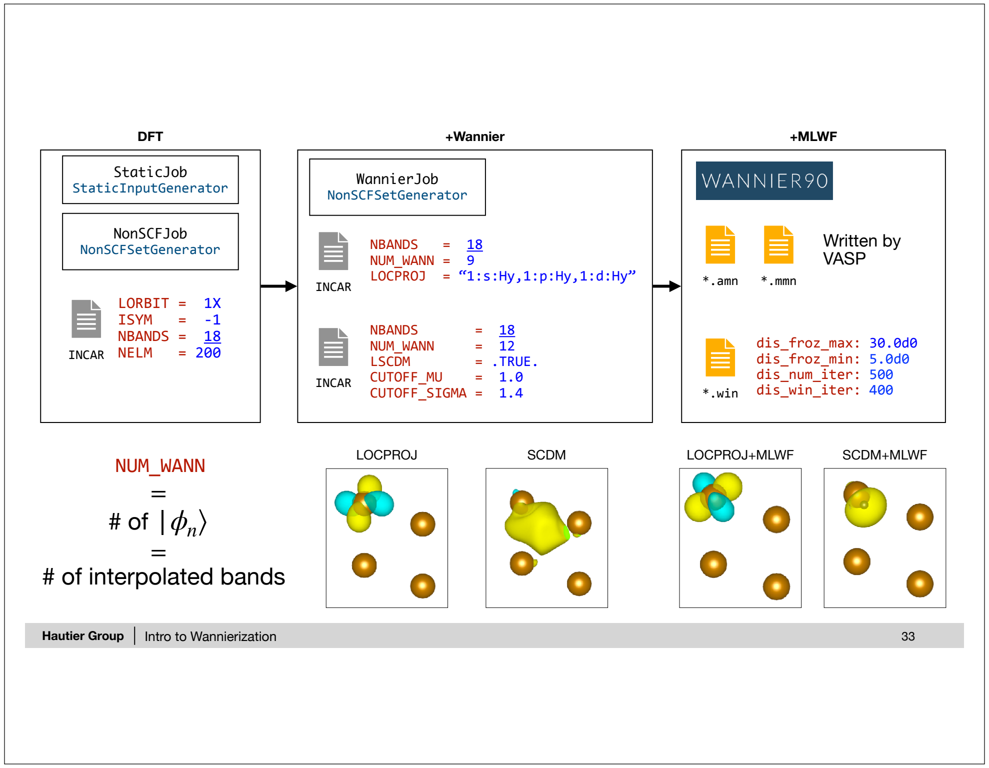
ED+AO+MLWF


ED+AO


PD+SCDM

Optimizing $U_{mn\mathbf{k}}$





**DFT**

StaticJob
StaticInputGenerator

NonSCFJob
NonSCFSetGenerator

INCAR

```
LORBIT =  1X
ISYM   =  -1
NBANDS =  18
NELM   = 200
```

**+Wannier**

WannierJob
NonSCFSetGenerator

INCAR

```
NBANDS   =  18
NUM_WANN =  9
LOCPROJ  = “1:s:Hy,1:p:Hy,1:d:Hy”
```

INCAR

```
NBANDS       =  18
NUM_WANN     =  12
LSCDM        = .TRUE.
CUTOFF_MU    =  1.0
CUTOFF_SIGMA =  1.4
```

**+MLWF**

WANNIER90

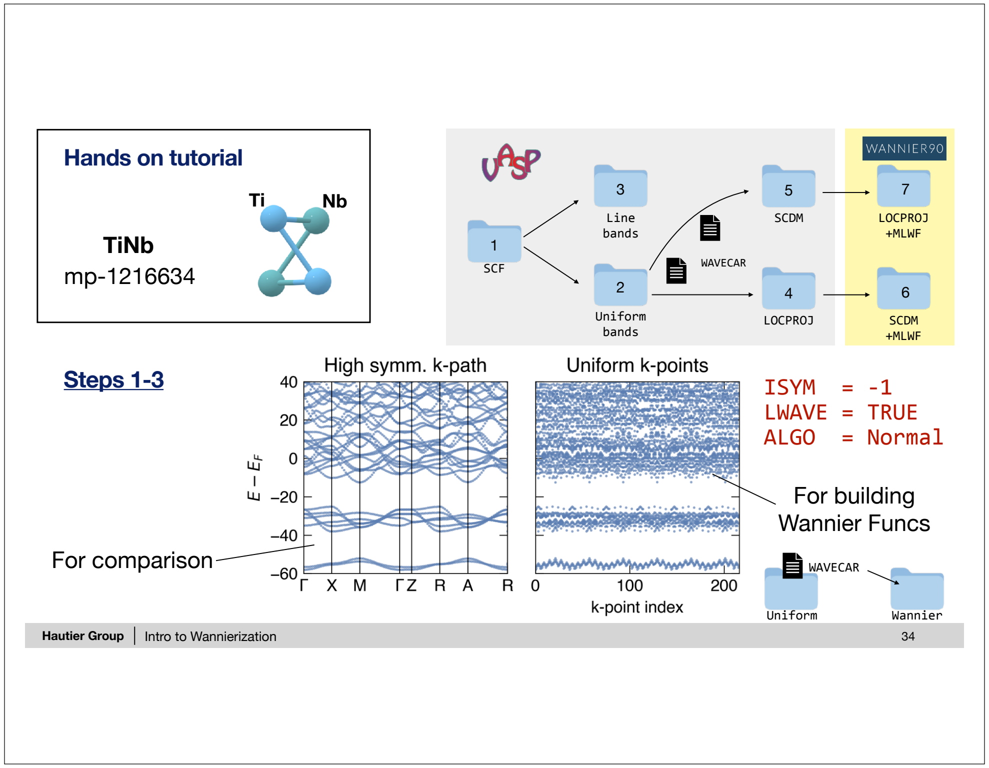
*.amn *.mmn Written by VASP

*.win

```
dis_froz_max: 30.0d0
dis_froz_min: 5.0d0
dis_num_iter: 500
dis_win_iter: 400
```

NUM_WANN
=
# of $|\phi_n\rangle$
=
# of interpolated bands

---



**Hands on tutorial**

**TiNb**
mp-1216634

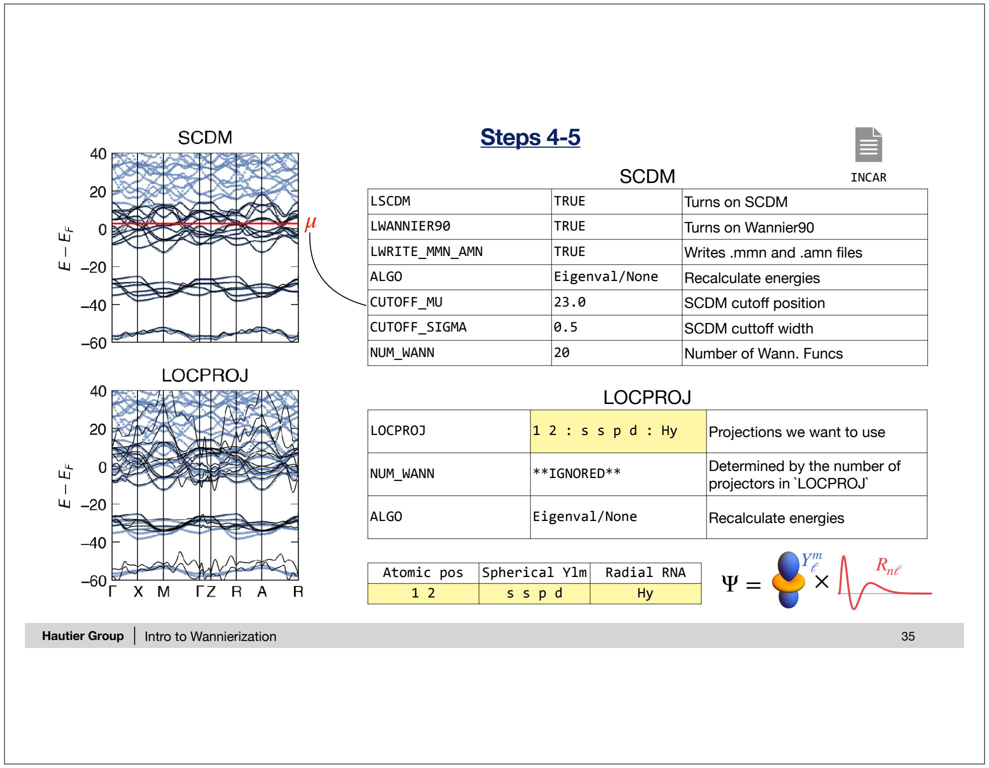
**Steps 1-3**

For comparison

For building Wannier Funcs

```
ISYM  = -1
LWAVE = TRUE
ALGO  = Normal
```

---



**Steps 4-5**

INCAR

SCDM

| | | |
|---|---|---|
| LSCDM | TRUE | Turns on SCDM |
| LWANNIER90 | TRUE | Turns on Wannier90 |
| LWRITE_MMN_AMN | TRUE | Writes .mmn and .amn files |
| ALGO | Eigenval/None | Recalculate energies |
| CUTOFF_MU | 23.0 | SCDM cutoff position |
| CUTOFF_SIGMA | 0.5 | SCDM cuttoff width |
| NUM_WANN | 20 | Number of Wann. Funcs |

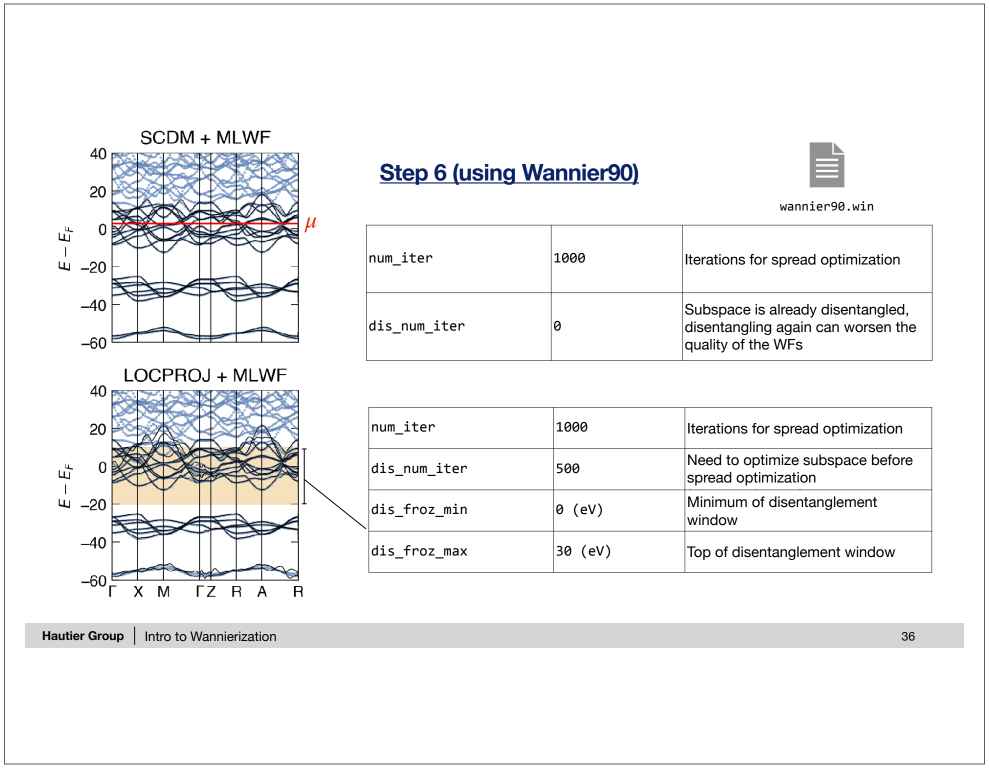
LOCPROJ

| | | |
|---|---|---|
| LOCPROJ | 1 2 : s s p d : Hy | Projections we want to use |
| NUM_WANN | **IGNORED** | Determined by the number of projectors in \`LOCPROJ\` |
| ALGO | Eigenval/None | Recalculate energies |

| Atomic pos | Spherical Ylm | Radial RNA |
|---|---|---|
| 1 2 | s s p d | Hy |

$$\Psi = Y_\ell^m \times R_{n\ell}$$

---



**Step 6 (using Wannier90)**

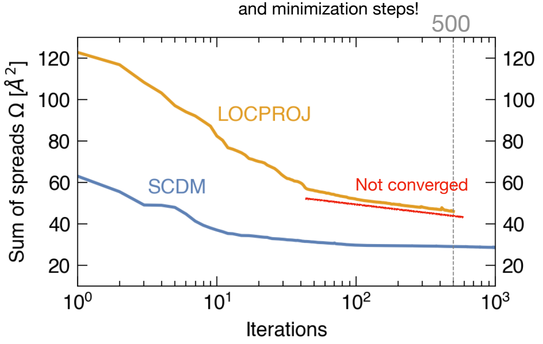
wannier90.win

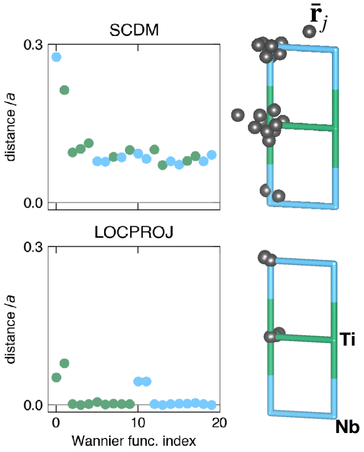
| | | |
|---|---|---|
| num_iter | 1000 | Iterations for spread optimization |
| dis_num_iter | 0 | Subspace is already disentangled, disentangling again can worsen the quality of the WFs |

| | | |
|---|---|---|
| num_iter | 1000 | Iterations for spread optimization |
| dis_num_iter | 500 | Need to optimize subspace before spread optimization |
| dis_froz_min | 0 (eV) | Minimum of disentanglement window |
| dis_froz_max | 30 (eV) | Top of disentanglement window |

## Analyzing metrics

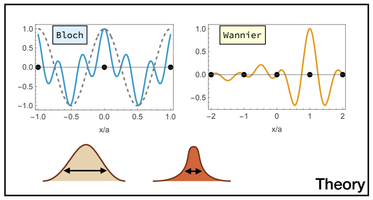
Wannier90 splits disentanglement and minimization steps!

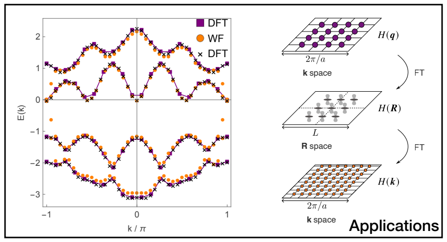


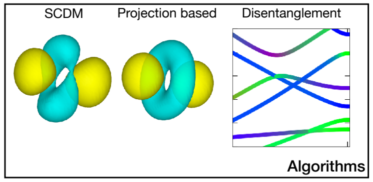


---

## Time for questions







WANNIER90

VASP

*.win

INCAR

Tutorial

---

## Clear problem: **many parameters!**

**Different types of spin currents in the comprehensive materials database of nonmagnetic spin Hall effect**

Yang Zhang, …, **Claudia Felser**, …

npj Computational Materials | (2021)7:167

**High-throughput calculations of spin Hall conductivity in non-magnetic 2D materials**

Jiaqi Zhou, Samuel Poncé, & Jean-Christophe Charlier

npj 2D materials and applications | (2025)9:39

### Observation

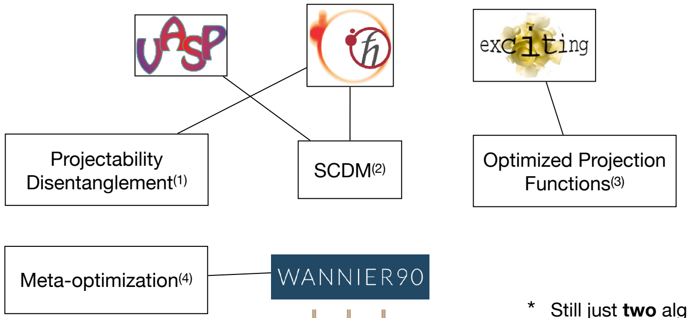
Uses local-orbital basis DFT
No f-electron systems
Brute-force sampling

Fixed disentanglement parameters.
Needs manual tuning of failed cases
(42 of 426)

Some approaches have emerged for automated Wannier…

---

## Automated Wannier: state of the art



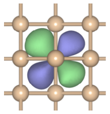
Projectability Disentanglement(1)

SCDM(2)

Optimized Projection Functions(3)

Meta-optimization(4)

WANNIER90

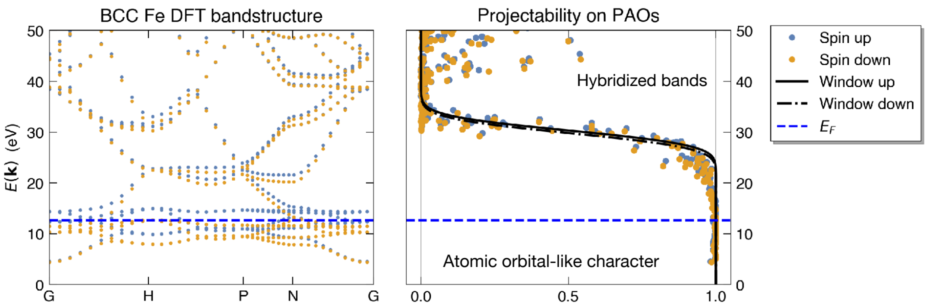


* Still just **two** algorithms for disentanglement (SCDM and SMV)

1. Vitale, V. et al. npj Comput Mater **6**, 66 (2020)
2. Qiao, J., Pizzi, G. & Marzari, N. npj Comput Mater **9**, 206 (2023)
3. Tillack, S. & Draxl, C. arXiv.2502.03213 (2025)
4. Tiwari, S., Cucco, B., Ha, V.-A. & Giustino, F. npj Comput Mater (2026)

## State of the art: **projectability disentanglement**

Qiao, J., Pizzi, G. & Marzari, N. npj Comput Mater **9**, 206 (2023)
Vitale, V. et al. npj Comput Mater **6**, 66 (2020)


BCC Fe DFT bandstructure

Projectability on PAOs

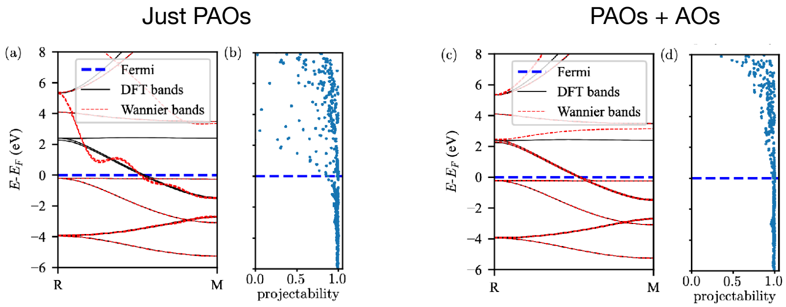
*Automatic disentanglement*

SCDM:
$|\psi_{n\mathbf{k}}\rangle f(\tilde{\mu},\sigma;E)\langle\psi_{n\mathbf{k}}|$

LOCPROJ:
Filters out $|\psi_{n\mathbf{k}}\rangle$

---

## Relying only on PAOs for AlCo can **fail**


Just PAOs

PAOs + AOs

`Co Pseudo` $3s$ $4s$ $3p$ $3d$

`Al Pseudo` $3s$ $3p$

PAOs + $4p$

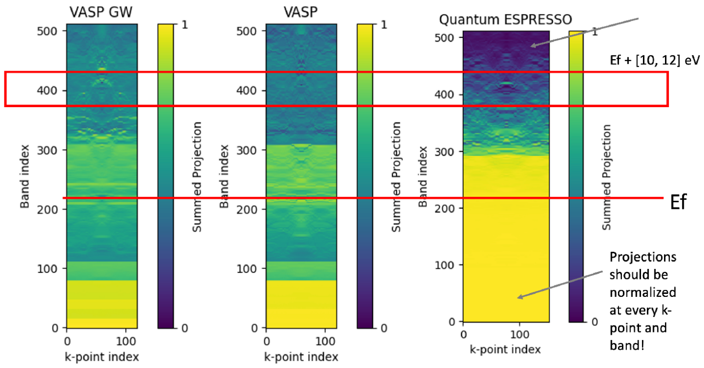
Jiang, Y. et al. npj Comput Mater 11, 353 (2025)

*Not yet released in QE*

---

## PD will probably not work in VASP

- VASP just sucks with projections… (still no clue how QE does it so well)



Ef + [10, 12] eV

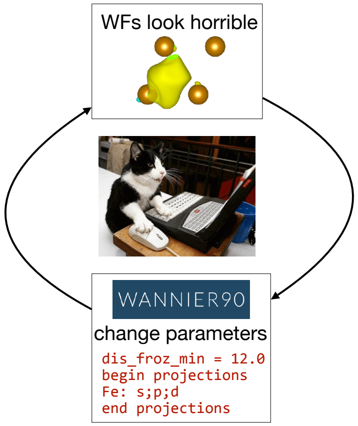
Ef

Projections should be normalized at every k-point and band!

Credit @ Omar Ashour

---

## What if we could *imitate* what a PhD student does?

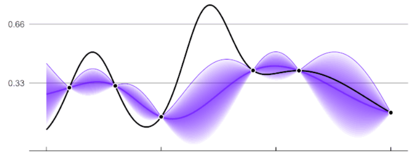

WFs look horrible

WANNIER90

change parameters

```
dis_froz_min = 12.0
begin projections
Fe: s;p;d
end projections
```

Bayesian optimization:
adding points to learn black-box function

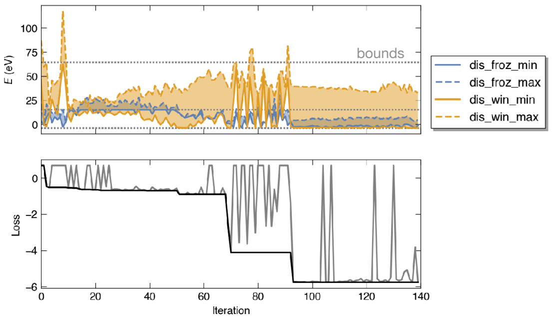


Keeps function evaluations minimal

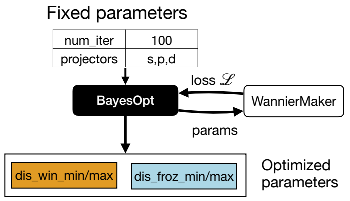
Finds the best places to search for maxima

* Tiwari, S., Cucco, B., Ha, V.-A. & Giustino, F.
*npj Comput Mater* (2026) doi:10.1038/s41524-026-02082-1

## Optimizing disentanglement windows



$$\mathscr{L}[U_{mn}] = \alpha_1 \frac{\Delta E(\mathbf{k})}{E_{\text{Hartree}}} + \alpha_2 \,\mathrm{Var}\left[\frac{\Omega}{5\,\text{Å}^2}\right]$$



Fixed parameters

| | |
|---|---|
| num_iter | 100 |
| projectors | s,p,d |

BayesOpt

loss $\mathscr{L}$

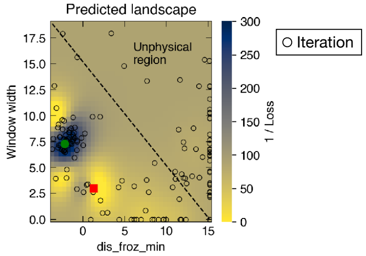
WannierMaker

params

dis_win_min/max

dis_froz_min/max

Optimized parameters



---

## Takeaways

1. Automated Wannierization is in its infancy,
   but needs an elegant and efficient implementation
2. Design philosophies:
   physically motivated vs hyper-parameter optimization
3. New methods ideally need to be compatible
   with **any DFT** code for widespread use