

Introduction to PAOFLOW

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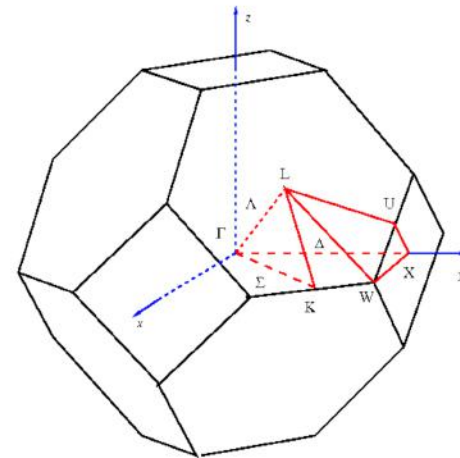
Some QE post processing

QE post processing

Band Structure of Silicon

Re-run the self-consistent calculation at equilibrium lattice parameter, then run a *non-self-consistent* (fixed-potential) calculation, with the same input as for scf, but

- variable `calculation` is set to 'bands' ;
- the number `nbnd` of Kohn-Sham states must be explicitly set;
- k-point list is chosen along suitable high-symmetry lines. See sample file `si.bands.in`, containing the $L - \Gamma - X - K - \Gamma$ path.



Important: outdir and prefix must be the same in bands and in scf calculations.

```
$ pw.x -in si.bands.in > si.bands.out
```

The list of k-points and of Kohn-Sham energies can be found after the line

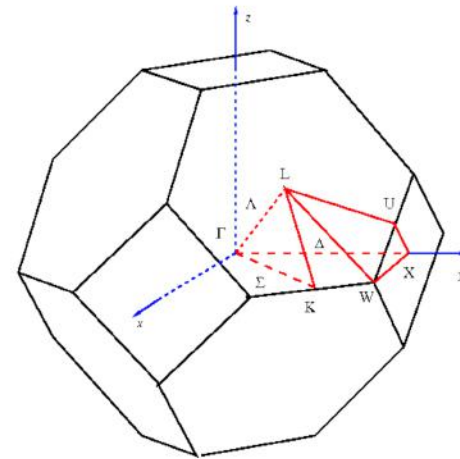
```
End of band structure calculation
```

QE post processing

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```
End of band structure calculation
```

QE post processing

Plotting Band Structure

There are various ways to plot the band structure. The simplest: use command **bands.x** with the following input (outdir and prefix as in previous steps):

```
&bands  
  prefix='...', outdir='...', filband = 'sibands.dat', lsym=.false.  
/
```

Output file **sibands.dat** can be plotted using command **plotband.x**.

Setting option `lsym=.true` instead, **bands.x** performs a symmetry analysis. An additional file **sibands.dat.rep** is generated, containing information on symmetry labels of the various bands.

Beware: the k -point path must be continuous in space; no two consecutive k -points can be the same, or else you may get funny-looking bands

QE post processing

Plotting Band Structure II

`plotband.x` prompts for terminal input:

```
$ plotband.x
Input file > sibands.dat
Reading      8 bands at      36 k-points
Range:    -6.3010    13.7920eV  Emin, Emax > -6.30 10.30
high-symmetry point:  0.5000 0.5000 0.5000    x coordinate    0.0000
high-symmetry point:  0.0000 0.0000 0.0000    x coordinate    0.8660
high-symmetry point:  0.0000 0.0000 1.0000    x coordinate    1.8660
high-symmetry point:  0.0000 0.5000 1.0000    x coordinate    2.3660
high-symmetry point:  0.0000 1.0000 1.0000    x coordinate    2.8660
high-symmetry point:  0.0000 0.0000 0.0000    x coordinate    4.2802
output file (xmgr) > sibands.plot
bands in xmgr format written to file sibands
output file (ps) > (press Return)
```

Output is in file `sibands.plot` and can be plotted with `gnuplot`. If symmetry analysis is performed, output is instead split into several files `sibands.plot.N.M`, where N labels the high-symmetry lines, M labels irreducible representations.

QE post processing

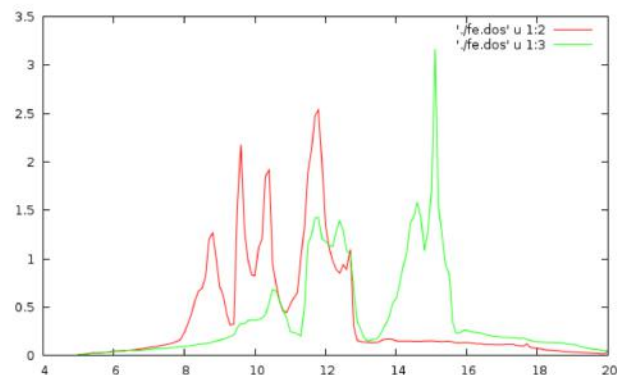
Density of States (DOS)

1. Run a non self-consistent calculation (`calculation='nscf'` in namelist `&control`), using a previously computed scf potential. Input file `fe_fm.nscf.in`:
 - has the same prefix and outdir of the previous scf step
 - uses a denser k-point mesh than in the previous scf step
 - uses the *linear tetrahedron method* (variable `occupations='tetrahedra'`)
2. Run code `dos.x`, using input file `fe.dos.in`: `$ dos.x -in fe.dos.in`, where
 - prefix and outdir are the same of the previous non-scf step
 - output is written to file `fildos`

Plot spin-up (column 2) and down (column 3) DOS as a function of E (column 1)

3. (step 1 is not strictly needed, but if you want a nice DOS you need tetrahedra and a dense k-point grid)

Reminder: Absolute values of Kohn-Sham eigenvalues have no direct physical meaning



Localized orbitals

Localized basis sets

Chemical interpretation of the wavefunction

Simple connection with plane-waves via Fourier transforms:

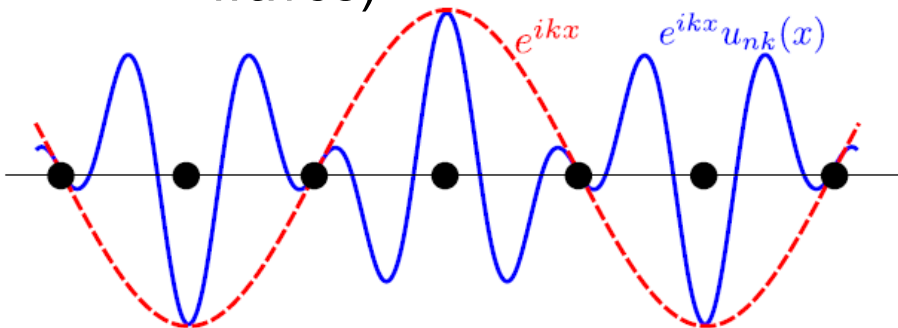
Construction of model Hamiltonians (e.g. strongly correlated systems)

Band structure interpolation

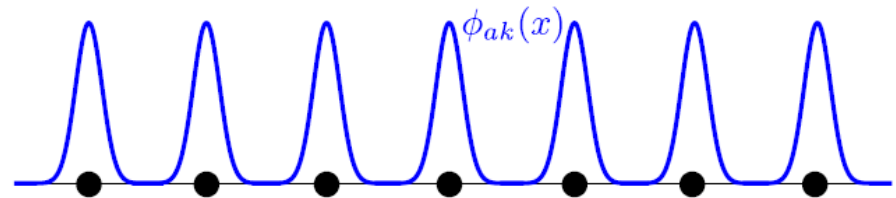
Transport properties

Many more...

Bloch states (plane waves)



Localized states (i.e. atomic orbitals)



Wannier functions

A convenient localized basis set.

Maximal localization: Unique basis set $U_{mn}(\vec{k})$

$$\psi_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r}) e^{-i\vec{k}\cdot\vec{r}}$$

$$w_n(\vec{r} - \vec{R}) = \int \sum_m U_{mn}(\vec{k}) \psi_{n\vec{k}}(\vec{r}) e^{-i\vec{k}\cdot\vec{R}} d^3k$$

Bloch



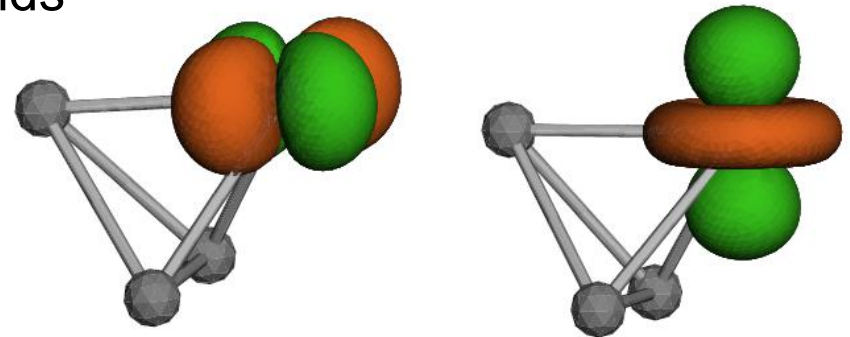
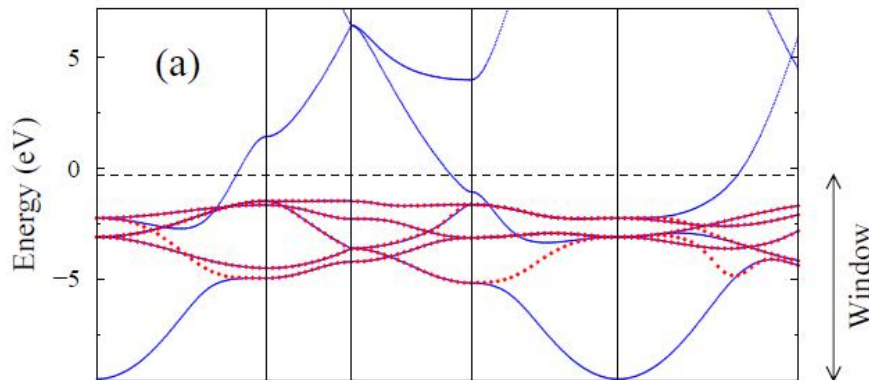
Wannier

Not straightforward (what projectors and how many?)

Internal iterative procedure for disentangling bands (e.g in metals)

Energy window?

Intractable for large number of bands



N. Marzari et. al. Rev. Mod. Phys. **84**, 1419 (2012)

Localized basis sets

Chemical interpretation of the wavefunction

Simple connection with plane-waves via Fourier transforms:

Construction of model Hamiltonians (e.g. strongly correlated systems)

PHYSICAL REVIEW B **88**, 165127 (2013)

Effective and accurate representation of extended Bloch states on finite Hilbert spaces

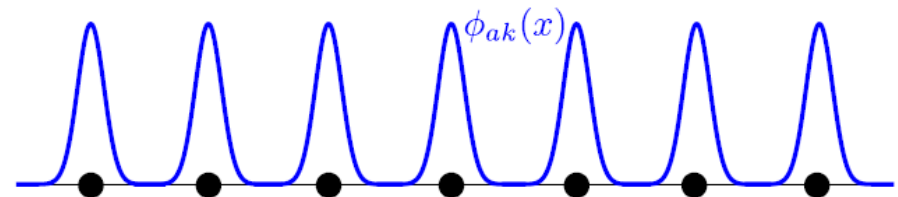
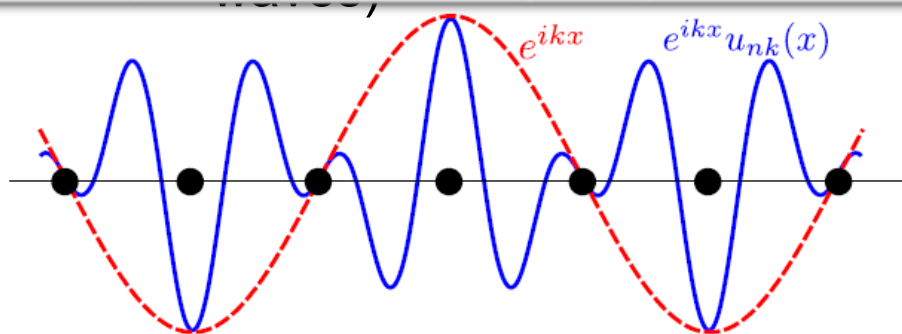
Luis A. Agapito,^{1,2,*} Andrea Ferretti,³ Arrigo Calzolari,^{1,3} Stefano Curtarolo,^{2,4} and Marco Buongiorno Nardelli^{1,2,†}

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The PAOFLOW method

Pseudo-atomic orbitals (PAO)

Readily available from pseudo-potentials: $\phi_{a\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \phi_a(\vec{r} - \vec{R})$

Connection to Bloch states (i.e Kohn-Sham states from DFT) via a simple projection
-- typically done to obtain Projected Density of States (PDOS):

$$\psi_{n\vec{k}}(\vec{r}) = \sum_a A_{an} \bar{k} \phi_{n\vec{k}}(\vec{r})$$

$$DOS = n(\epsilon) = \sum_n \delta(\epsilon - \epsilon_n)$$

$$\sum_n \langle \psi_n | \psi_n \rangle \delta(\epsilon - \epsilon_n) =$$

$$\sum_n \langle \psi_n | \left(\sum_a |\phi_a\rangle \langle \phi_a| \right) | \psi_n \rangle \delta(\epsilon - \epsilon_n) =$$

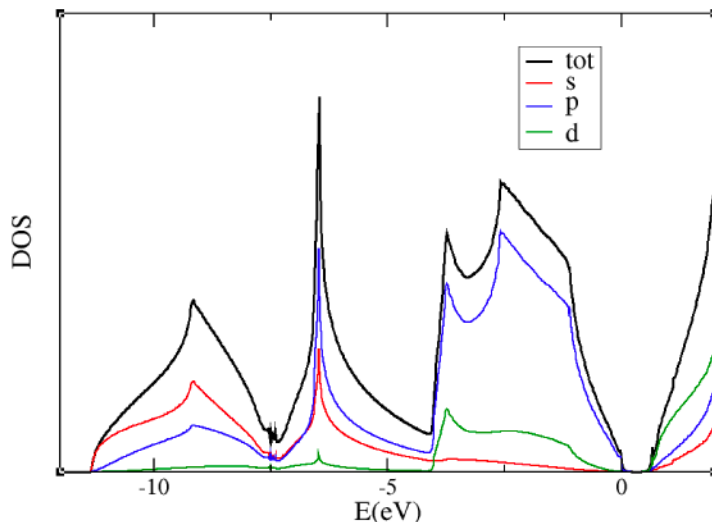
$$\sum_n \sum_a \langle \psi_n | \phi_a \rangle \langle \phi_a | \psi_n \rangle \delta(\epsilon - \epsilon_n) =$$

$$\sum_n \sum_a A_{an}^* A_{an} \delta(\epsilon - \epsilon_n) = \sum_i n_i(\epsilon)$$

$$PDOS = \sum_i n_i(\epsilon) = \sum_n A_{an}^* A_{an} \delta(\epsilon - \epsilon_n)$$

We assume the basis is orthonormal

Silicon



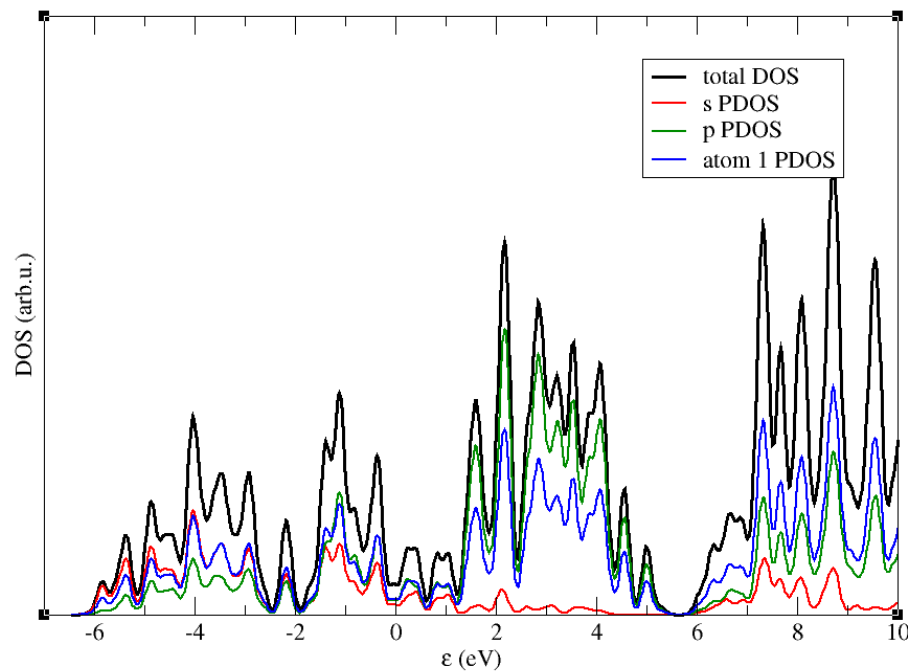
QE post processing

Projected Density of States (PDOS)

1. Run a non self-consistent calculation as for the DOS case
2. Run code `projwfc.x`, using input file `proj.in`
\$ `projwfc.x` < `proj.in` , where
 - gaussian broadening `degauss` is used (tetrahedra not yet implemented)
 - `prefix` and `outdir` are the same of the previous non-scf step
 - the prefix to all output files in in variable `filpdos`

Hands-on: Silicon – PDOS

1. `pw.x < scf_Si.in > scf_Si.out`
2. `projwfc.x < proj.in > proj.out`
3. `sumpdos *(x\)* > X.dat` (for the x orbitals) or
`sumpdos silicon.pdos_atm#X1\(* > atomX.dat` (for the X atom)



Hands-on: Silicon – PDOS

Atomic states used for projection
(read from pseudopotential files):

```
state # 1: atom 1 (Si ), wfc 1 (l=0 m= 1)
state # 2: atom 1 (Si ), wfc 2 (l=1 m= 1)
state # 3: atom 1 (Si ), wfc 2 (l=1 m= 2)
state # 4: atom 1 (Si ), wfc 2 (l=1 m= 3)
state # 5: atom 1 (Si ), wfc 3 (l=2 m= 1)
state # 6: atom 1 (Si ), wfc 3 (l=2 m= 2)
state # 7: atom 1 (Si ), wfc 3 (l=2 m= 3)
state # 8: atom 1 (Si ), wfc 3 (l=2 m= 4)
state # 9: atom 1 (Si ), wfc 3 (l=2 m= 5)
state # 10: atom 1 (Si ), wfc 4 (l=3 m= 1)
state # 11: atom 1 (Si ), wfc 4 (l=3 m= 2)
state # 12: atom 1 (Si ), wfc 4 (l=3 m= 3)
state # 13: atom 1 (Si ), wfc 4 (l=3 m= 4)
state # 14: atom 1 (Si ), wfc 4 (l=3 m= 5)
state # 15: atom 1 (Si ), wfc 4 (l=3 m= 6)
state # 16: atom 1 (Si ), wfc 4 (l=3 m= 7)
state # 17: atom 2 (Si ), wfc 1 (l=0 m= 1)
state # 18: atom 2 (Si ), wfc 2 (l=1 m= 1)
state # 19: atom 2 (Si ), wfc 2 (l=1 m= 2)
state # 20: atom 2 (Si ), wfc 2 (l=1 m= 3)
state # 21: atom 2 (Si ), wfc 3 (l=2 m= 1)
state # 22: atom 2 (Si ), wfc 3 (l=2 m= 2)
state # 23: atom 2 (Si ), wfc 3 (l=2 m= 3)
state # 24: atom 2 (Si ), wfc 3 (l=2 m= 4)
state # 25: atom 2 (Si ), wfc 3 (l=2 m= 5)
state # 26: atom 2 (Si ), wfc 4 (l=3 m= 1)
state # 27: atom 2 (Si ), wfc 4 (l=3 m= 2)
state # 28: atom 2 (Si ), wfc 4 (l=3 m= 3)
state # 29: atom 2 (Si ), wfc 4 (l=3 m= 4)
state # 30: atom 2 (Si ), wfc 4 (l=3 m= 5)
state # 31: atom 2 (Si ), wfc 4 (l=3 m= 6)
state # 32: atom 2 (Si ), wfc 4 (l=3 m= 7)
```

Our basis or localized orbitals

Hands-on: Silicon – PDOS

$$\rho(\mathbf{r}) = \sum_n |\psi|^2 = \sum_n \left(\sum_a A_{an}^* \phi_a^* \right) \left(\sum_b A_{bn} \phi_b \right) = \sum_{ab} P_{ab} \phi_a^* \phi_b$$

$$P_{ab} = \sum_n A_{an}^* A_{bn} \equiv \text{density matrix}$$

$$\text{charge of A} = \sum_{a \in A} P_{aa}$$

Lowdin Charges:

Atom # 1: total charge = 3.9897, s = 0.9061,

Atom # 1: total charge = 3.9897, p = 2.3837, pz = 0.7946, px = 0.7946, py = 0.7946,

Atom # 1: total charge = 3.9897, d = 0.6981, dz2 = 0.0861, dxz = 0.1753, dyz = 0.1753, dx2-y2 = 0.0861, dxy = 0.1753,

Atom # 1: total charge = 3.9897, f = 0.0018, fz3 = 0.0003, fxz2 = 0.0002, fyz2 = 0.0002, fzx2-zy2 = 0.0002, fxyz = 0.0003, fx3-3xy2 = 0.0003, f3yx2-y3 = 0.0003,

Atom # 2: total charge = 3.9897, s = 0.9061,

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Spilling Parameter: 0.0026

Pseudo-atomic orbitals (PAO)

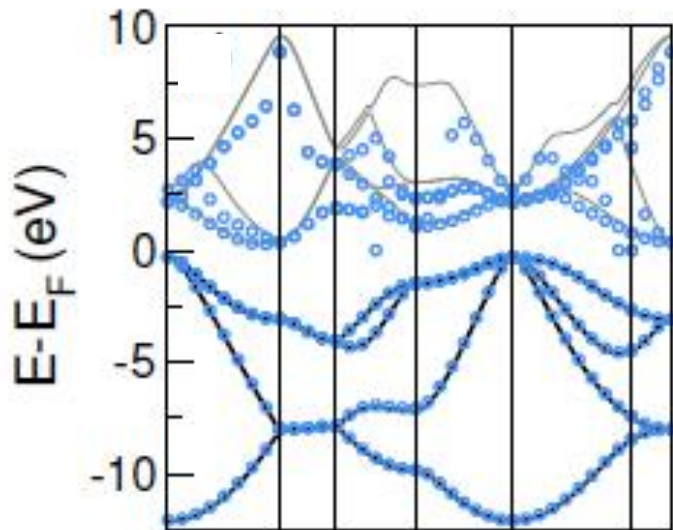
Readily available from pseudo-potentials: $\phi_{a\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \phi_a(\vec{r} - \vec{R})$

Connection to Bloch states (i.e Kohn-Sham states from DFT) via a simple projection
-- typically done to obtain Projected Density of States (PDOS):

$$\psi_{n\vec{k}}(\vec{r}) = \sum_a A_{an}^{\vec{k}} \phi_{n\vec{k}}(\vec{r}) \longrightarrow \mathbf{H}^{\vec{k}} = \mathbf{A}^{\vec{k}} \mathbf{E}^{\vec{k}} \mathbf{A}^{\vec{k}\dagger}$$

\downarrow
 LCAO
 Hamiltonian

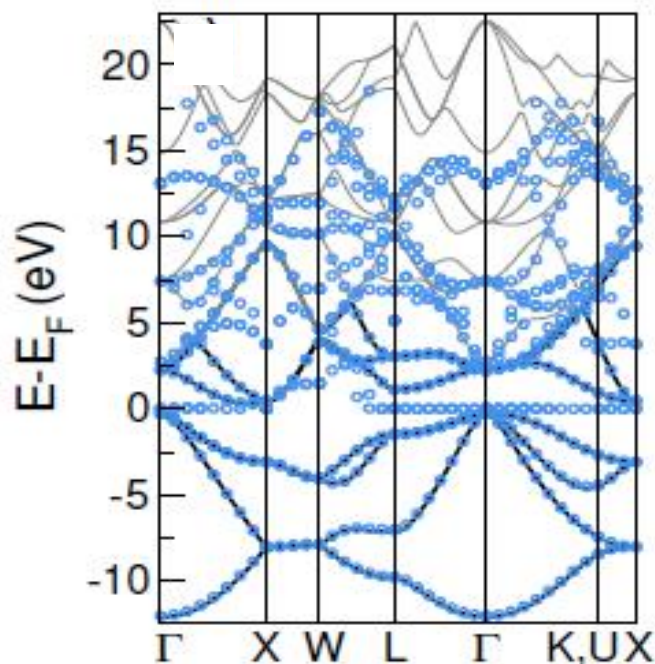
\downarrow
 KS
 eigenvalues



Si ($2s^2 2p^2$ basis set): 8 atomic orbitals
Valence bands reproduced to high accuracy
Conduction bands deviate strongly from KS eigenvalues.

L. A. Agapito et. al. Phys. Rev. B 88, 165127 (2013)

Projectability of bands



LCAO band structure with *spd* basis set.
Some low energy conduction bands improve.

A set of null eigenvalues are inserted

Projectability:

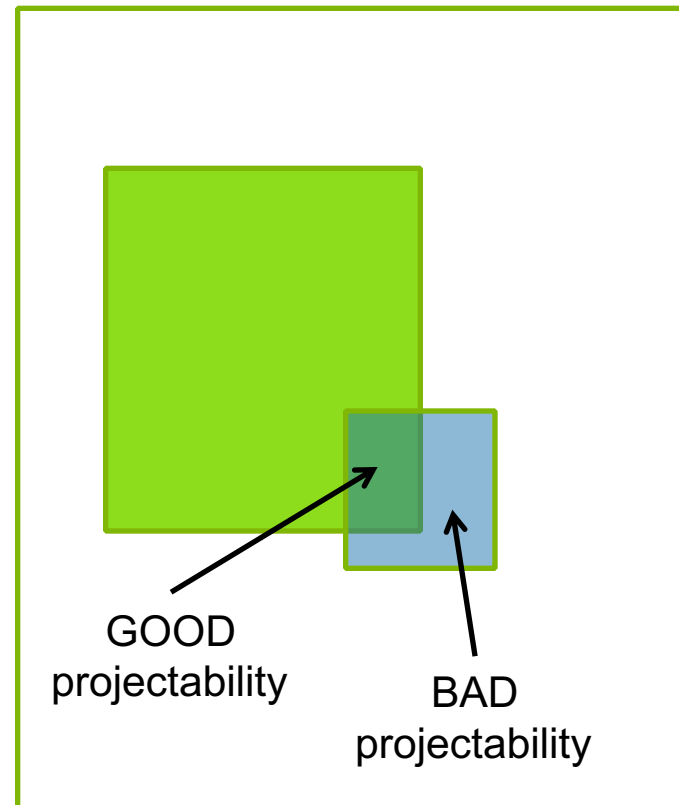
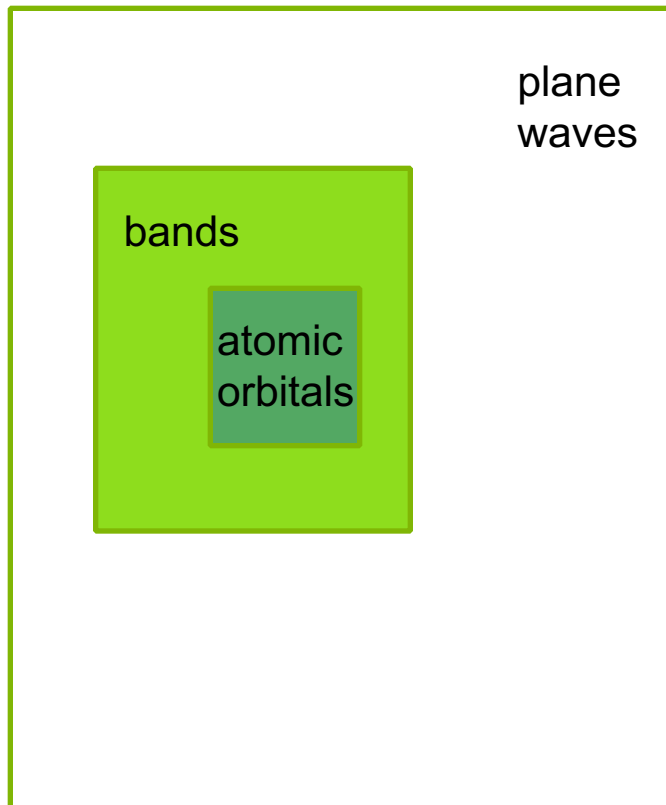
$$\mathcal{P}_n = \min\{\sum_u a_{un}^{k*} a_{un}^k, \forall \mathbf{k} \in \text{BZ}\}$$

High projectability bands (i.e. $\mathcal{P}_n \approx 1$)
yield accurate LCAO band structure.

Low projectability bands (i.e. $\mathcal{P}_n \ll 1$)
yield poor LCAO bands and lead to
null eigenstates.

n	Si Ω_1		Si Ω_2	
	\mathcal{P}_n	rms	\mathcal{P}_n	rms
1	0.9927	0.0478	0.9953	0.0792
2	0.9622	0.0572	0.9933	0.0555
3	0.9622	0.0252	0.9952	0.0382
4	0.9622	0.0203	0.9967	0.0266
5	0.4755	1.9200	0.9934	0.0267
6	0.0660		0.9771	0.0316
7	0.0941		0.9728	0.0380
8	0.0652		0.8464	0.1382

Accurate PAO Hamiltonians



Accurate tight-binding Hamiltonian matrices from *ab initio* calculations: Minimal basis sets

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$$\bar{H} = AEA^\dagger$$

Exclude the bad projectability states from the set of bands to be represented (**filtering**) – orthogonal projection

$$Q_N = I_M - A(A^\dagger A)^{-1}A^\dagger$$

Introduces a spurious null space that must be eliminated

Shift by a fixed energy outside of the region of good projectability bands (**shifting**)

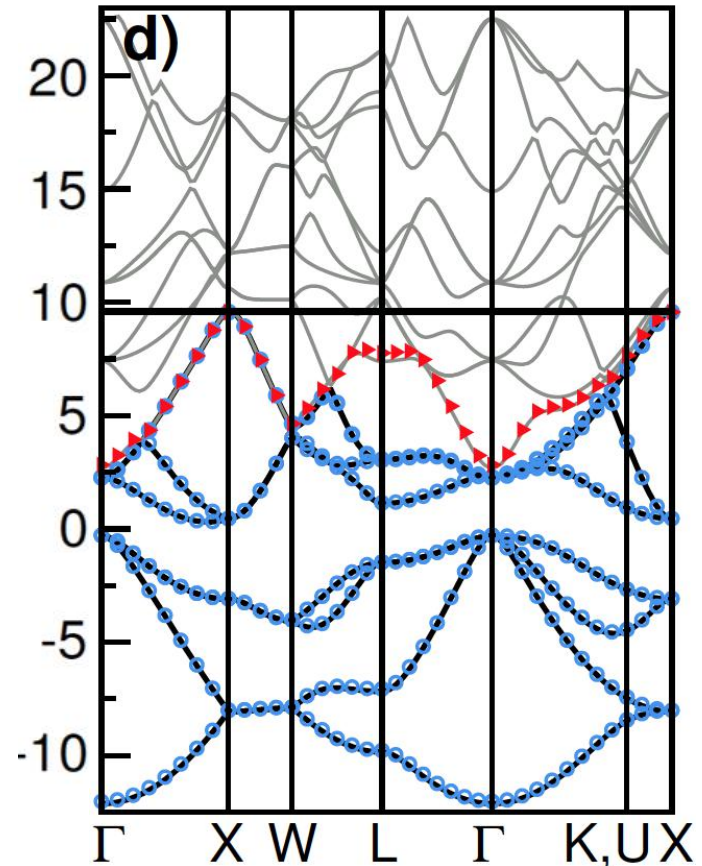
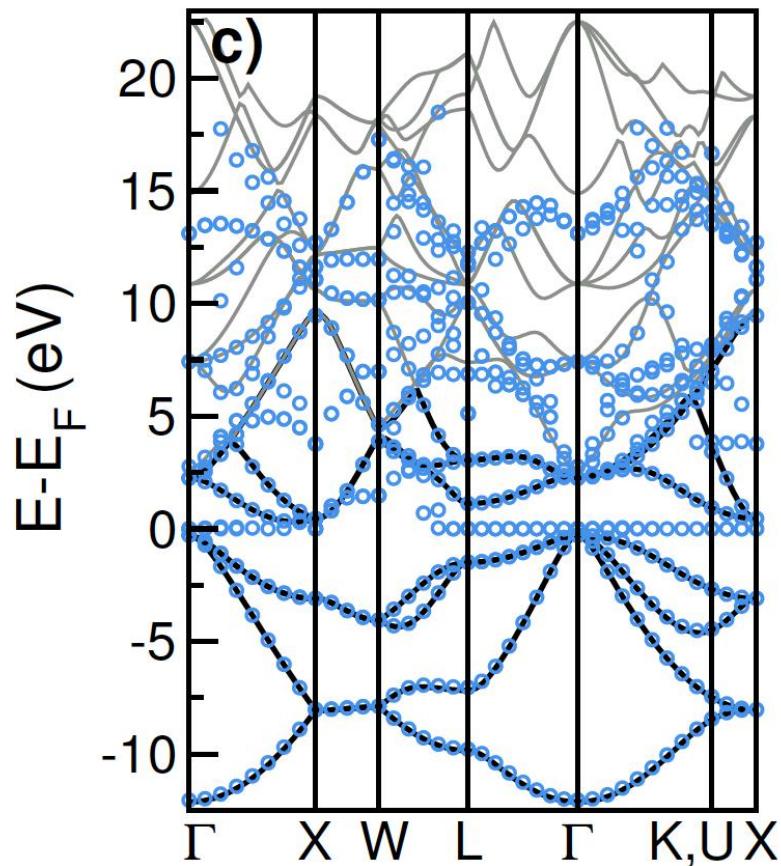
$$\bar{H}_\kappa = \bar{H} + \kappa Q_N$$

Accurate PAO Hamiltonians

$$\bar{H} = AEA^\dagger$$

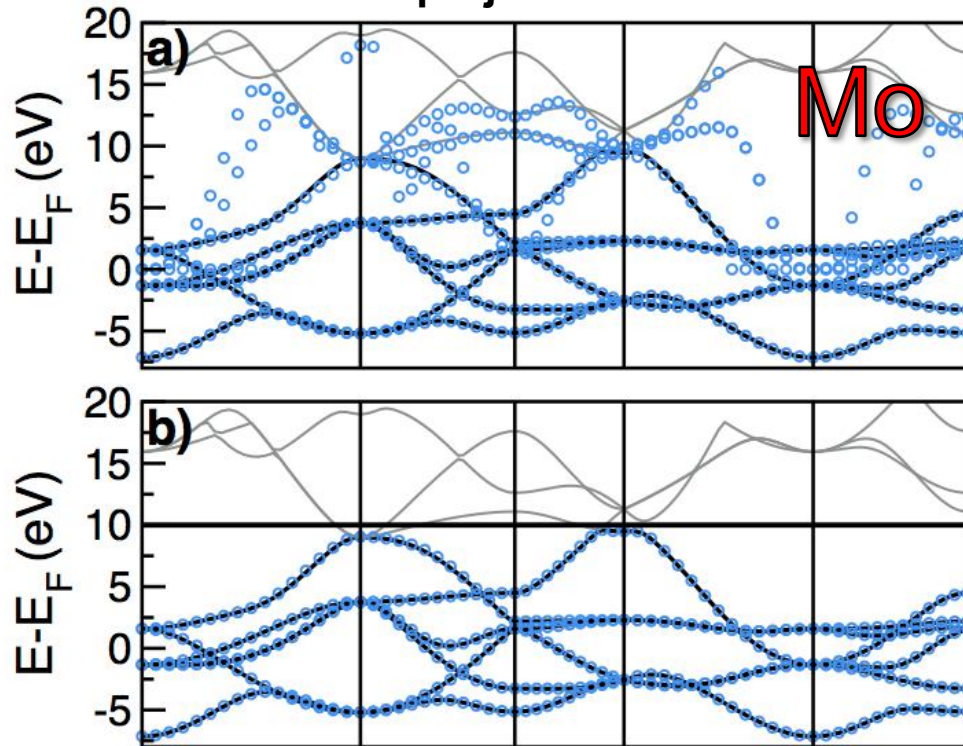


$$\bar{H}_\kappa = \bar{H} + \kappa Q_N$$

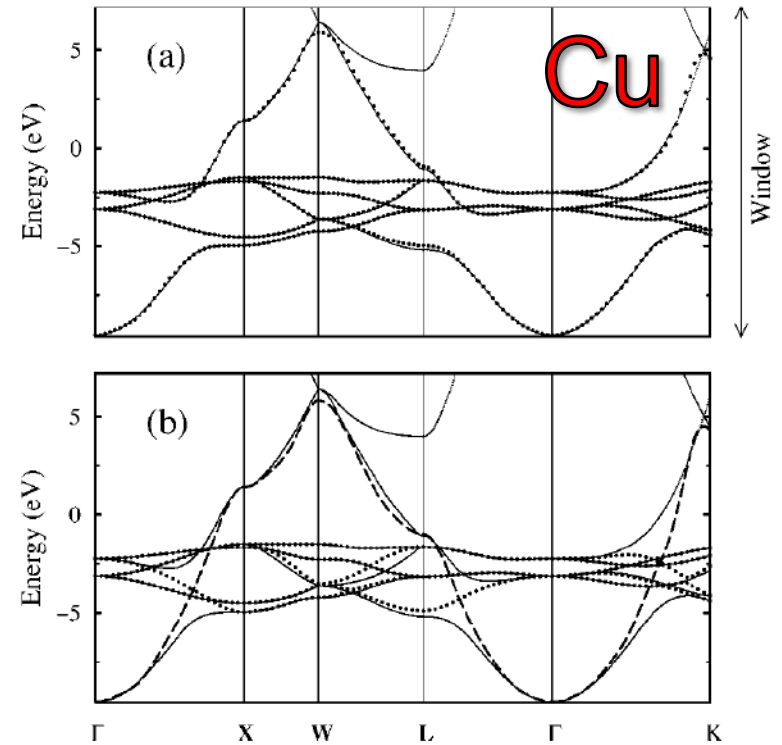


Accurate PAO Hamiltonians

projections



Wannier functions



Effective description of entangled bands in metals

PAOFLOW

1. Go to the Example1 directory on the tutorial repository
2. Run scf.in and nscf.in
3. Go to the jupyter notebook!



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Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci



PAOFLOW: A utility to construct and operate on *ab initio* Hamiltonians from the projections of electronic wavefunctions on atomic orbital bases, including characterization of topological materials



Marco Buongiorno Nardelli ^{a,e,*}, Frank T. Cerasoli ^a, Marcio Costa ^f, Stefano Curtarolo ^{b,e,h}, Riccardo De Gennaro ^g, Marco Fornari ^{c,d,e}, Laalitha Liyanage ^a, Andrew R. Supka ^{c,d}, Haihang Wang ^a

Computational Materials Science 200 (2021) 110828



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Advanced modeling of materials with PAOFLOW 2.0: New features and software design



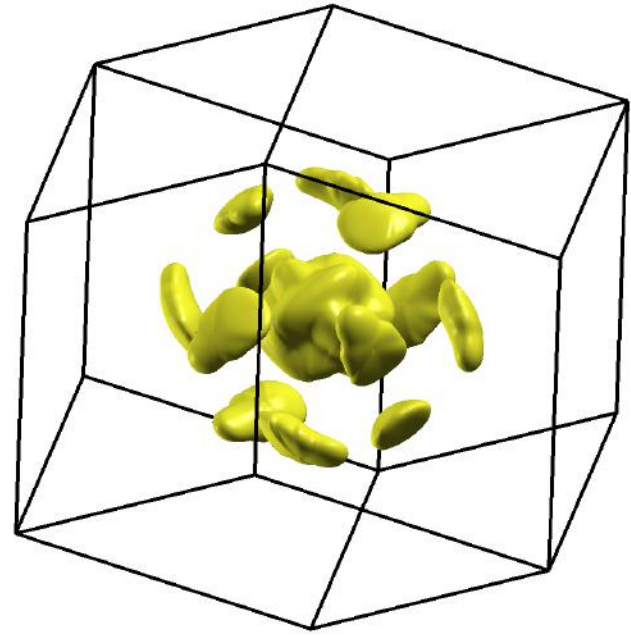
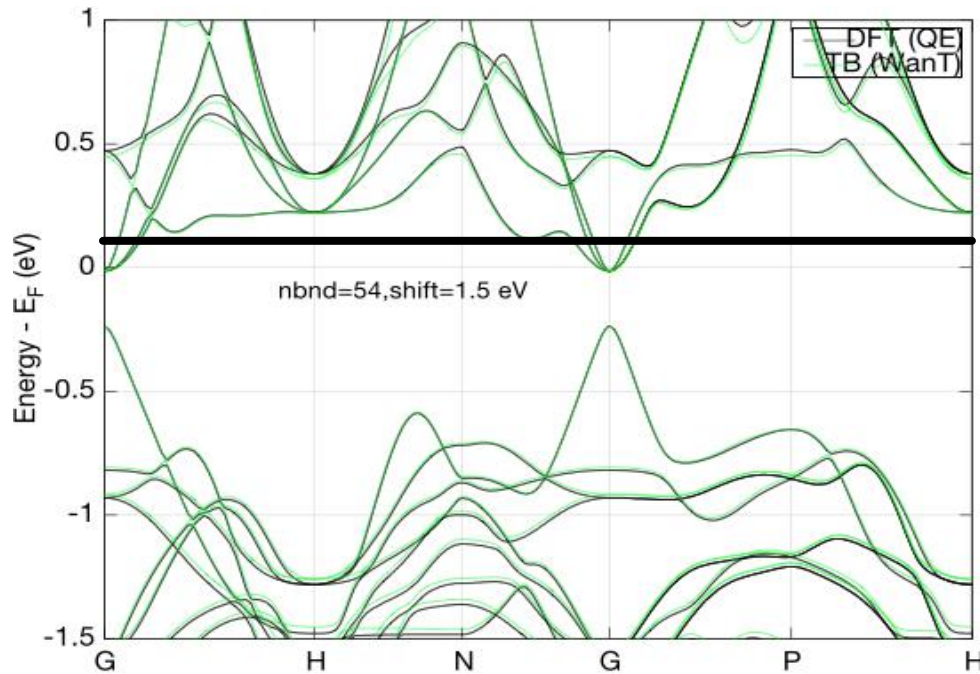
Frank T. Cerasoli ^a, Andrew R. Supka ^{b,c}, Anooja Jayaraj ^a, Marcio Costa ^d, Ilaria Siloi ^e, Jagoda Sławińska ^f, Stefano Curtarolo ^g, Marco Fornari ^{b,c,g}, Davide Ceresoli ^h, Marco Buongiorno Nardelli ^{a,g,*}

PAOFLOW capabilities

- Construction of PAO Hamiltonians from the DFT wavefunctions onto pseudo atomic orbitals
- Construction of PAO Hamiltonians from analytical tight binding models
- Hamiltonian data for further processing (ACBN0, PAOtransport, etc.)
- External fields and non scf ACBN0 correction
- Spin orbit correction of non SO calculations
- Bands along standard paths in the BZ
- Real space electronic charge density
- Interpolation of Hamiltonians on arbitrary Monkhorst and Pack k-meshes
- Adaptive smearing for BZ and Fermi surface integration
- Density of states (and projected DOS)
- Fermi surfaces and spin textures
- Boltzmann transport (conductivity, Seebeck coefficient, electronic contribution to thermal conductivity)
- dielectric function (absorption coefficients and EELS)
- Berry curvature and anomalous Hall conductivity (including magnetic circular dichroism spectra)
- spin Berry curvature and spin Hall conductivity (including spin circular dichroism spectra)
- Band topology (Z_2 invariants, Berry and spin Berry curvature along standard paths in BZ, critical points)

K-point interpolation

$$H_{ab}(\vec{R}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}} H_{ab}^{\vec{k}} \longrightarrow H_{ab}^{\vec{K}} = \sum_{\vec{R}} e^{i\vec{K}\cdot\vec{R}} H_{ab}(\vec{R})$$



nature
materials

ARTICLES

PUBLISHED ONLINE: 5 OCTOBER 2015 | DOI: 10.1038/NMAT4430

Convergence of multi-valley bands as the electronic origin of high thermoelectric performance in CoSb_3 skutterudites, Y. Tang, Z.M. Gibbs, L.A. Agapito, G. Li, H. Kim, M. Buongiorno Nardelli, S. Curtarolo and G.J. Snyder

Transport properties

The standard approaches to electron transport in bulk semiconductors are based on the **semiclassical Boltzmann theory**.

Dynamics of carriers and response to external fields follow **classical motion equation**, whereas scattering events are included in a perturbative approach, via quantum mechanical **Fermi Golden Rule**.

Semiclassical transport

- probability density distribution function: $f(\mathbf{r}, \mathbf{p}, t)$
- equation of motion: $\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{p}} \cdot \mathbf{F} + \frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} = \left(\frac{\partial f}{\partial t} \right)_{coll}$
- relaxation-time approximation: $\left(\frac{\partial f}{\partial t} \right)_{coll} \approx -\frac{f - f_{eq}}{\tau_{relax}}$
- Fermi Golden Rule: $\frac{1}{\tau_{relax}(\epsilon)} = \frac{n_{imp}}{\hbar} \int d\mathbf{p}' |V_{\mathbf{p}\mathbf{p}'}|^2 (1 - \cos\theta) \delta(\epsilon - \epsilon_{\mathbf{p}})$
- Boltzman conductivity: $\sigma = \frac{Ne^2 \tau_{relax}}{m^*}$

Boltzmann Transport Equations

Accurate evaluation of Boltzmann transport integrals:

$$I^{\alpha}_{ij} = \frac{1}{V} \sum_{n, \vec{k}} (\epsilon_{n \vec{k}} - \mu)^{\alpha} v_i(n, \vec{k}) v_j(n, \vec{k}) \tau_{n \vec{k}} \left(- \frac{\partial f(\mu, T)}{\partial \epsilon_{n \vec{k}}} \right)$$

Band
velocities:

$$v_i(n, \vec{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_{n \vec{k}}}{\partial k_i}$$

Scattering
time:

$$\tau_{n \vec{k}}$$

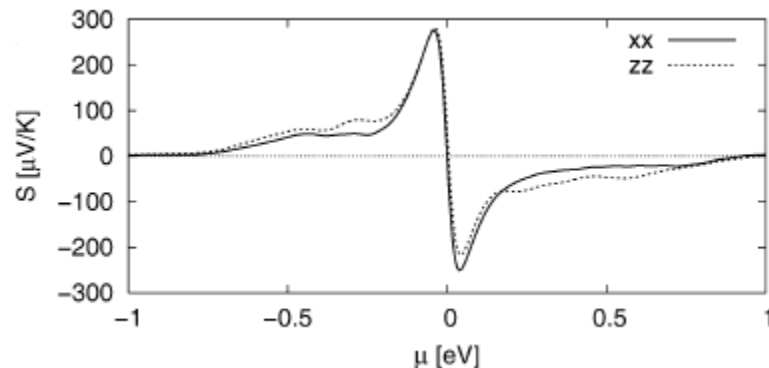
Fermi-Dirac
distribution:

$$f(\mu, T)$$

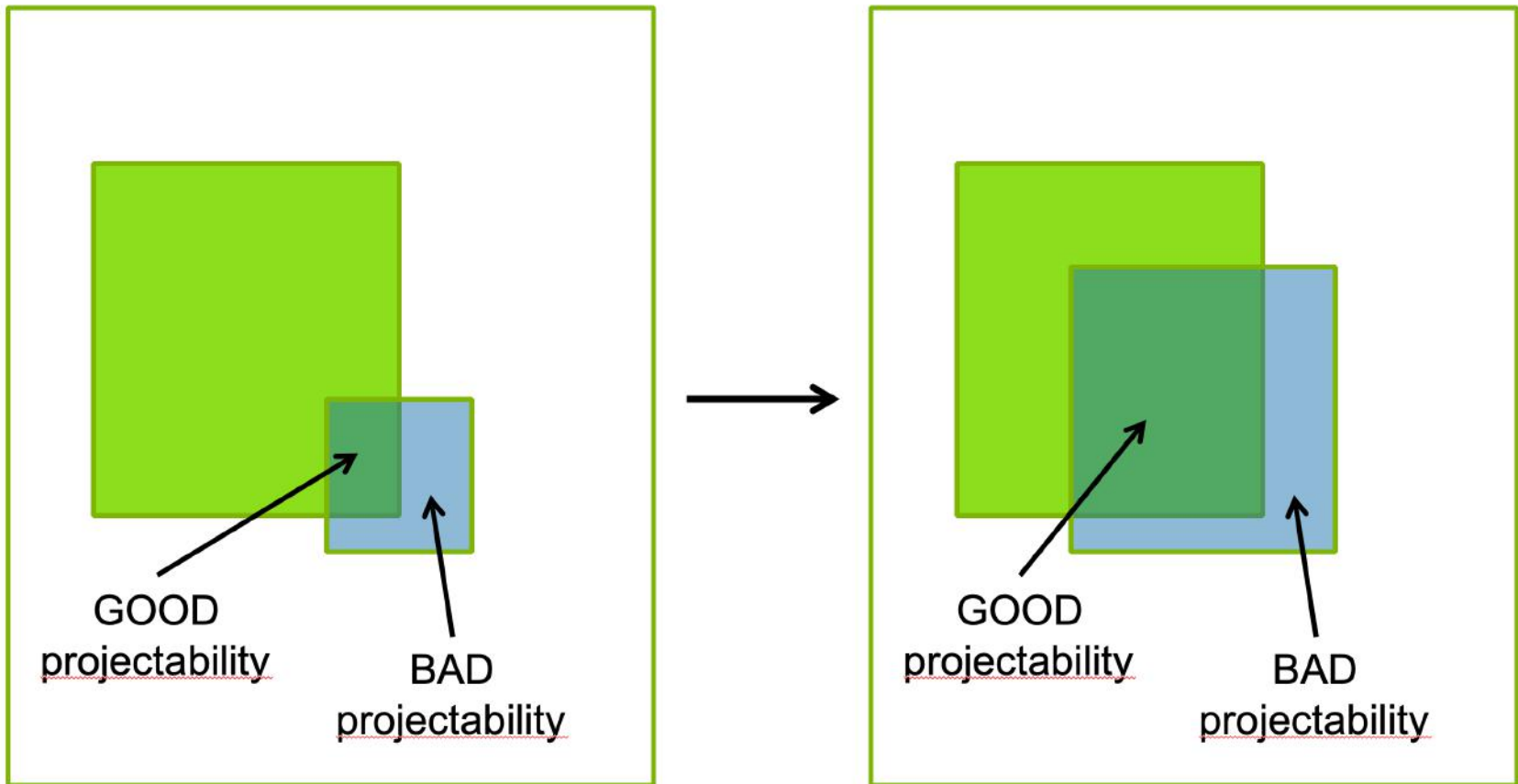
Requires very fine sampling of bands around Fermi energy –
projection Hamiltonian!

e.g. Seebeck coefficient of
 Bi_2Te_3

$$S = -I_0^{-1} \cdot I_1$$



Increase the basis set

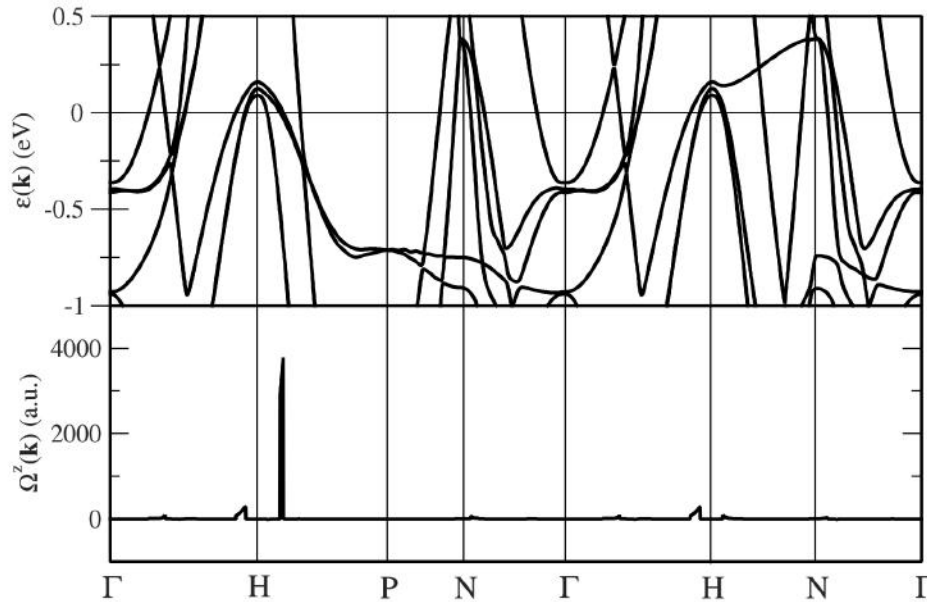


From SZ to DZ to DZP to TZP...etc.

PAOFLOW internal bases
(go to jupyter notebook)

Some more advanced applications
(go to jupyter notebook)

Berry curvature and Anomalous Hall conductivity: Fe



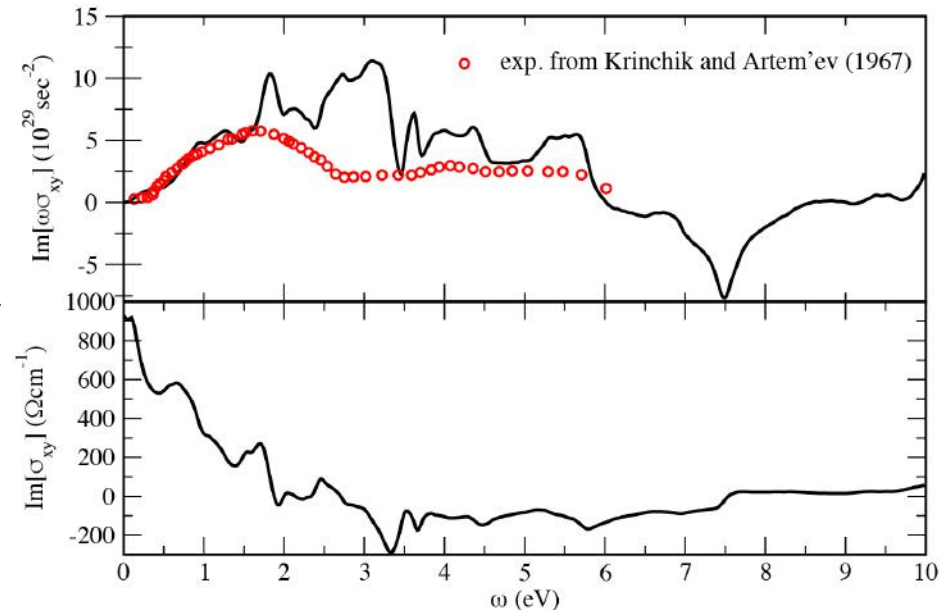
$$\Omega^z(\mathbf{k}) = \sum_n f_n \Omega_n^z(\mathbf{k})$$

Anomalous Hall conductivity:

$$\sigma_{xy} = -\frac{e^2}{\hbar} \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \Omega^z(\mathbf{k})$$

Berry curvature from Kubo formula:

$$\Omega_n^z(\mathbf{k}) = - \sum_{n' \neq n} \frac{2 \text{Im} \langle \psi_{n\mathbf{k}} | v_x | \psi_{n'\mathbf{k}} \rangle \langle \psi_{n'\mathbf{k}} | v_y | \psi_{n\mathbf{k}} \rangle}{(\omega_{n'} - \omega_n)^2}$$



$$\sigma(\omega)_{xy} = \frac{e^2}{\hbar} \int_{V_G} \frac{d^3k}{(2\pi)^3} \sum_{n \neq n'} (f_{n,\mathbf{k}} - f_{n',\mathbf{k}}) \times \frac{\text{Im} \langle \psi_{n\mathbf{k}} | v_x | \psi_{n'\mathbf{k}} \rangle \langle \psi_{n'\mathbf{k}} | v_y | \psi_{n\mathbf{k}} \rangle}{(\omega_{n'} - \omega_n)^2 - (\omega + i\delta)^2}$$

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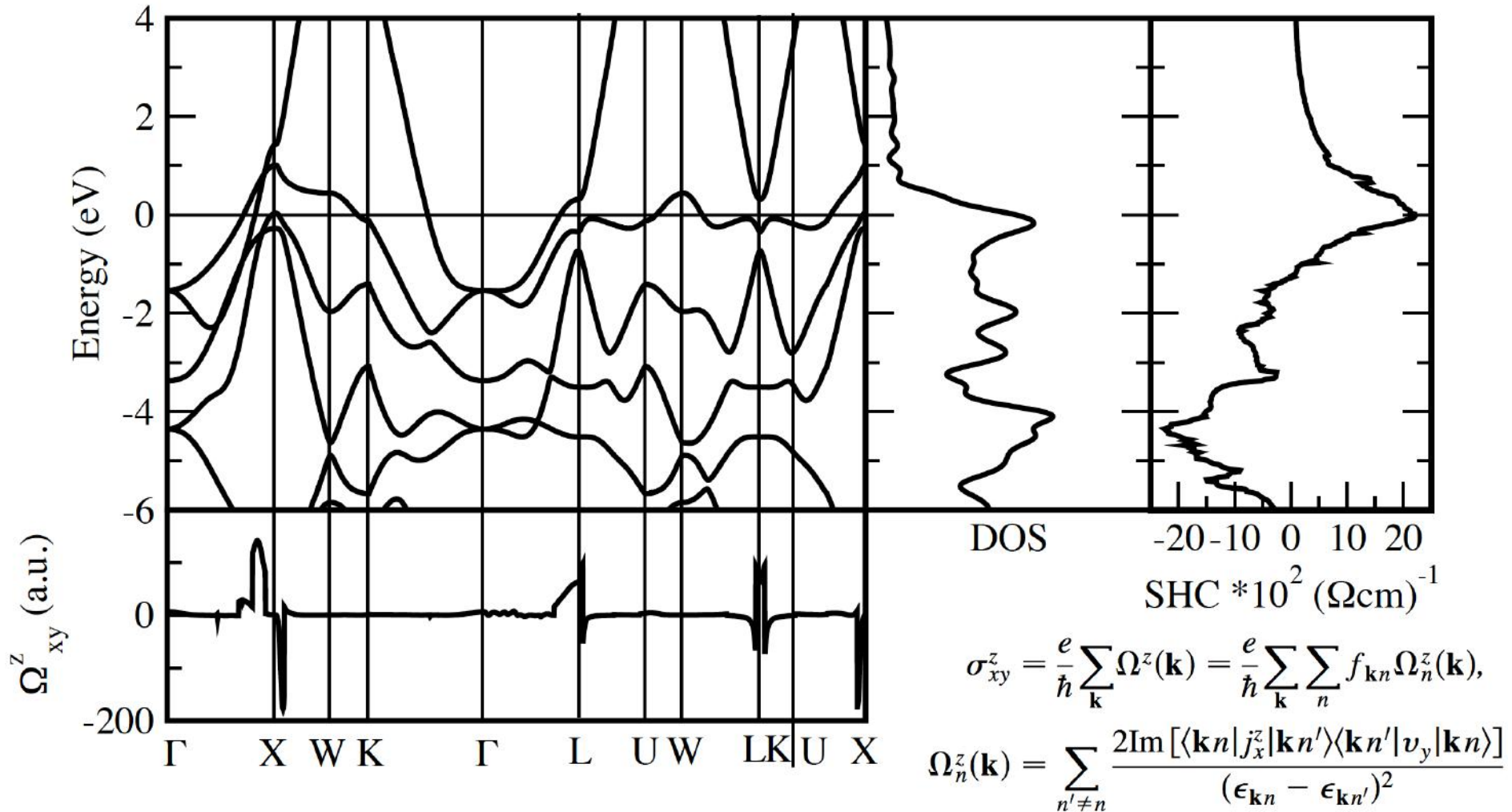
PHYSICAL REVIEW LETTERS

week ending
23 JANUARY 2004

First Principles Calculation of Anomalous Hall Conductivity in Ferromagnetic bcc Fe

Yugui Yao,^{1,2,3} Leonard Kleinman,¹ A. H. MacDonald,¹ Jairo Sinova,^{4,1} T. Jungwirth,^{5,1} Ding-sheng Wang,³ Enge Wang,^{2,3} and Qian Niu¹

Spin Hall conductivity



PRL 100, 096401 (2008)

PHYSICAL REVIEW LETTERS

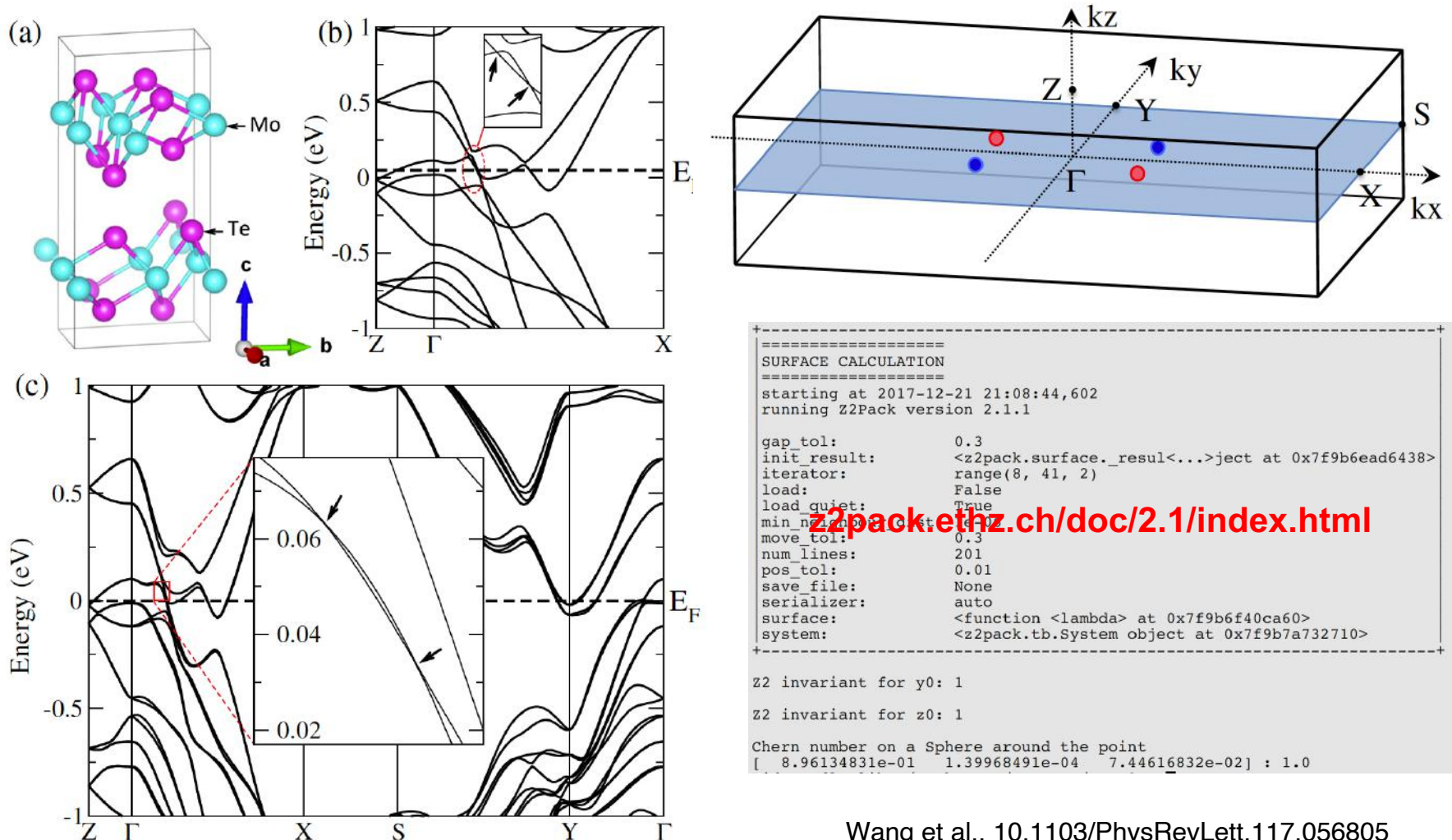
week ending
7 MARCH 2008

Intrinsic Spin Hall Effect in Platinum: First-Principles Calculations

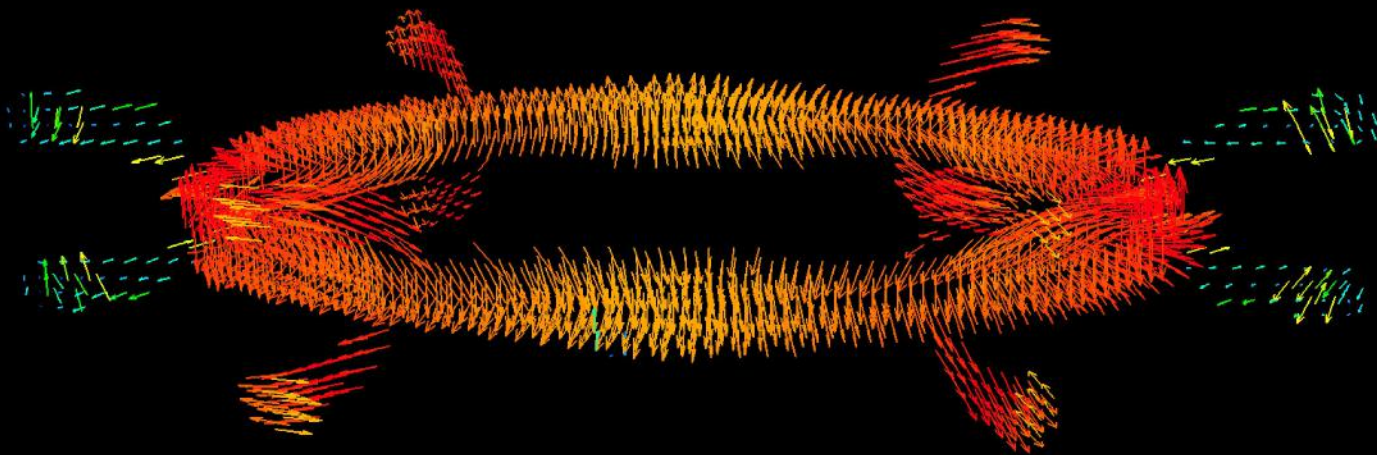
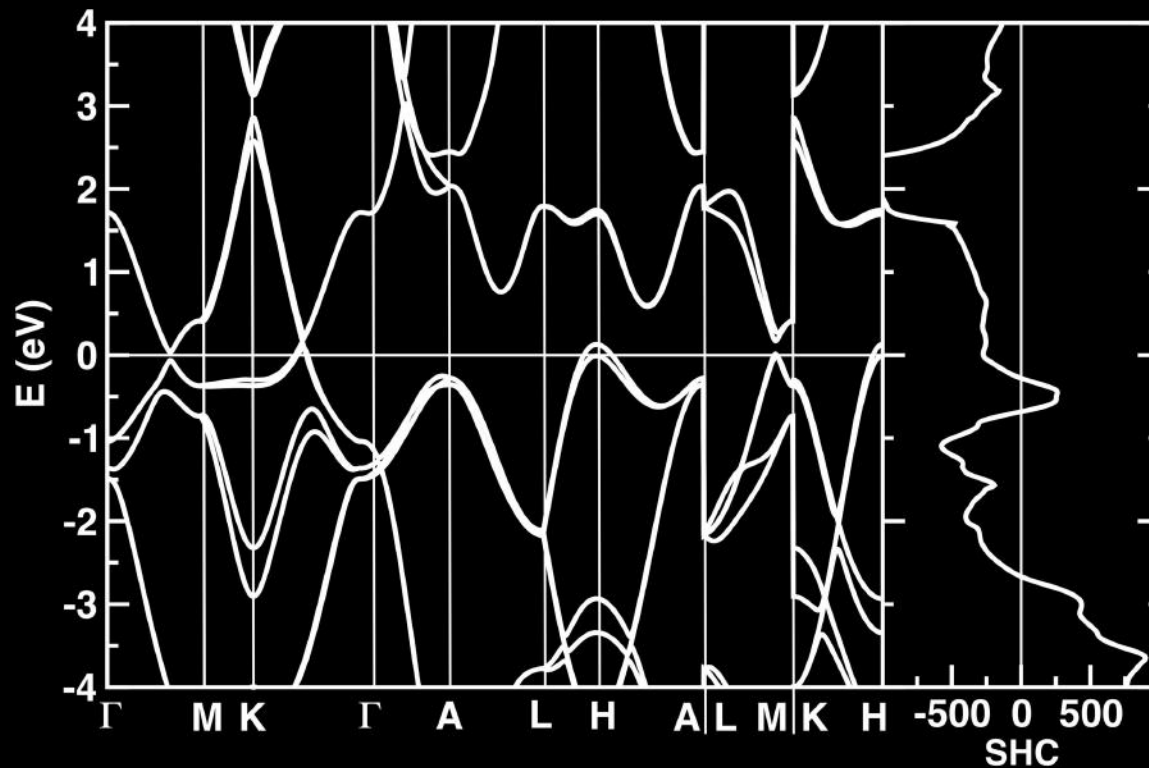
G. Y. Guo,^{1,*} S. Murakami,² T.-W. Chen,¹ and N. Nagaosa^{3,4}

Topological invariants

MoTe₂: A Type-II Weyl Topological Metal



Wang et al., 10.1103/PhysRevLett.117.056805



Nodal chain and Weyl points in HfC

PAOFLOW Examples

example01 : Si with spd pseudopotential

example02 : Al with spd pseudopotential

example03 : Pt with lsda (nspin = 2)

example04 : Fe non collinear with spin orbit - Anomalous Hall conductivity

example05 : Pt non collinear with spin orbit - Spin Hall conductivity

example06 : AIP with non self consistent ACBN0

example07 : Al starting from projections with overlap matrix of the atomic orbital
(prior to orthogonalization)

example08 : 2D SnTe - Spin Hall conductivity

example09 : Weyl point search in MoP2

example10 : Transport in GaAs with temperature and energy dependent model for
relaxation time