

WANNIER BERRI

Berryology made easy

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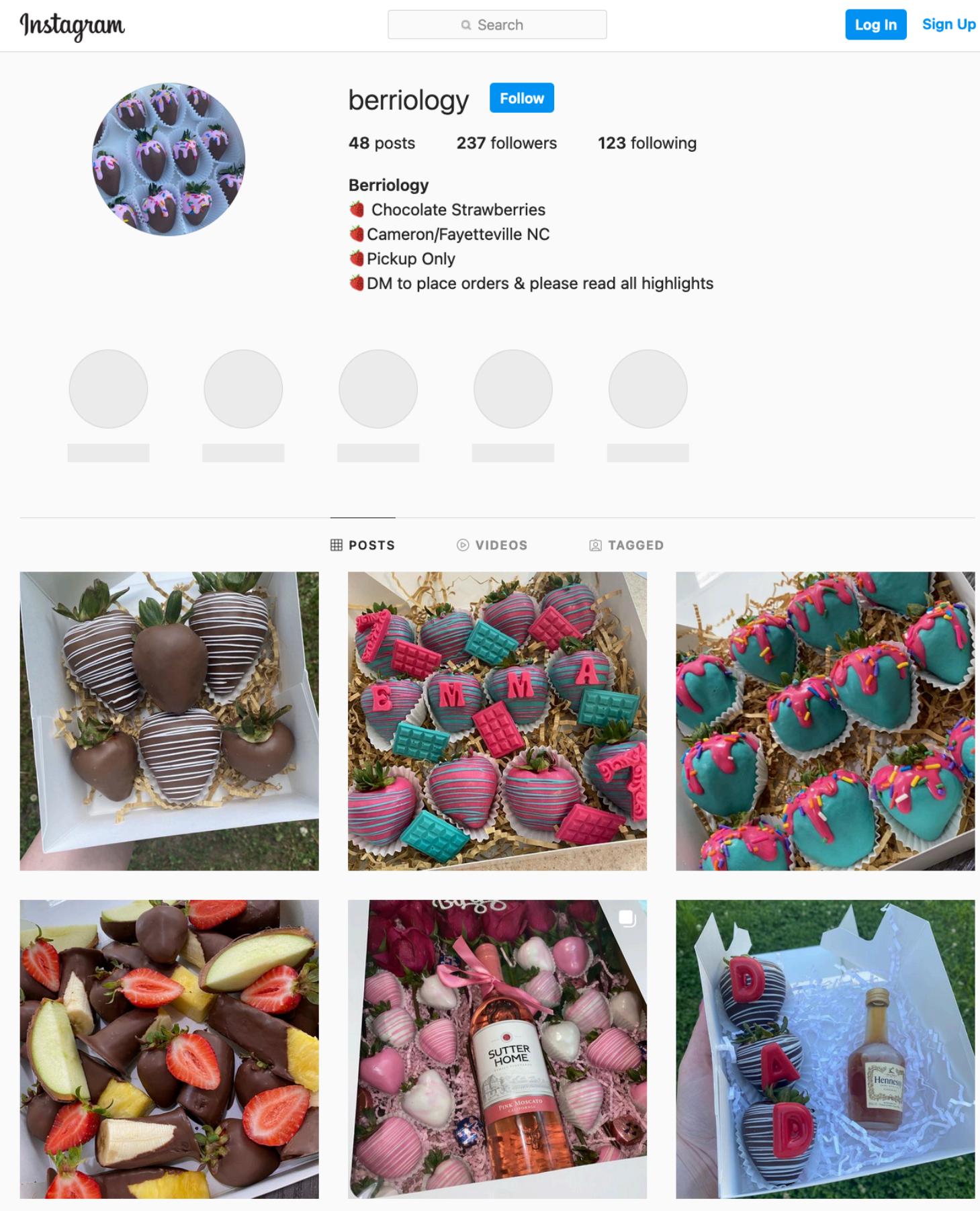
Seoul National University
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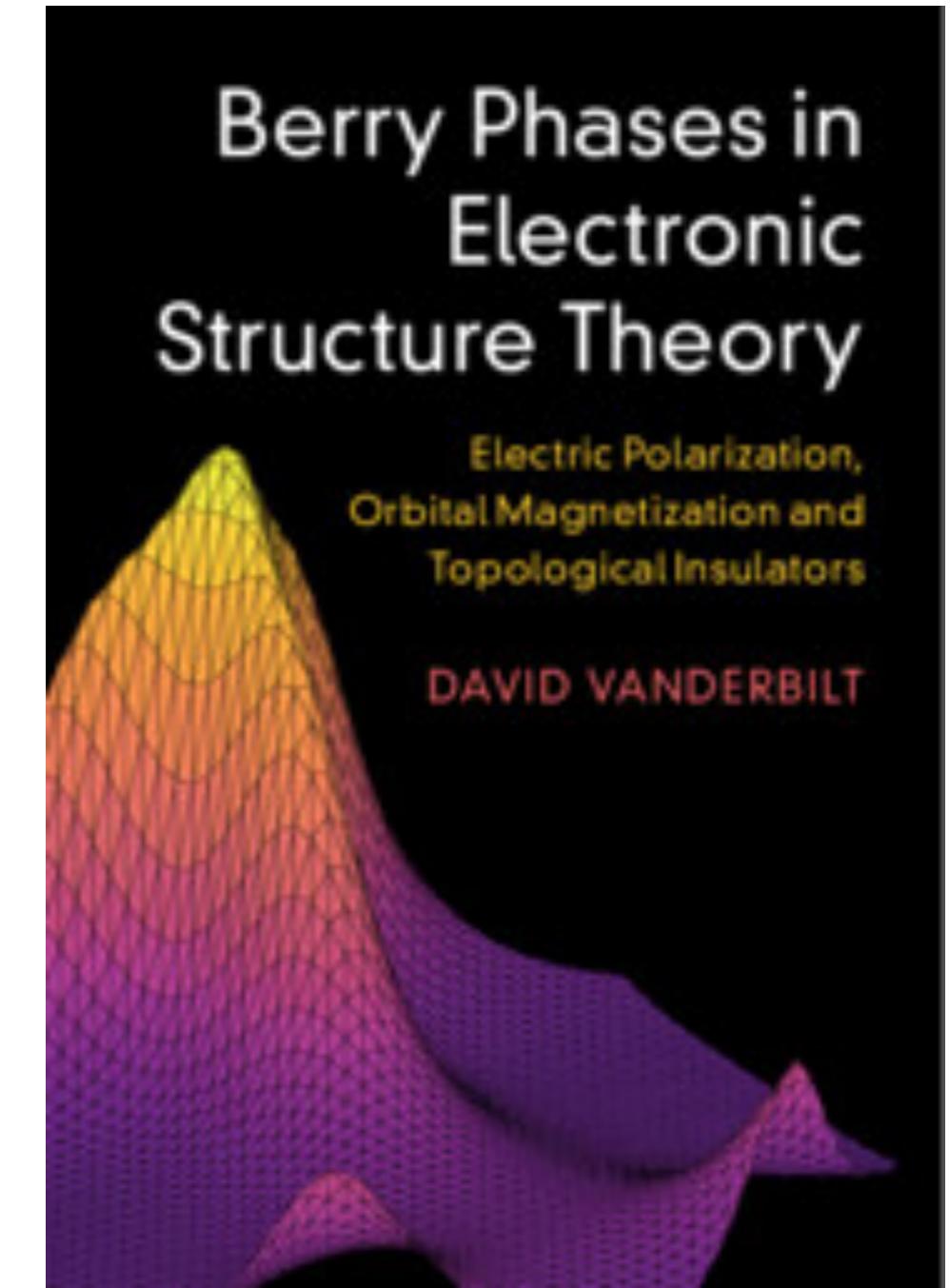
wannier-berri.org



berriology



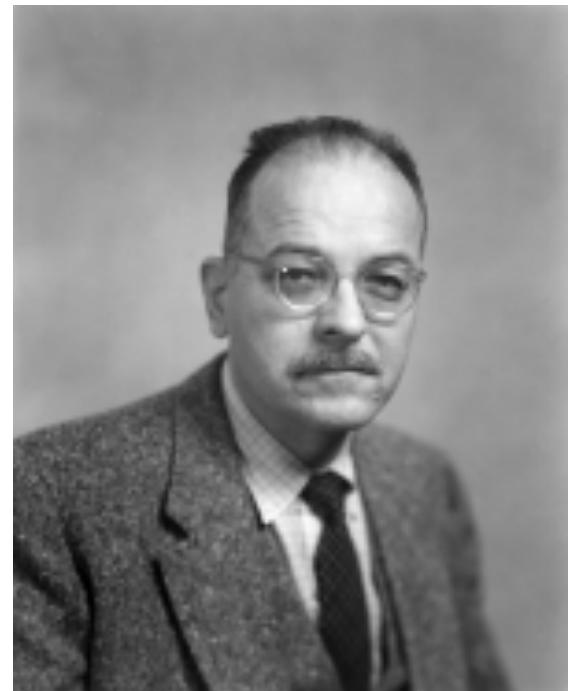
berriology



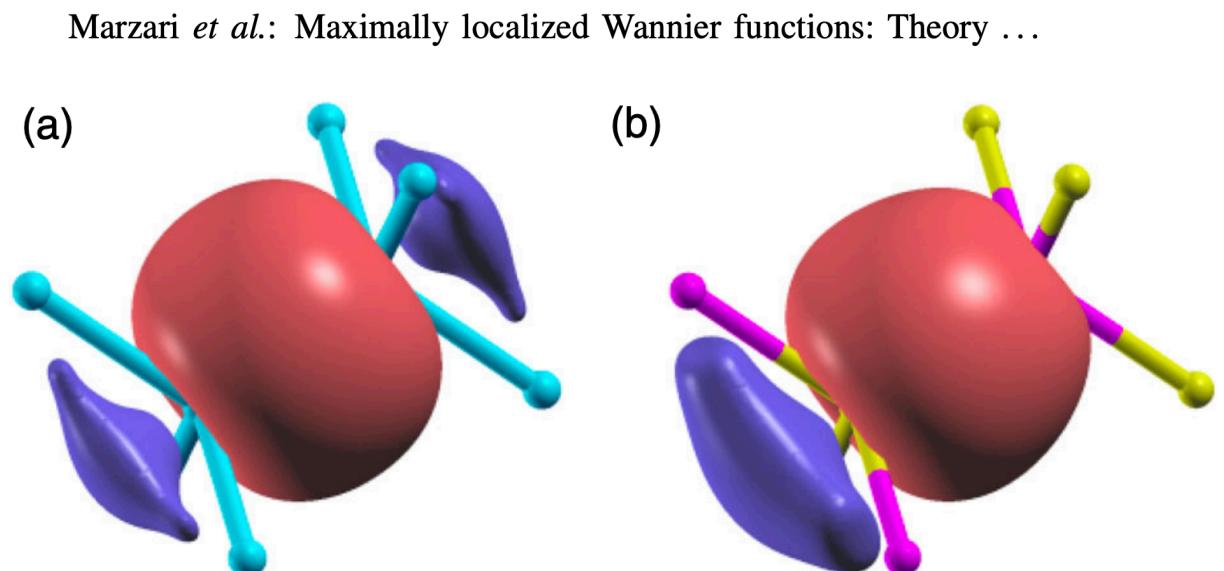
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the name

WANNIER

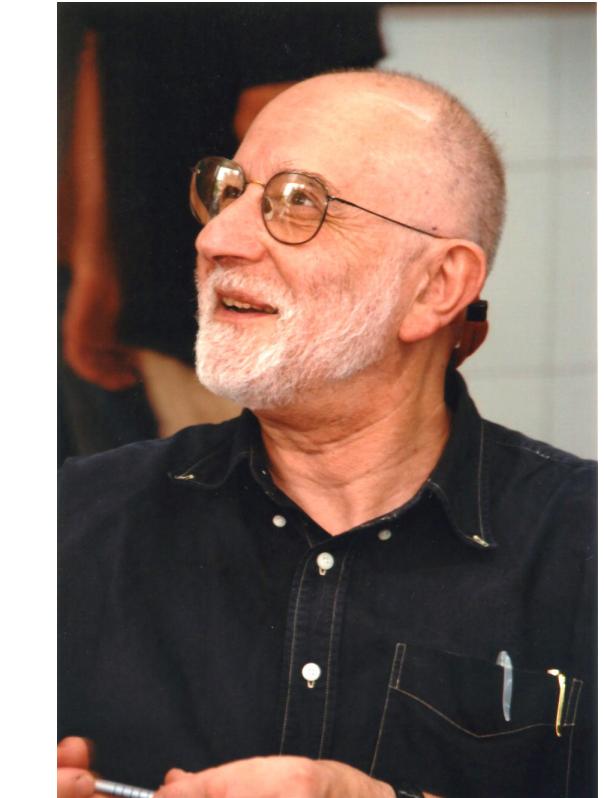


Gregory Wannier



BERRI

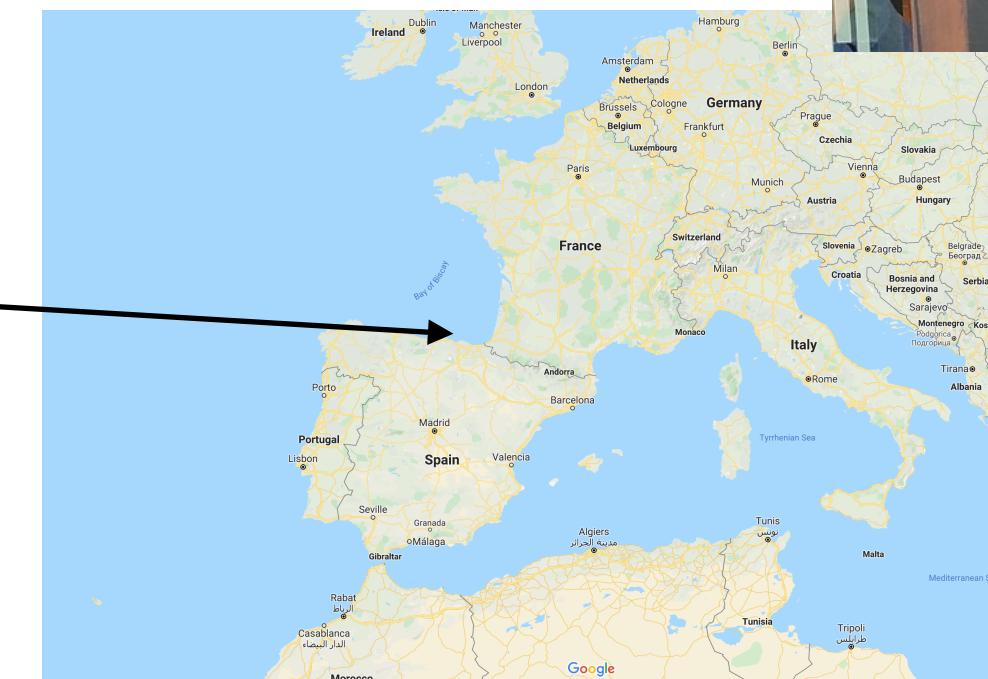
= “new” (basque)



Michael Berry

ikerbasque
Basque Foundation for Science

Basque Country
is here



Why Wannier interpolation?

Example : anomalous Hall conductivity

$$\sigma_{xy}^{\text{AHE}} = -\frac{e^2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \Omega_z(\mathbf{k})$$

$$\Omega_z(\mathbf{k}) = \sum_n f_{n\mathbf{k}} \Omega_{n,z}(\mathbf{k})$$

$$\Omega_{n,z}(\mathbf{k}) = -2\text{Im}\langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} | \times | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle.$$

YATES *et al.* PHYSICAL REVIEW B 75, 195121 (2007)

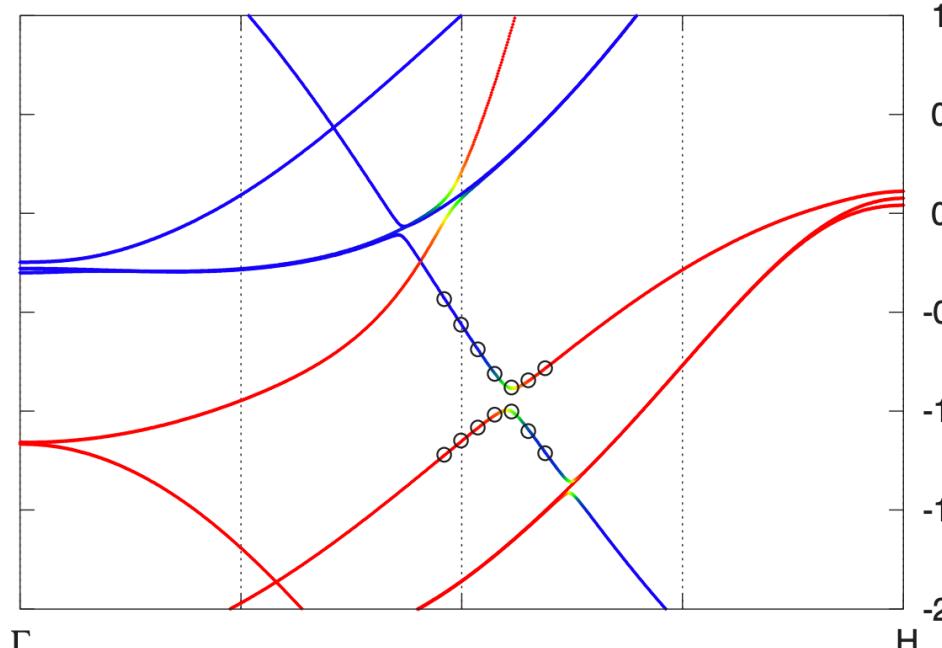


FIG. 1. (Color online) Wannier-interpolated bands of bcc Fe along Γ -H. The bands are colorcoded according to the value of the spin projection $\langle S_z \rangle$: red for spin-up and blue for spin-down. The energies are given in eV and the Fermi level is at 0 eV. The vertical dashed lines indicate k points on the *ab initio* mesh used for constructing the WFs. For comparison, points from a full *ab initio* calculation are shown as open circles.

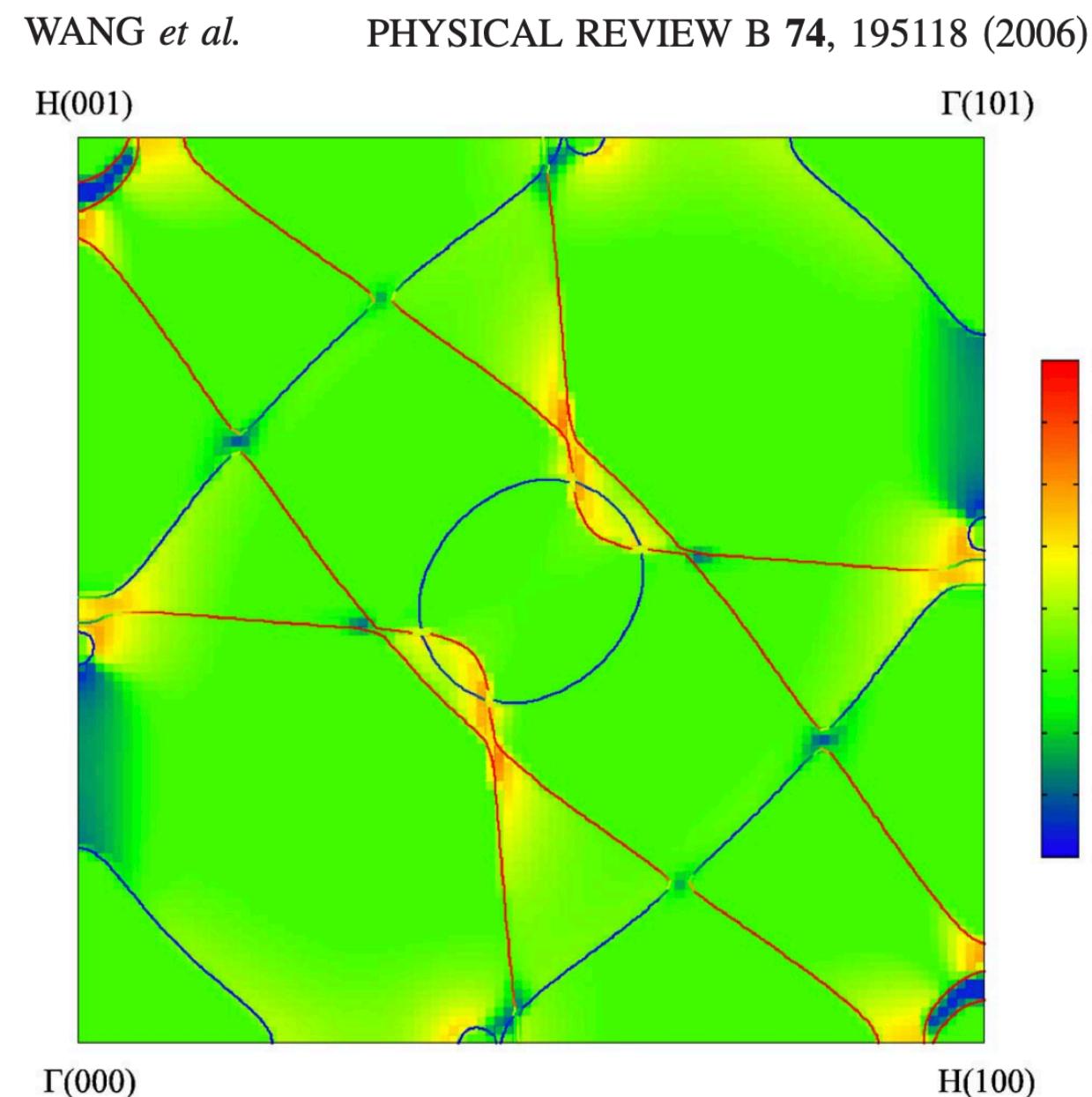


FIG. 6. (Color online) Calculated total Berry curvature $-\Omega_z$ in the plane $k_y=0$ (note log scale). Intersections of the Fermi surface with this plane are again shown.

- Faster evaluation on dense k -grids
- Derivatives without finite-differences
- Problem of gauge freedom

What are Wannier functions?

Maximally localized Wannier functions: Theory and applications

Nicola Marzari, Arash A. Mostofi, Jonathan R. Yates, Ivo Souza, and David Vanderbilt
Rev. Mod. Phys. **84**, 1419 – Published 10 October 2012

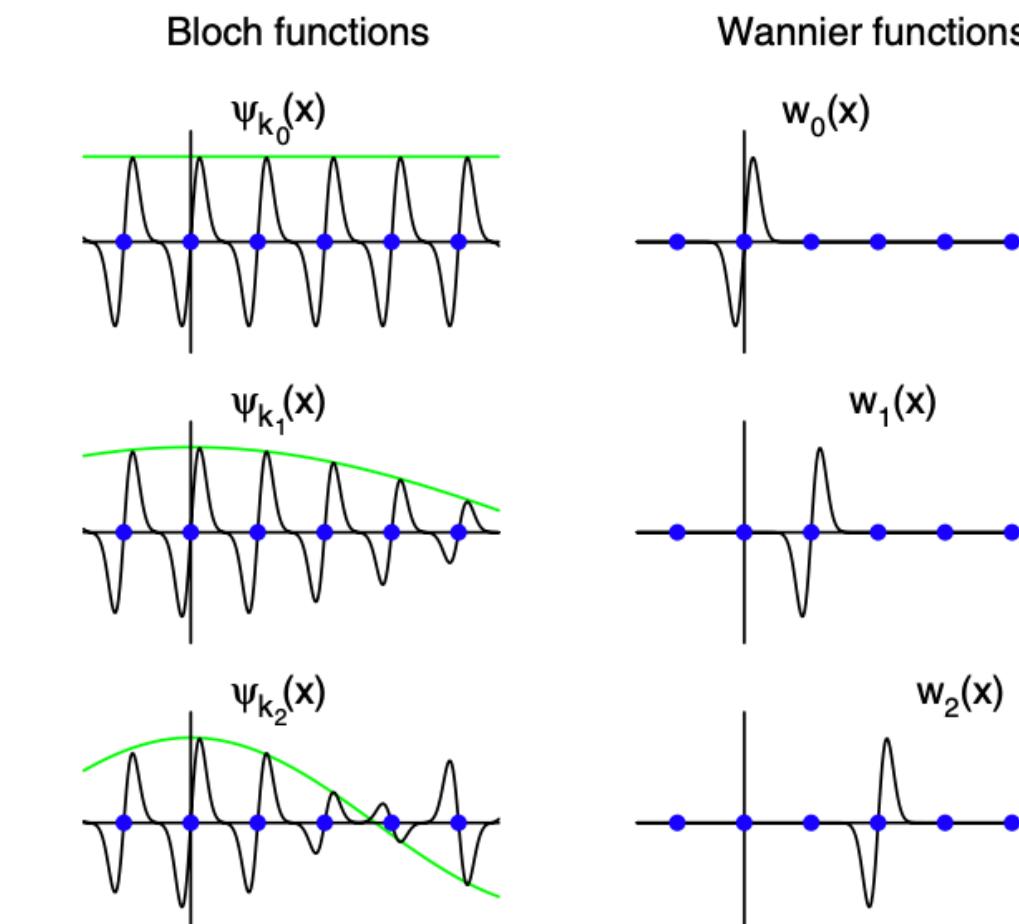
5

$$|\psi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R}n\rangle \quad \text{— Bloch function}$$

↔

$$|\mathbf{R}n\rangle = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{n\mathbf{k}}\rangle \quad \text{— Wannier function}$$

Multiband case: $|\mathbf{R}n\rangle = \frac{V}{(2\pi)^3} \int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{m=1}^J U_{mn}^{(\mathbf{k})} |\psi_{m\mathbf{k}}\rangle.$



Maximally localised WF (MLWF) : find $U(\mathbf{k})$ that minimises spread:

$$\Omega = \sum_n [\langle \mathbf{0}_n | r^2 | \mathbf{0}_n \rangle - \langle \mathbf{0}_n | \mathbf{r} | \mathbf{0}_n \rangle^2] = \sum_n [\langle r^2 \rangle_n - \bar{\mathbf{r}}_n^2]$$

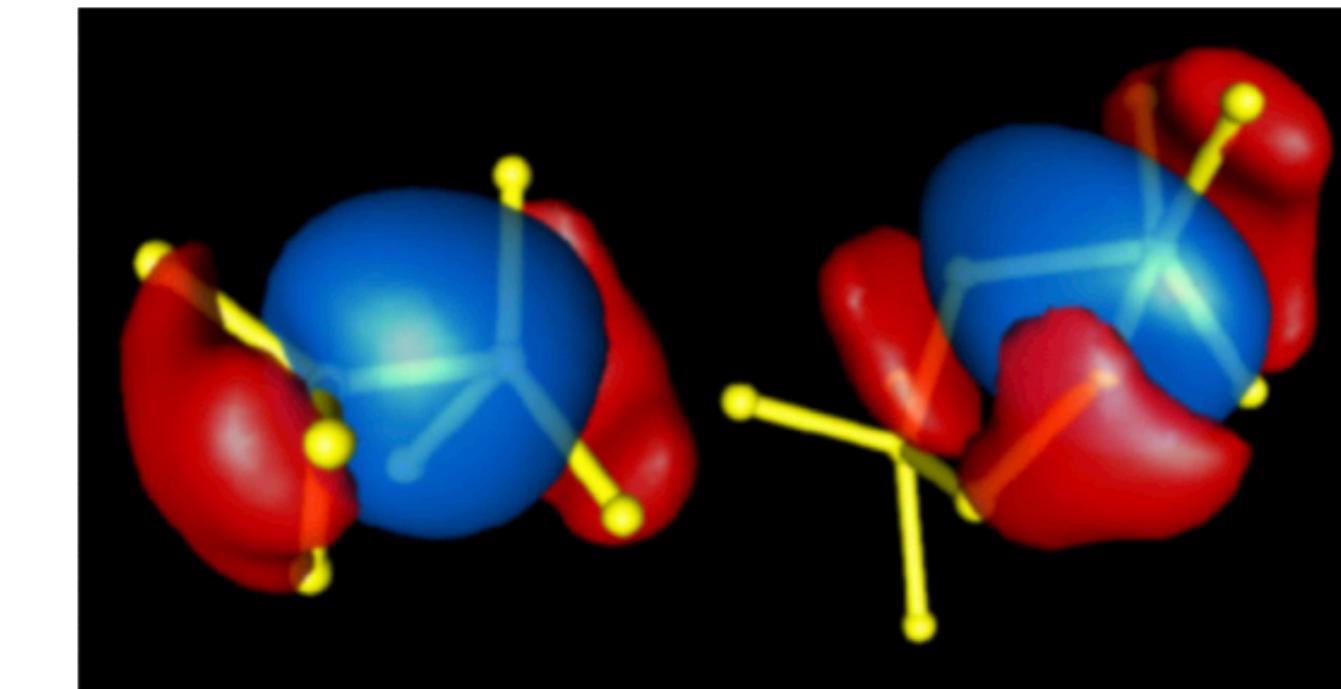


FIG. 4 (color online). MLWFs in amorphous Si, either around distorted but fourfold-coordinated atoms or in the presence of a fivefold defect. Adapted from Fornari *et al.*, 2001.

Wannier Interpolation

ab initio calculation



Bloch wavefunctions $|u_{n\mathbf{q}}\rangle$ and Energies $E_{n\mathbf{k}}$ on a **(coarse) regular grid**

Matrix elements: $\langle u_{n\mathbf{q}} | u_{m\mathbf{q}+\mathbf{b}} \rangle$,
 $\langle u_{n\mathbf{q}} | \hat{s} | u_{m\mathbf{q}} \rangle$

WANNIER90

Wannier functions $|\mathbf{R}_j\rangle$
 and matrix elements $X(\mathbf{R})$

$$\langle i\mathbf{0} | \mathbf{r} | j\mathbf{R} \rangle$$

$$\langle i\mathbf{0} | \hat{H} | j\mathbf{R} \rangle$$

$$\langle i\mathbf{0} | \hat{s} | j\mathbf{R} \rangle$$

WANG et al. PHYSICAL REVIEW B 74, 195118 (2006)

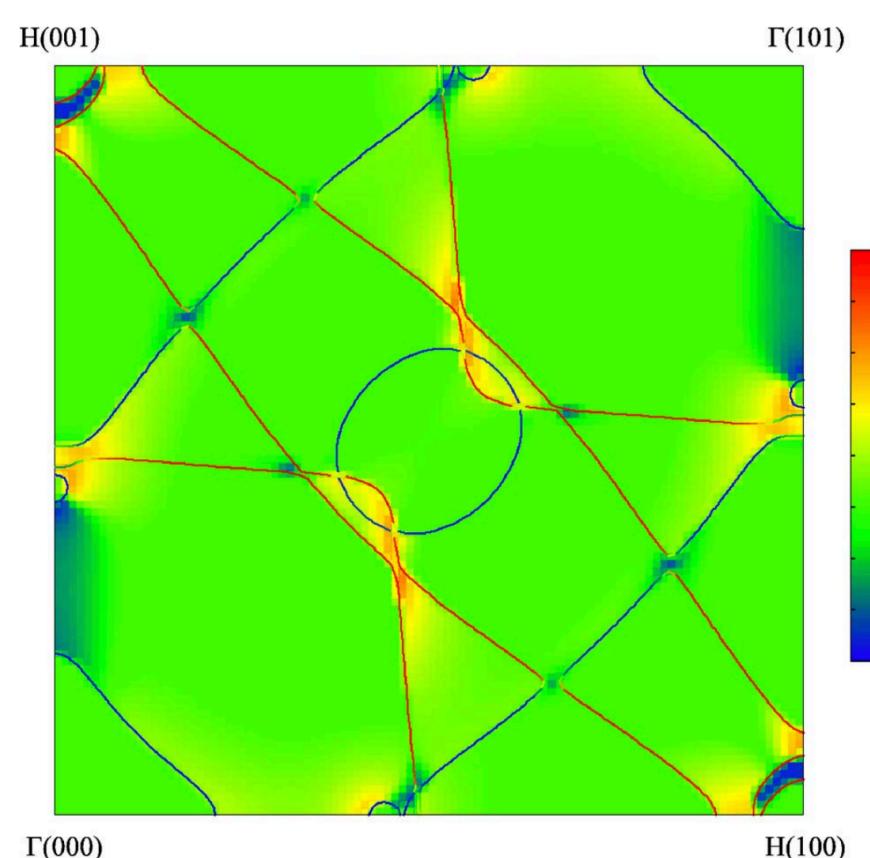


FIG. 6. (Color online) Calculated total Berry curvature $-\Omega_z$ in the plane $k_y=0$ (note log scale). Intersections of the Fermi surface with this plane are again shown.

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 postw90.X

interpolate to
 arbitrary k-points

$$X(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\mathbf{R}} X(\mathbf{R})$$

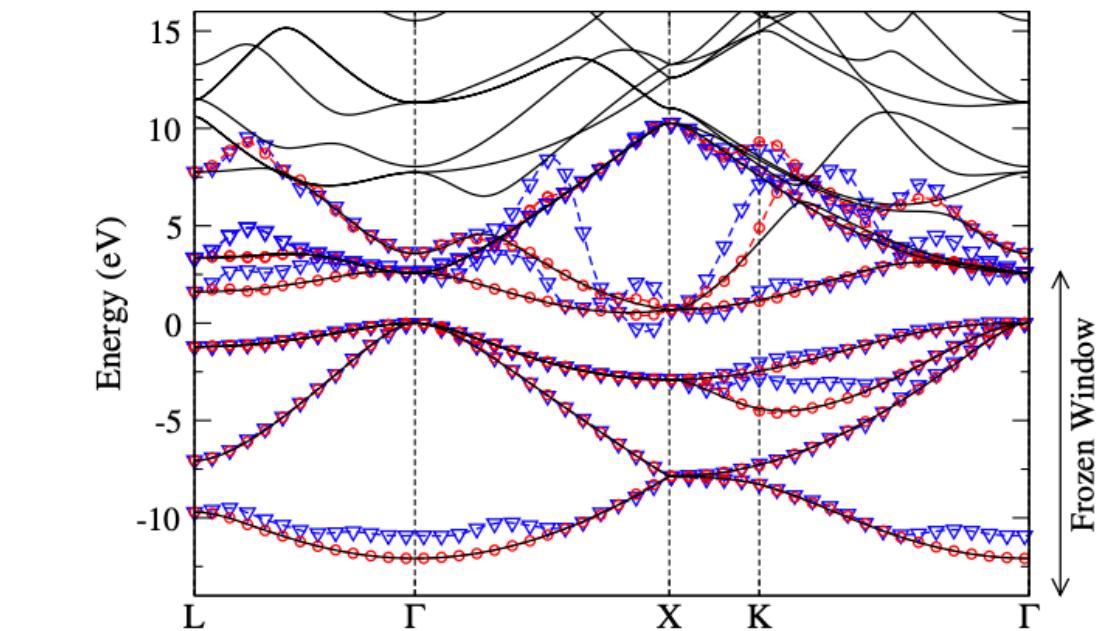


FIG. 5 (color online). Band structure of bulk crystalline Si. Solid lines: Original bands generated directly from a DFT calculation. Triangles: Wannier-interpolated bands obtained from the subspace selected by an unconstrained projection onto atomic sp^3 orbitals. Circles: Wannier-interpolated bands obtained with the same procedure and the additional constraint of reproducing exactly the original valence manifold and parts of the conduction manifold, using a frozen energy window (see text).

YATES et al. PHYSICAL REVIEW B 75, 195121 (2007)

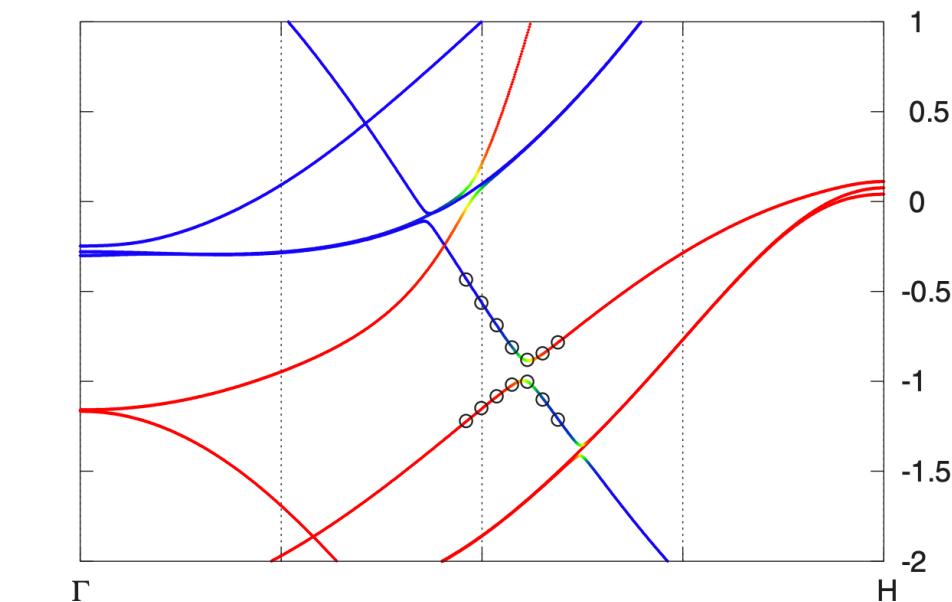


FIG. 1. (Color online) Wannier-interpolated bands of bcc Fe along Γ -H. The bands are colorcoded according to the value of the spin projection $\langle S_z \rangle$: red for spin-up and blue for spin-down. The energies are given in eV and the Fermi level is at 0 eV. The vertical dashed lines indicate k points on the *ab initio* mesh used for constructing the WFs. For comparison, points from a full *ab initio* calculation are shown as open circles.

Wannier Interpolation vs tight-binding

$$H_{ij}^W(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}(\mathbf{R}+\mathbf{t}_j-\mathbf{t}_i)} \langle \mathbf{0}i | \hat{H} | \mathbf{R}j \rangle$$

$$\sum_j H_{ij}(\mathbf{k}) U_{jn}(\mathbf{k}) = \epsilon_{n\mathbf{k}} U_{in}(\mathbf{k})$$

$$|u_{n\mathbf{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j-\mathbf{r})} |\phi_i\rangle U_{in}(\mathbf{k})$$

$$\sqrt{N} |\nabla_{\mathbf{k}} u_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j-\mathbf{r})} |\phi_i\rangle \nabla_{\mathbf{k}} U(\mathbf{k}) + i \sum_{\mathbf{R}} (\mathbf{R} + \mathbf{t}_j - \mathbf{r}) e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j-\mathbf{r})} |\phi_i\rangle U(\mathbf{k})$$

$$\mathbf{A}_{mn}(\mathbf{k}) \equiv i \langle u_{m\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle = (U^\dagger \cdot \nabla_{\mathbf{k}} U)_{mn} + (U^\dagger \cdot \mathbf{A}^W \cdot U)_{mn}$$

internal term

$$(U^\dagger \cdot \nabla_{\mathbf{k}} U)_{mn} = -i \frac{(U^\dagger \cdot \nabla_{\mathbf{k}} H^W \cdot U)_{mn}}{\epsilon_n - \epsilon_m}$$

external term

$$\mathbf{A}_{ij}^W(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}(\mathbf{R}+\mathbf{t}_j-\mathbf{t}_i)} \langle \mathbf{0}i | \mathbf{r} - \mathbf{t}_j - \mathbf{R} | \mathbf{R}j \rangle$$

In tight-binding approximaton

$$\langle \mathbf{0}i | \mathbf{r} | \mathbf{R}j \rangle = \delta_{ij} \delta_{\mathbf{0},\mathbf{R}} \mathbf{t}_j \implies \mathbf{A}^W = 0$$

if we consider \mathbf{t}_j as free parameters, the magnitude the external and internal terms will change, but the total remains the same but **only for gauge-invariant quantities**.

Wannier Interpolation is free from truncation error

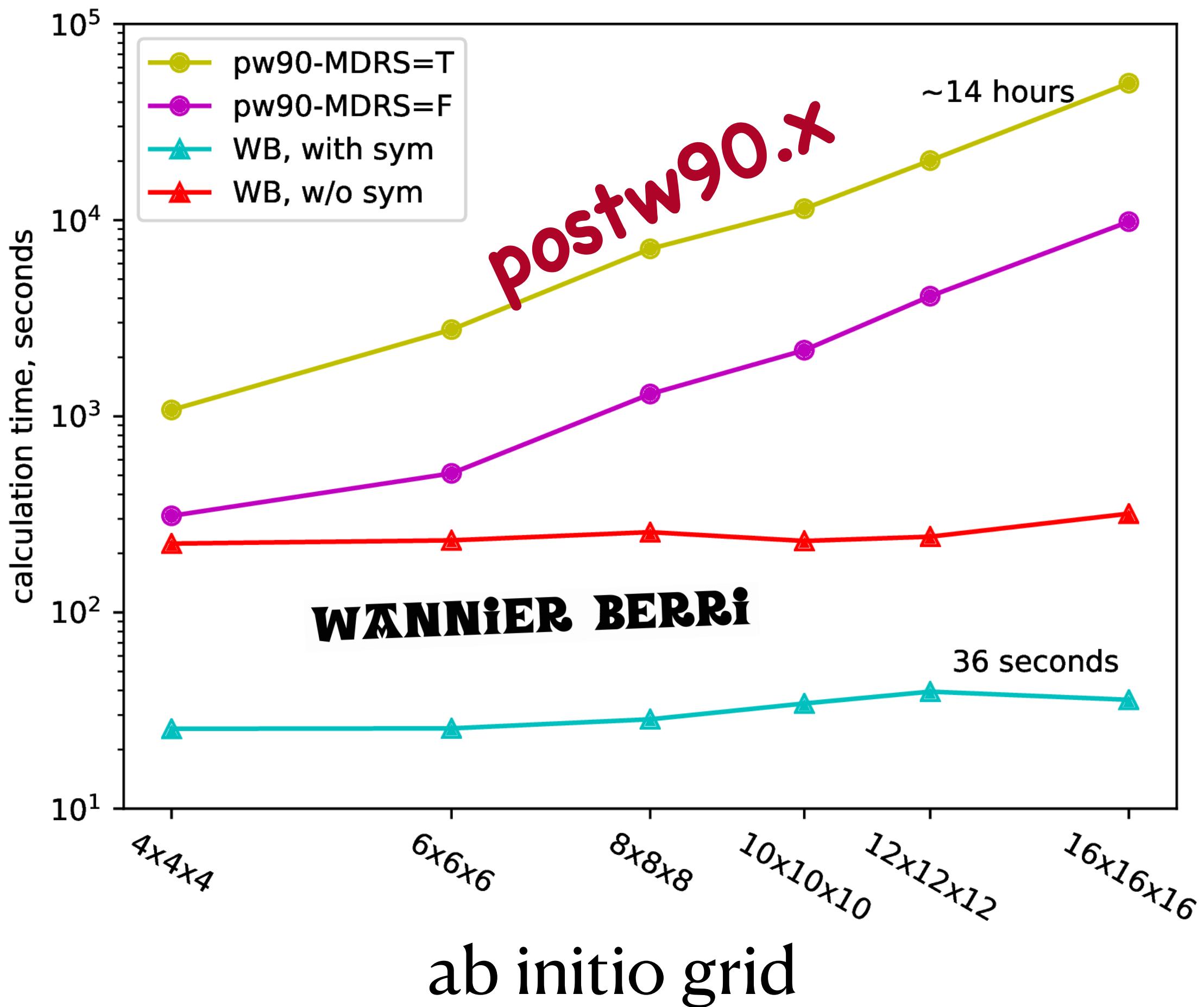
How do we make berryology and Wannier interpolation easy(ier)?

- Fast (many k-points per minute)
- Efficient (require less k-points)
- Easy implementation of new things
- Implementation on a user side

32-core node

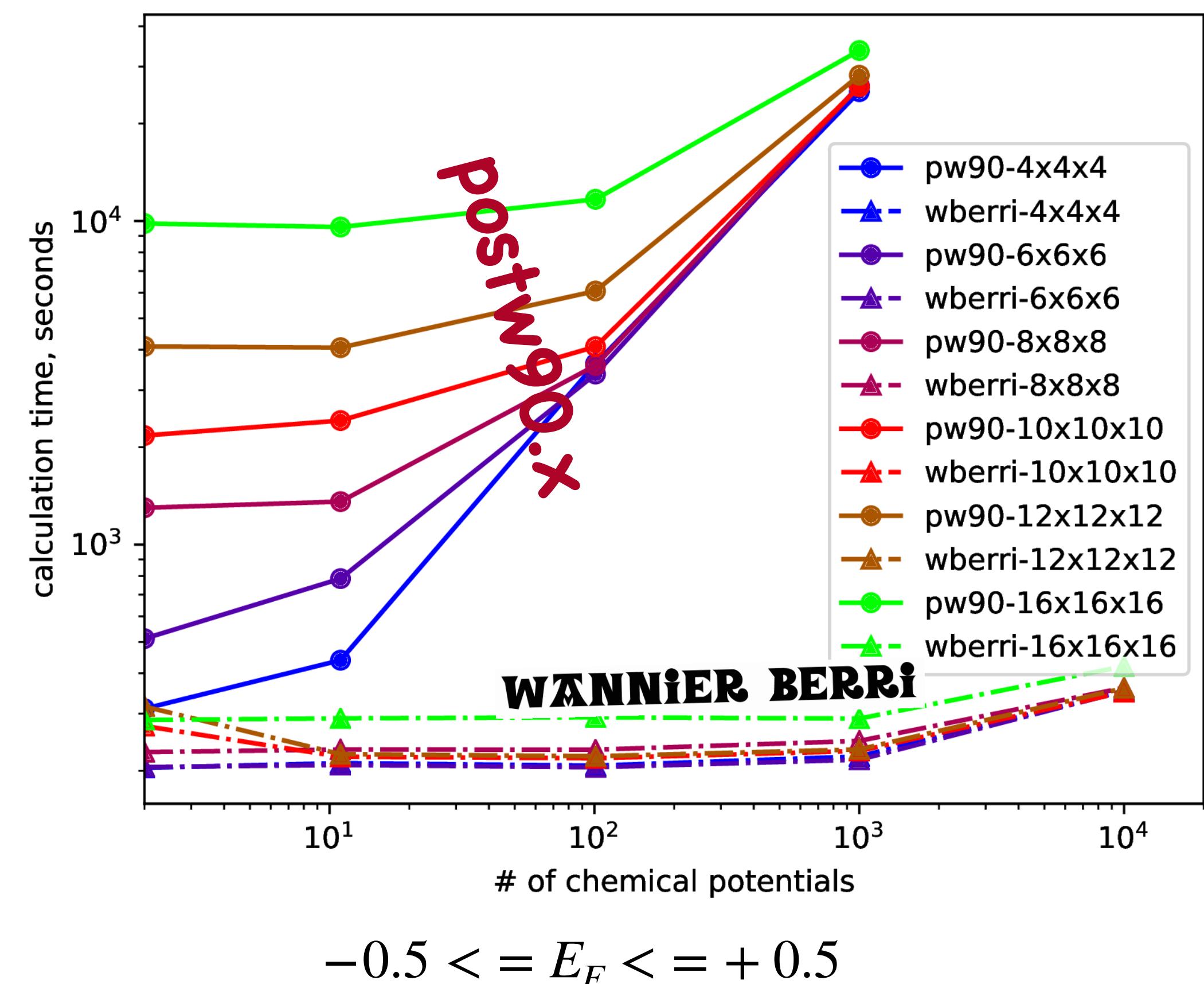
How we make it faster

interpolate to 200x200x200, single Fermi level



MDRS=minimal distance replica selection (use_ws_distance=T – default value)

interpolate to 200x200x200, multiple Fermi level



adaptive refinement switched off

mixed Fourier transform

ab initio \mathbf{q} -grid – coarse $\sim 20 \times 20 \times 20$

Bloch functions $|\psi_{n\mathbf{q}}\rangle$

$$\text{Wannier functions: } |\mathbf{R}n\rangle = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_m U_{mn}(\mathbf{k}) |\psi_{m\mathbf{k}}\rangle \quad (1)$$

$$X_{mn}(\mathbf{R}) = \langle \mathbf{0}m | \hat{X} | \mathbf{R}m \rangle, \text{ where } \hat{X} = \hat{H}, \hat{\mathbf{r}}, \hat{\sigma}, \dots \quad (2)$$

$$X(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} X(\mathbf{R}) \quad (3)$$

– interpolation \mathbf{k} -grid – dense $\sim 500 \times 500 \times 500$

$$N_{\mathbf{k}} \gg N_{\mathbf{R}} \approx N_{\mathbf{q}}$$

I. “slow FT”: – as implemented in `postw90.x`

- (i) $t_{\text{slow}} \propto N_{\mathbf{k}} \cdot N_{\mathbf{R}}$
- (ii) all \mathbf{k} -points treated independently
- (iii) requires little memory
- (iv) easy to parallelise

II. FFT : extend the $X(\mathbf{R})$ with zeros for large $|\mathbf{R}|$

- (i) $t_{\text{FFT}} \propto N_{\mathbf{k}} \log N_{\mathbf{k}}$ – *may be* faster for $N_{\mathbf{k}} \gtrsim N_{\mathbf{R}}$
- (ii) requires a lot of memory
- (iii) hard to parallelise
- (iv) cannot exclude symmetry-equivalent points
- (v) cannot do adaptive refinement.

III. mixed FT: divide $N_{\mathbf{k}} = N_{\mathbf{K}} \cdot N_{\text{FFT}}$

$$\tilde{X}(\mathbf{R}, \mathbf{K}) = e^{i\mathbf{K}\cdot\mathbf{R}} X(\mathbf{R}), \text{ – “slow FT”}$$

$$t_{\text{mix},1} \propto N_{\mathbf{K}} \cdot N_{\mathbf{R}}$$

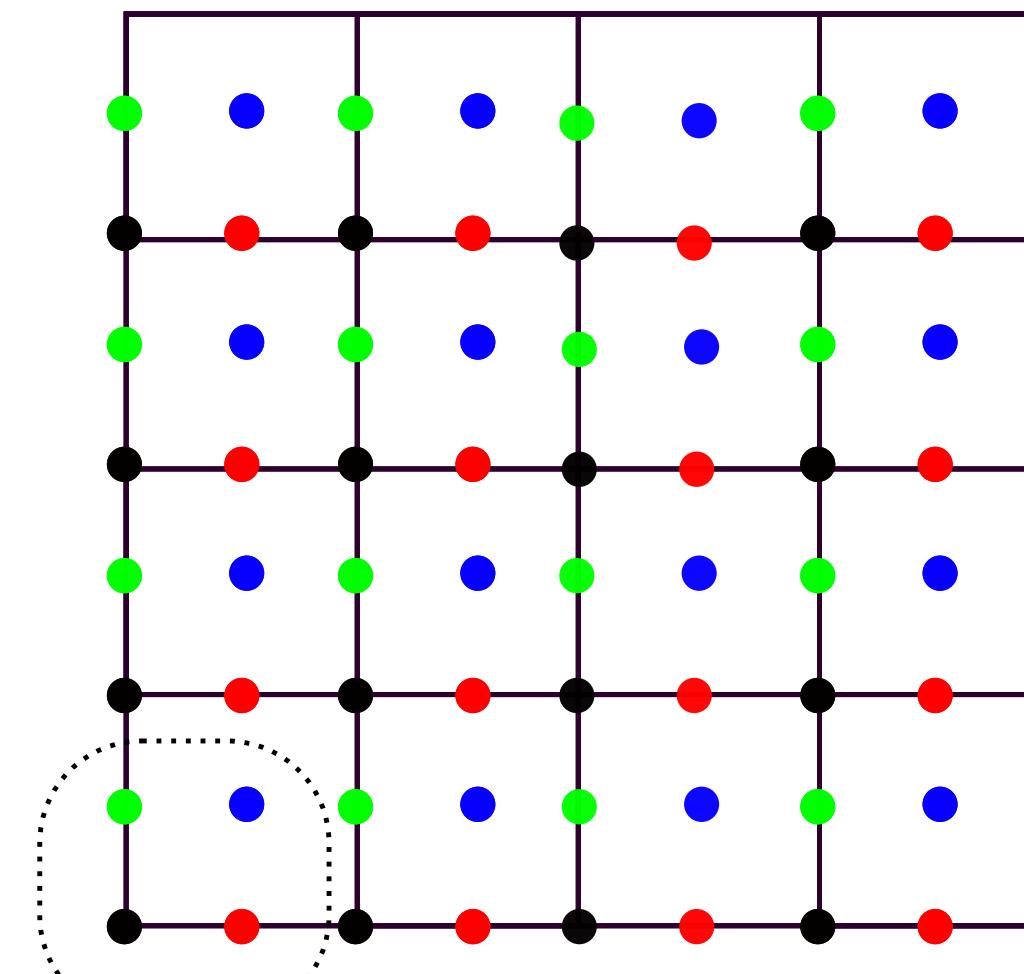
$$X(\mathbf{K} + \mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} X(\mathbf{R}, \mathbf{K}) \text{ – as FFT}$$

$$t_{\text{mix},2} \propto N_{\mathbf{K}} \cdot N_{\text{FFT}} \log N_{\text{FFT}}$$

A good choice is $N_{\text{FFT}} \gtrsim N_{\mathbf{R}} \approx N_{\mathbf{q}}$

- (i) $t_{\text{mix}} \propto N_{\mathbf{k}} \log N_{\mathbf{R}} \approx < t_{\text{slow}}, t_{\text{FFT}}$
- (ii) all \mathbf{K} -points treated independently
- (iii) reasonable memory consumption
- (iv) operations over k-grid is vectorised (good for Python)
- (v) time weakly depends on the size of *ab initio* grid
- (vi) parallelisation over \mathbf{K} -points
- (vii) apply symmetries and adaptive refinement by \mathbf{K} -points

4x4 FFT Grid

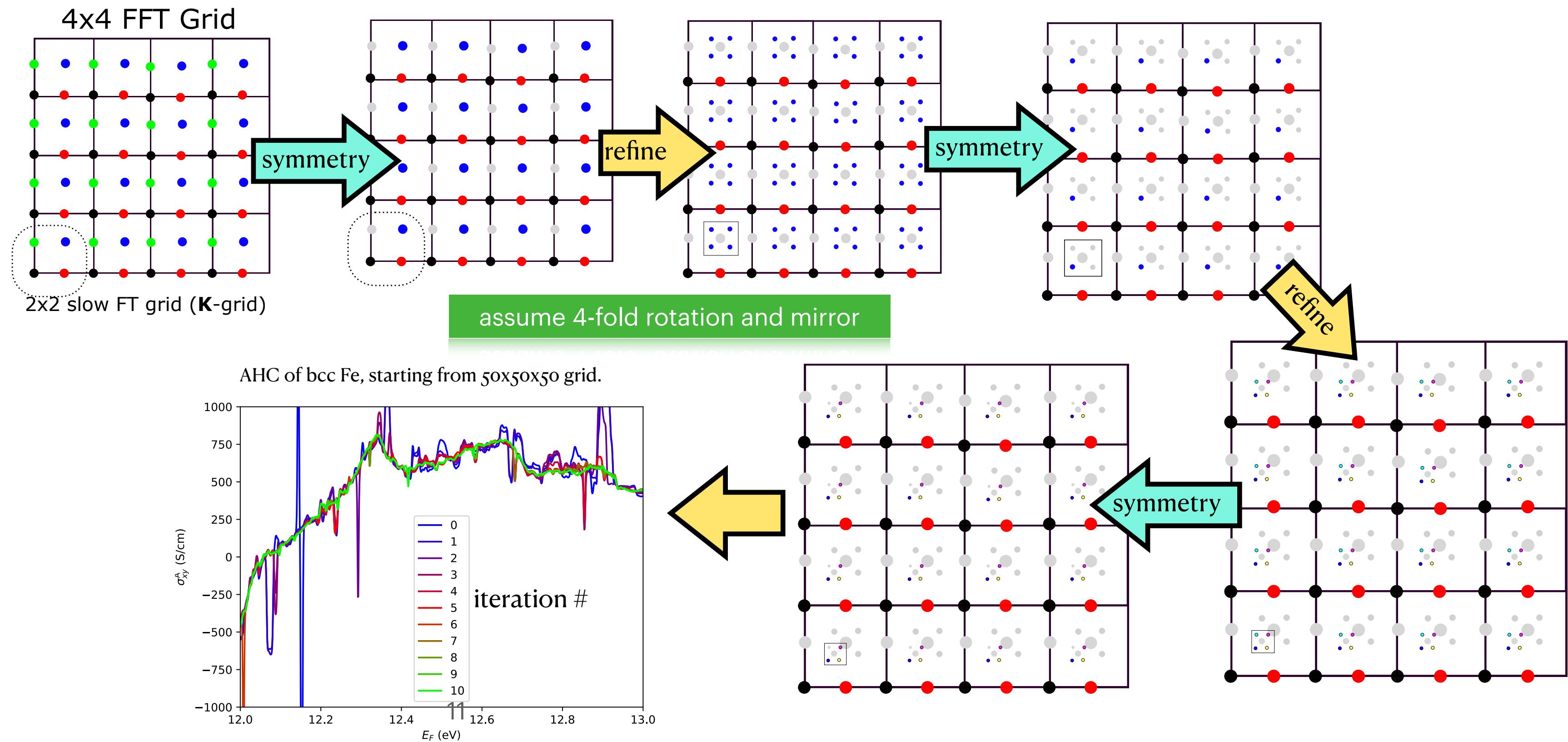


2x2 slow FT grid (\mathbf{K} -grid)

How we make it efficient

- use of symmetries
- recursive refinement
- tetrahedron method
- Fermi sea formulas

symmetries and adaptive refinement



Fermi surface vs Fermi sea

ohmic conductivity

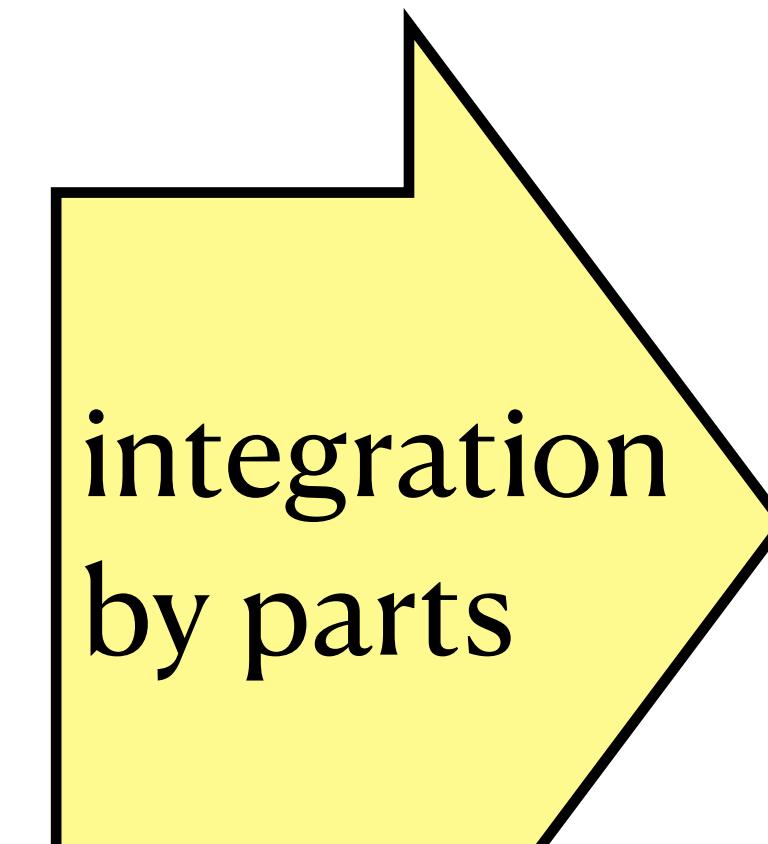
$$\sigma_{ab} = -\frac{\tau e^2}{\hbar^2} \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial E_{n\mathbf{k}}}{\partial k_a} \frac{\partial f_{n\mathbf{k}}}{\partial k_b}$$

Berry dipole

$$D_{ab} = - \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial f_{n\mathbf{k}}}{\partial k_a} \Omega_{n\mathbf{k}}^b$$

GME tensor

$$K_{ab} = - \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial f_{n\mathbf{k}}}{\partial k_a} m_{n\mathbf{k}}^b$$



only $E_{n\mathbf{k}} = E_F$

at $T = 0$

only $E_{n\mathbf{k}} \leq E_F$

contribute

$$\sigma_{ab} = \frac{\tau e^2}{\hbar^2} \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial^2 E_{n\mathbf{k}}}{\partial k_a \partial k_b} f_{n\mathbf{k}}$$

$$D_{ab} = \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial \Omega_{n\mathbf{k}}^b}{\partial k_a} f_{n\mathbf{k}}$$

$$K_{ab} = \sum_n \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial m_{n\mathbf{k}}^b}{\partial k_a} f_{n\mathbf{k}}$$

requires less
k-points

PHYSICAL REVIEW B 97, 035158 (2018)

f — Fermi distribution

$\Omega_{n\mathbf{k}} = -2\text{Im}\langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} | \times | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle$ — Berry curvature

$$\mathbf{m}_{n\mathbf{k}} = \mathbf{m}_{n\mathbf{k}}^{\text{spin}} + \mathbf{m}_{n\mathbf{k}}^{\text{orb}}$$

$$\mathbf{m}_{n\mathbf{k}}^{\text{orb}} = \frac{e}{2\hbar} \text{Im}\langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} | \times (H - E_{n\mathbf{k}}) | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle$$

— orbital moment

Gyrotropic effects in trigonal tellurium studied from first principles
Stepan S. Tsirkin,^{1,2} Pablo Aguado Puente,^{1,2} and Ivo Souza^{1,3}

Implementation of new things

- object-oriented programming
- modular structure
- abstract classes
- routine that evaluates the integral has no idea what it integrates.

Implementation on the user side

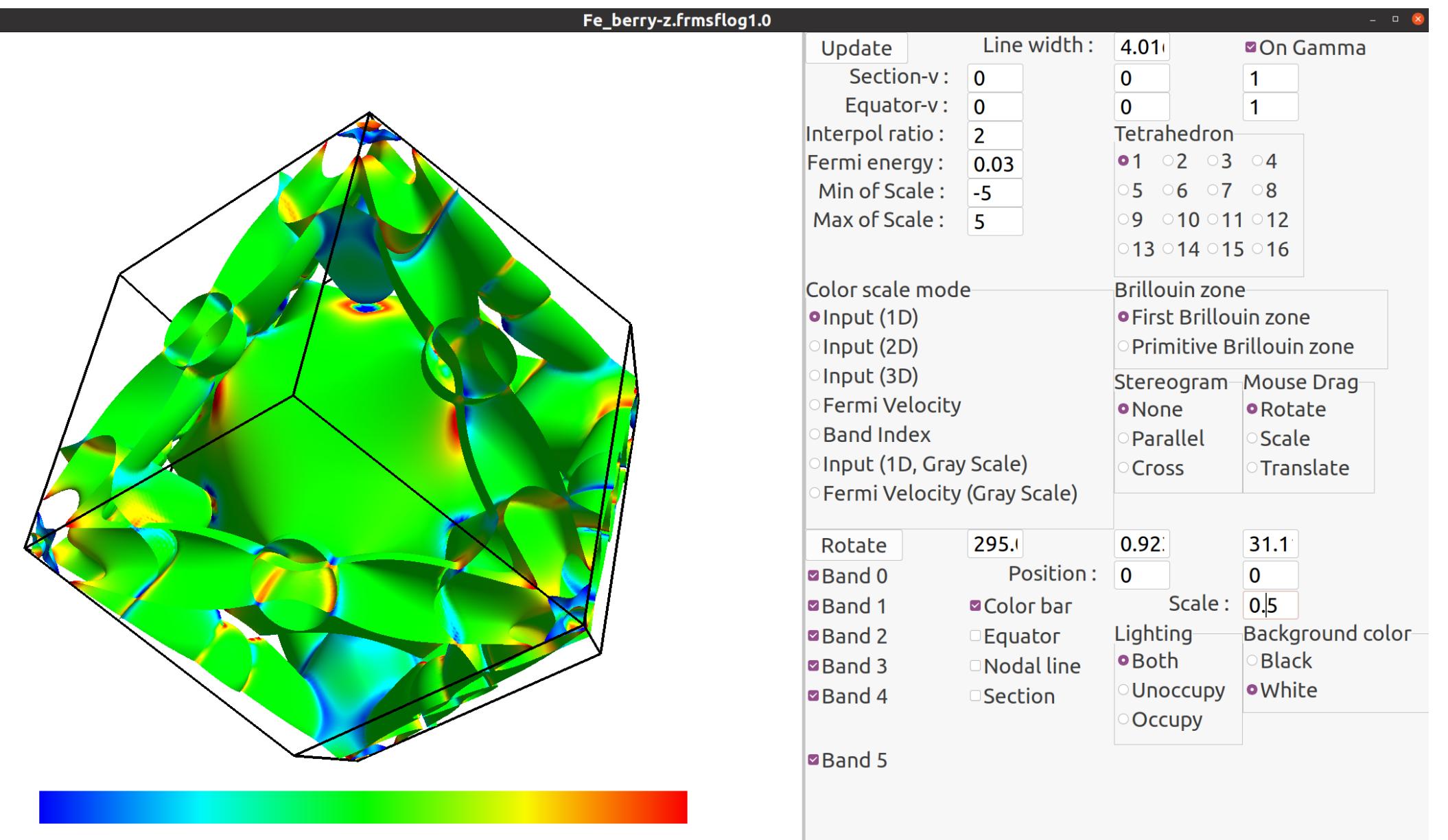
- Write function and pass it to WannierBerri as a parameter (see tutorial)
- If it works - share with community

visualisation

```
WB.tabulate(system,  
            grid=WB.Grid(system,length=100),  
            quantities=[ "berry" ],  
            fout_name='Fe ',  
            numproc=num_proc,  
            ibands=np.arange(4,10),  
            Ef0=12.6)
```

or any other quantity $X_n(\mathbf{k})$
may be added

saves to a format .frmsf



<https://fermisurfer.osdn.jp/>

Further information:

- 1)  GitHub

<https://github.com/wannier-berri/wannier-berri>

- 2) web page :

<http://wannier-berri.org>

- 3) mailing list:

<https://physik.lists.uzh.ch/sympa/info/wannier-berri>

- 4) contact me: stepan.tsirkin@uzh.ch

Wannier school

Trieste, May 2022:

Wannier90
WannierTools
WannierBerri
EPW
Z2pack
PythonTB
TBmodels

Open postdoc position

**San Sebastian
(Spain)**