Wannier Functions

Lecture II

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ICTS School, Bangalore, January 7 2014

Acknowledgments

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Arash Mostofi - Imperial College
Jonathan Yates - University of Oxford
Ivo Souza - San Sebastian
Givoanni Pizzi - EPFL

Maximally localized Wannier functions: Theory and applications
Nicola Marzari, Arash A. Mostofi, Jonathan R. Yates, Ivo Souza, David Vanderbilt
Rev. Mod. Phys. 84, 1419-1475 (2012)

www.wannier.org

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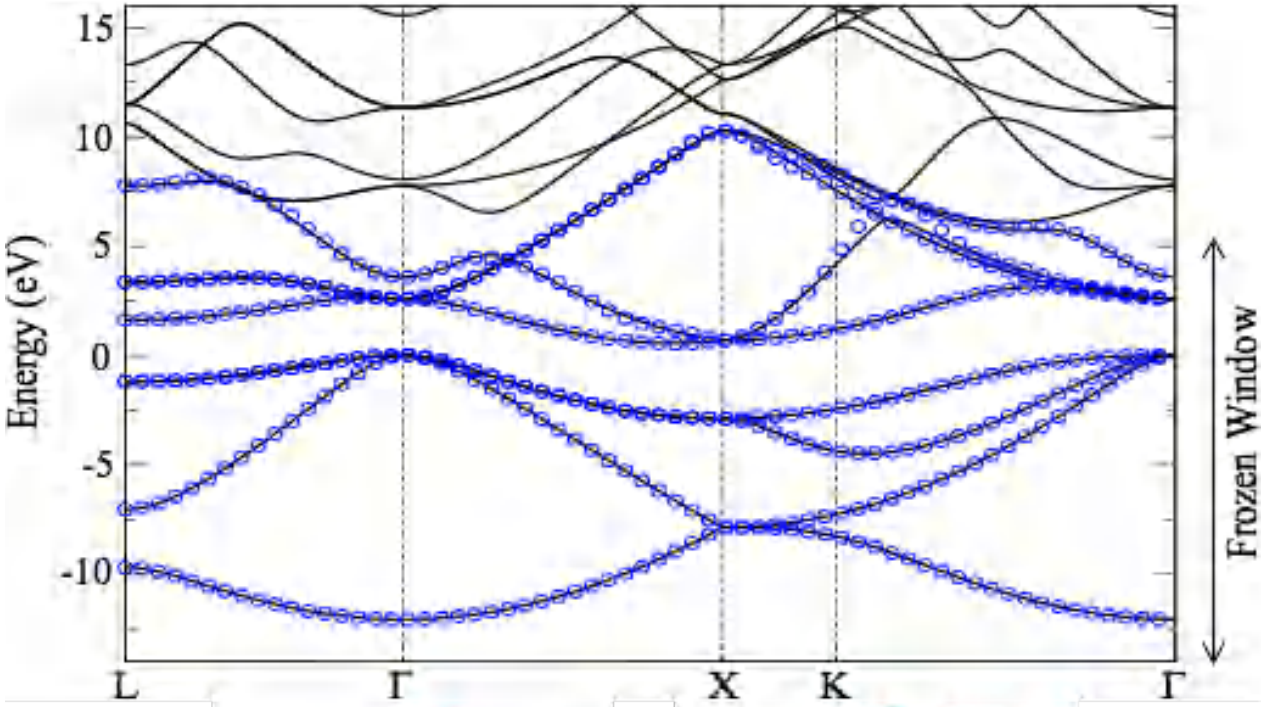
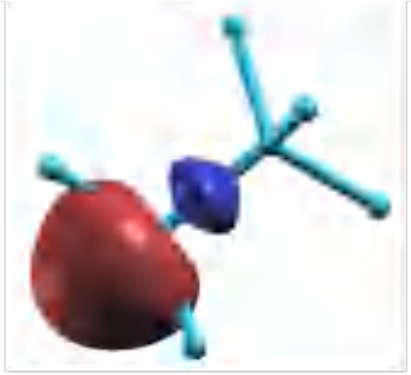
Outline

- Wannier interpolation
- Electric polarization and anomalous Hall
- Chemical bonding and polar properties
  - Covalent semiconductors and polymers
  - Perovskites
  - Liquid water
- Hybrid Wannier functions and centers (?)
- Summary and Conclusions

Silicon - conduction & valence states



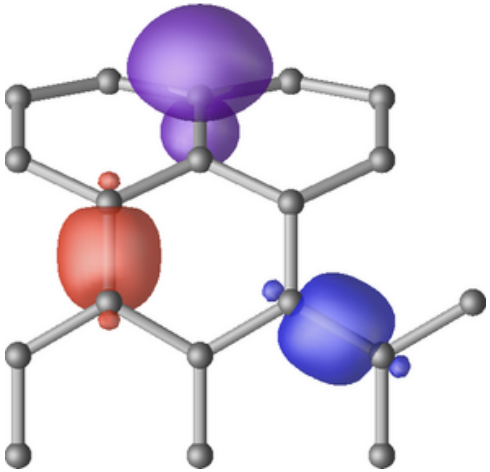


Max-loc WFs ↔ "Exact" Tight-Binding

Compact mapping of Bloch states into local orbitals

$$\omega_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})d\mathbf{k}$$

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N_R}}\sum_R e^{i\mathbf{k}\cdot\mathbf{R}}\,\omega_n(\mathbf{r}-\mathbf{R})$$



Multiband case:

$$w_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}}\sum_m U_{mn}^{(\mathbf{k})}\psi_{m\mathbf{k}}(\mathbf{r})\,d\mathbf{k}$$

Wannier interpolation

Multiple bands:

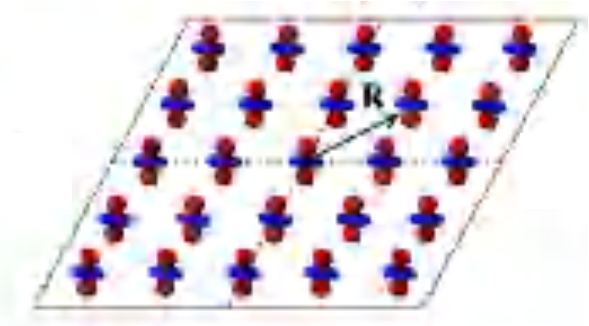
$$w_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}} \underbrace{\sum_m U^{(\mathbf{k})}_{mn}\,\psi_{m\mathbf{k}}(\mathbf{r})}_{\tilde{\psi}_{n\mathbf{k}}(\mathbf{r})}\, d\mathbf{k}$$

Change of notation:

$$w_n(\mathbf{r}-\mathbf{R}) \longrightarrow |\mathbf{R}n\rangle$$

"Exact TB" Hamiltonian in real space:

$$H_{\mathbf{0}n,\mathbf{R}m} = \langle \mathbf{0}n|H|\mathbf{R}m\rangle$$



Wannier interpolation

Corresponding k-space Hamiltonian:

$$H_{nm}(\mathbf{k}) = \langle \tilde{\psi}_{n\mathbf{k}} | H | \tilde{\psi}_{m\mathbf{k}} \rangle$$

$$= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \, H_{\mathbf{0}n,\mathbf{R}m}$$

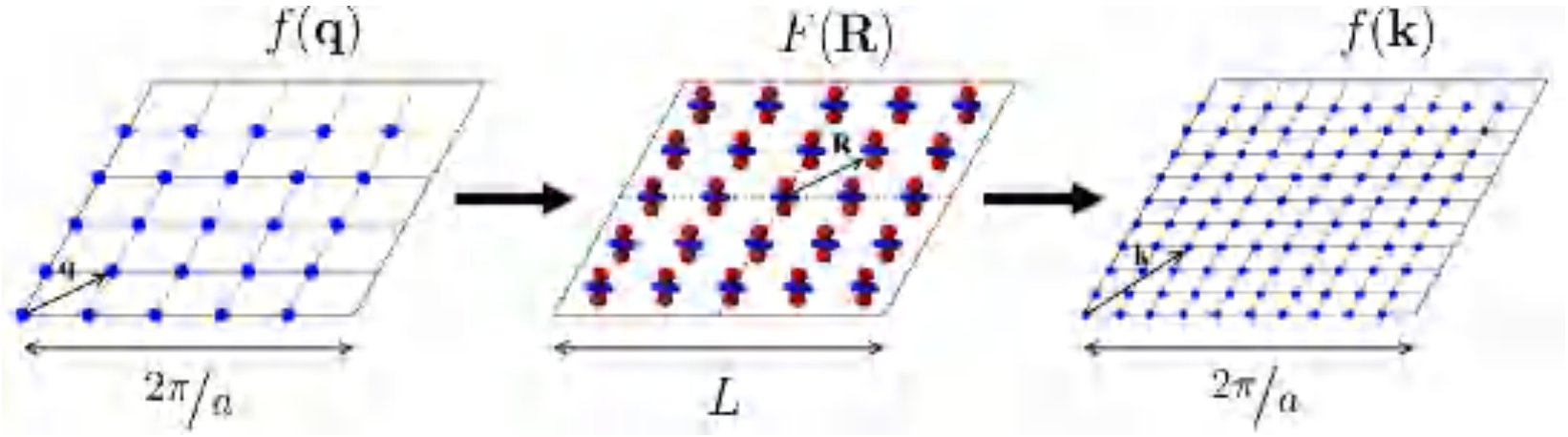
$$= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \, \langle \mathbf{0}n | H | \mathbf{R}m \rangle$$

Diagonalize & recover

$E_n(\mathbf{k})$, $U_{mn}(\mathbf{k})$

Gone in circles?
Not quite...

Wannier interpolation



DFT calc. on coarse grid

Construct WFs

Cheap calc. on fine grid

Wannier interpolation

Corresponding k-space Hamiltonian:

$$H_{nm}(\mathbf{k}) = \langle \tilde{\psi}_{n\mathbf{k}} | H | \tilde{\psi}_{m\mathbf{k}} \rangle$$

$$= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \, H_{\mathbf{0}n,\mathbf{R}m}$$

$$= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \, \langle \mathbf{0}n | H | \mathbf{R}m \rangle$$

Diagonalize & recover

$$E_n(\mathbf{k}) \ , \ U_{mn}(\mathbf{k})$$

DO THIS ON MUCH FINER GRID !

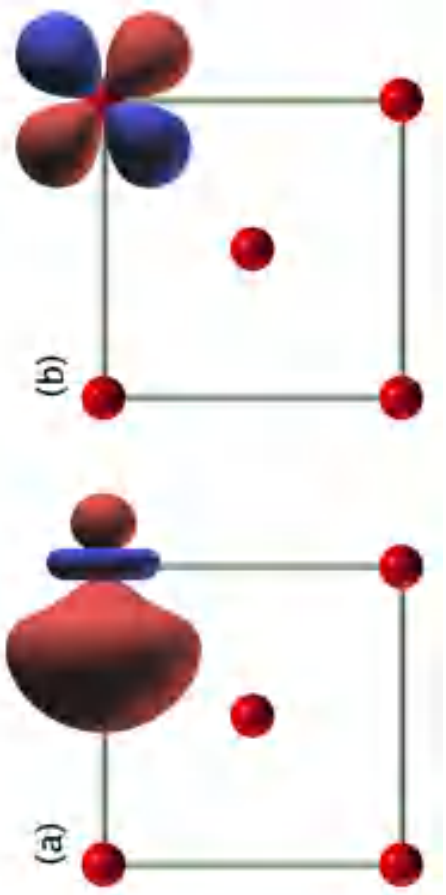
Wannier interpolation of other operators

$$\mathcal{O}_{nm}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \mathbf{0}n|\hat{\mathcal{O}}|\mathbf{R}m\rangle$$

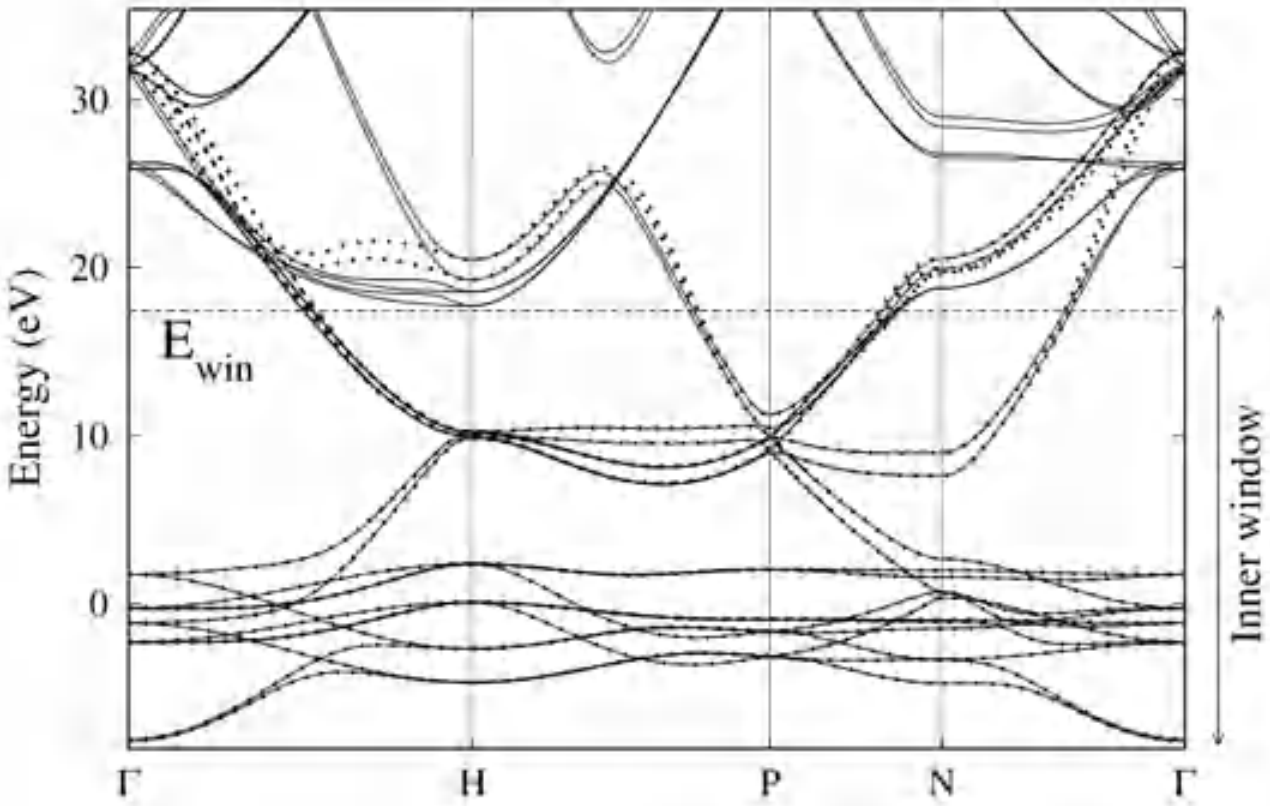
$\hat{\mathcal{O}} = H$: First-principles TB Hamiltonian

$\hat{\mathcal{O}} = \hat{X}\,,\ \hat{Y}\,,\ \hat{Z}$: Berry-related quantities

bcc Iron



18 spinor Wannier functions
Keep up to 4th neighbour overlaps
Cost 1/2000 of full calculation



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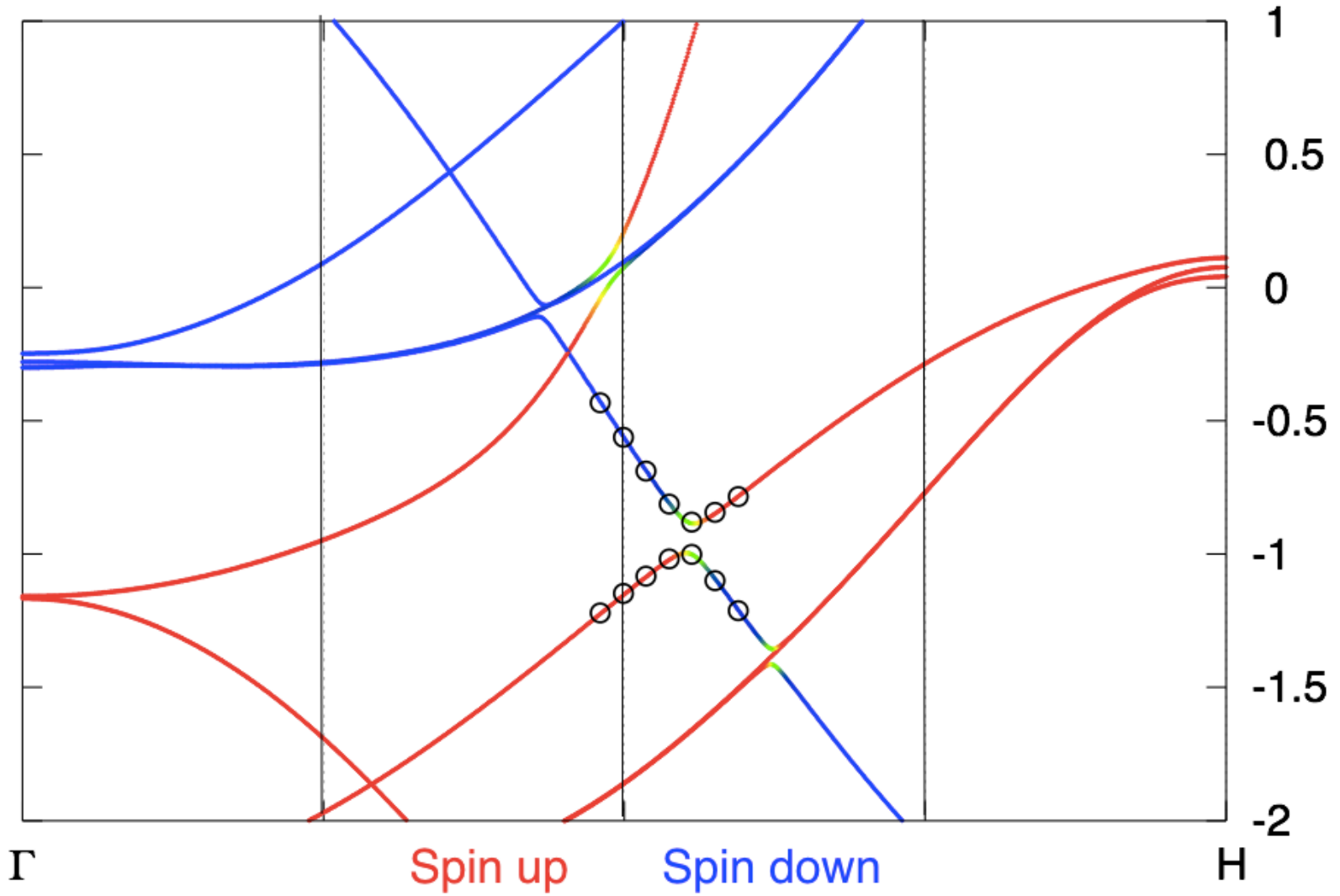
Avoided Crossing in bcc Fe



Wannier90 code

Authors

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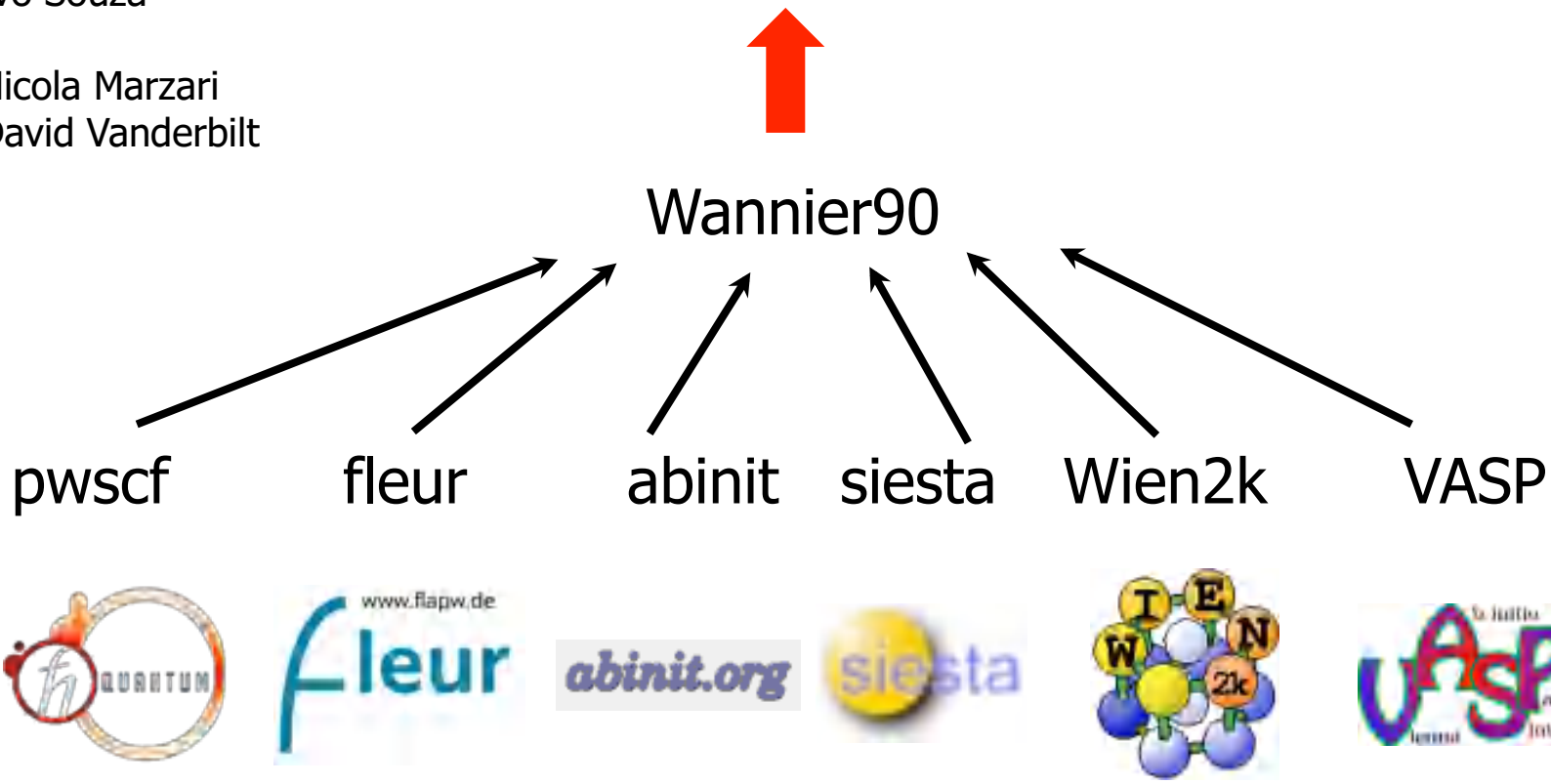
David Vanderbilt

Wannier interpolation, transport, etc.



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Wannier90 v2.0

wannier90.x
- serial executable
- minimisation of spread
- plot MLWF, bands, fermi surfaces
- ballistic transport

postw90.x
- parallel (MPI) executable

DOS
- DOS, Wannier projected DOS, net spin (all using fixed and adaptive smearing)

Berry Phase properties
- Calculation of properties related to the k-space Berry curvature and Berry connection, including anomalous Hall conductivity, orbital magnetisation, and interband optical conductivity

BoltzWann
- Calculation of electronic transport properties for bulk materials using the semiclassical Boltzmann transport equation

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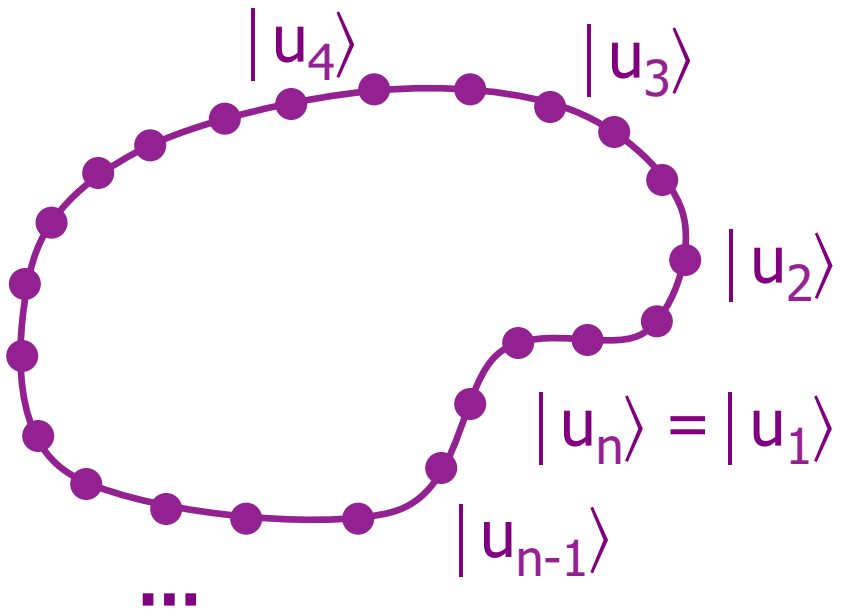
Tutorial: Berry phases

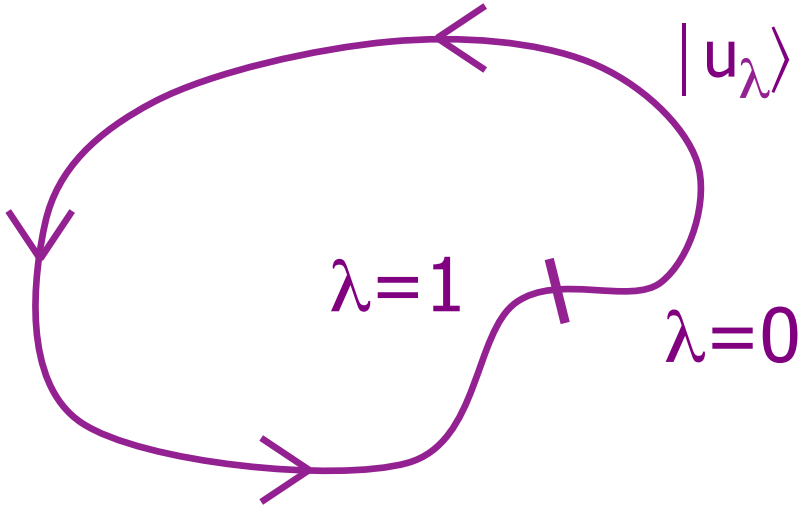


Now take limit that density of points $\to\infty$

$$\phi \quad -\mathrm{Im}\,\ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n\ \ 1}|u_n\rangle\right]$$

Check: $|\widetilde{u}_2\rangle = e^{i\beta}|u_2\rangle$ has no effect.

Tutorial: Berry phases



$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle$$

$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle}$$

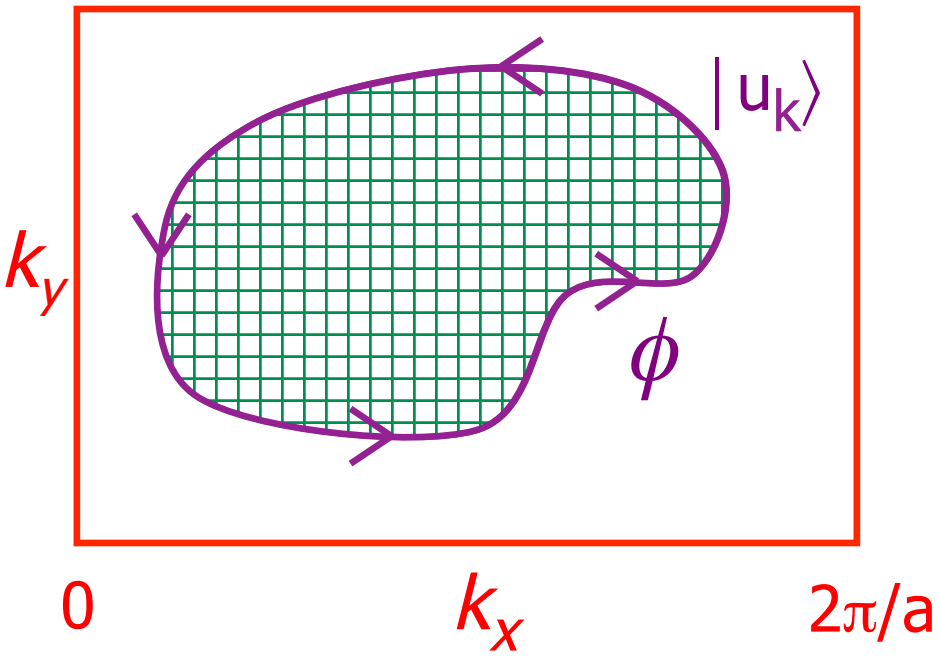
"Gauge" transformation:

$$\tilde{u}_\lambda \rangle = e^{-i\beta(\lambda)} | u_\lambda \rangle$$

Not hard to prove:

ϕ is well-defined modulo 2π.

Berry phase and curvature in the BZ



Berry potential:

$$\mathbf{A}(\mathbf{k}) = -\mathrm{Im}\,\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle$$

Berry phase:

$$\phi = \oint \mathbf{A}(\mathbf{k})\cdot d\mathbf{k}$$

Berry curvature:

$$\boldsymbol{\Omega}(\mathbf{k}) = \nabla \times \mathbf{A}$$

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x}\middle|\frac{du}{dk_y}\right\rangle$$

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

Bloch function

Stoke's theorem:

$$\phi = \int \Omega_z(\mathbf{k})\, d^2k$$

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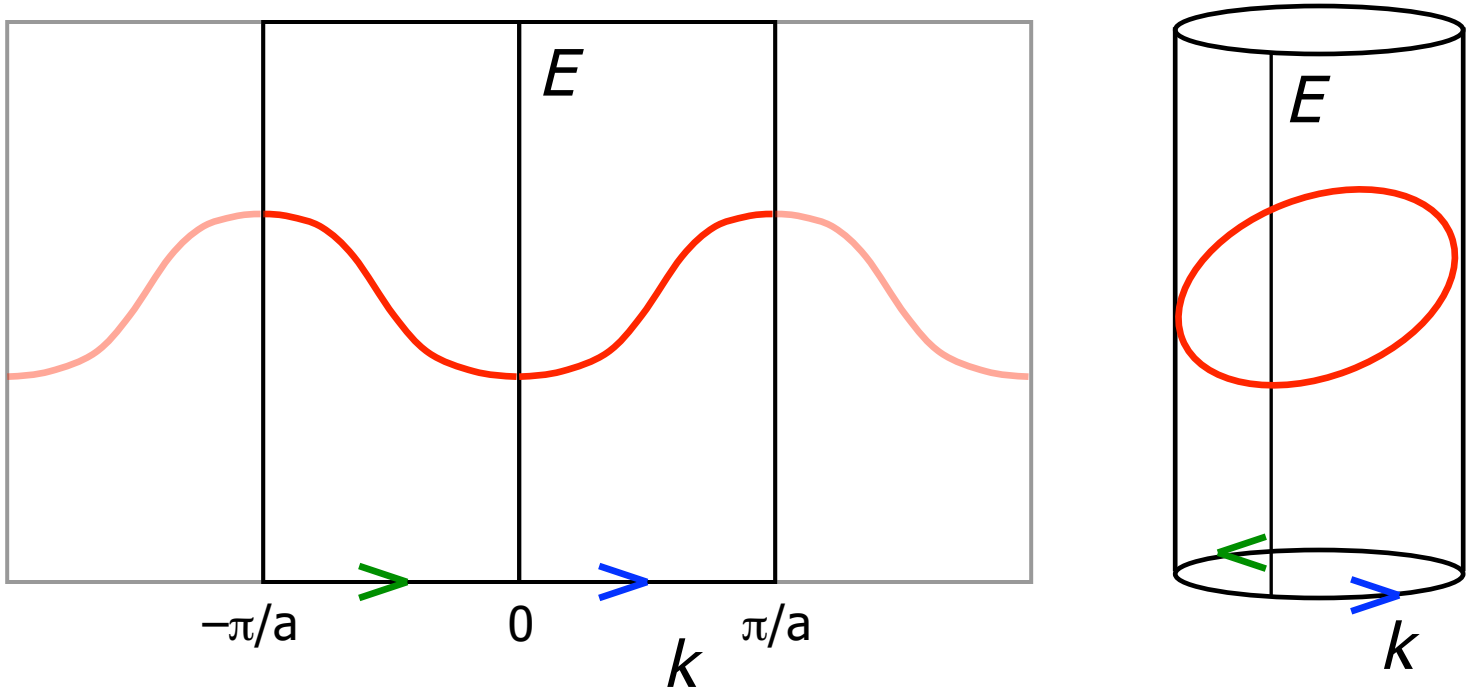
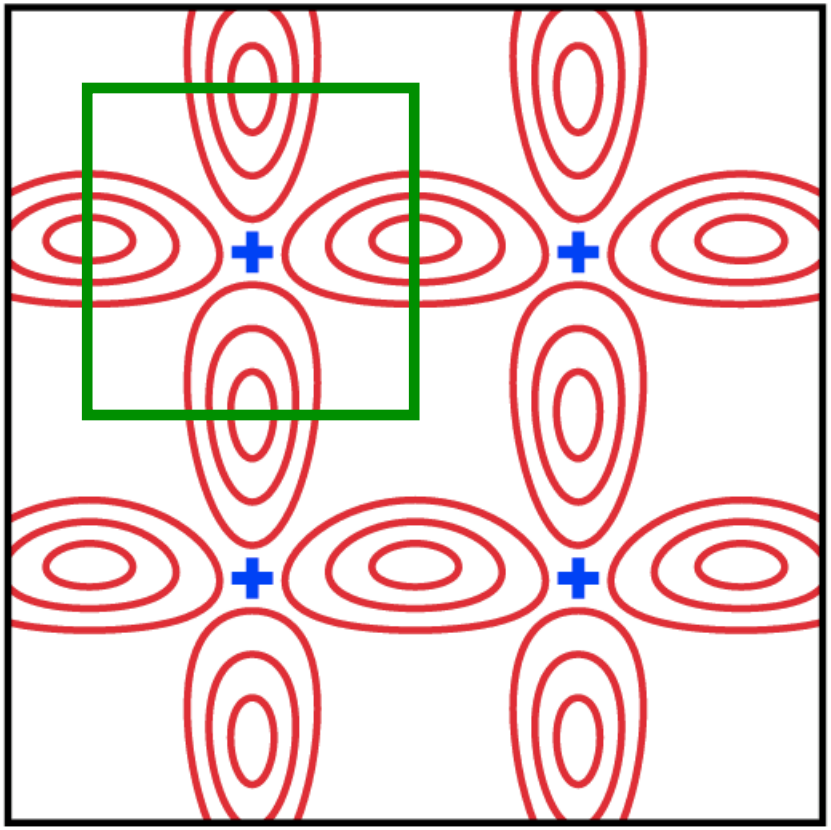
1D: BZ is really a loop

- Reciprocal space is really periodic
- Brillouin zone can be regarded as a loop



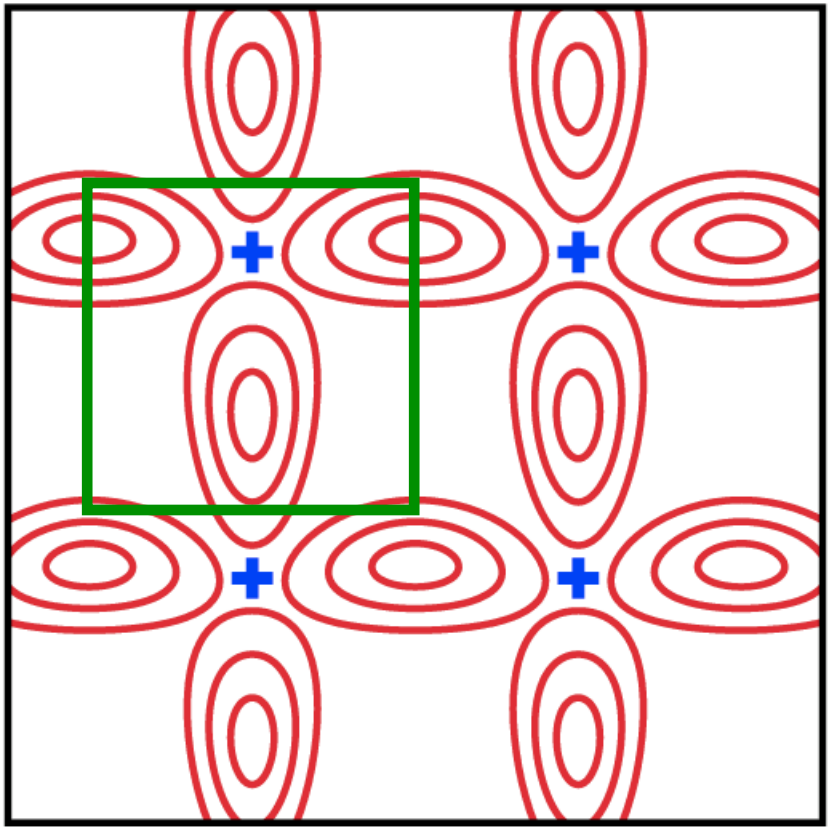
$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



$$\boldsymbol{d}_{\text{cell}} = \int_{\text{cell}} \boldsymbol{r}\, \rho(\boldsymbol{r})\, \mathrm{d}^3 r$$

$$\boldsymbol{d}_{cell} \approx \mathbf{0}$$

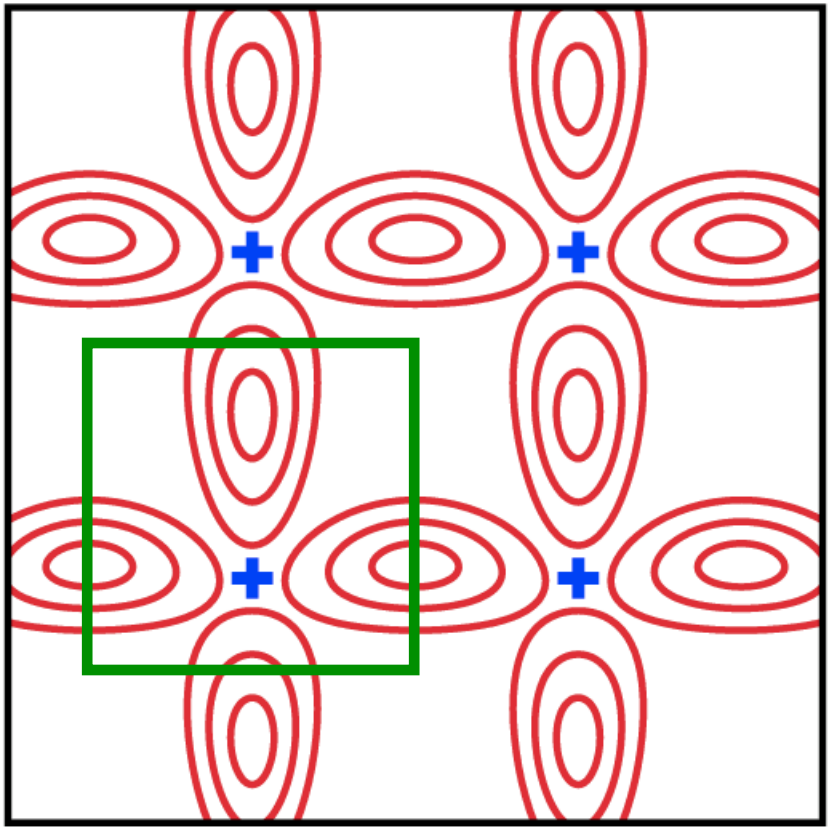
$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



$$\boldsymbol{d}_{\text{cell}} = \int_{\text{cell}} \boldsymbol{r}\, \rho(\boldsymbol{r})\, \mathrm{d}^3 r$$

$\boldsymbol{d}_{cell} =$ 

$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



$$\boldsymbol{d}_{\text{cell}} = \int_{\text{cell}} \boldsymbol{r}\, \rho(\boldsymbol{r})\, \mathrm{d}^3 r$$

$\boldsymbol{d}_{cell} =$ 

Modern Theory of Polarization

Problem:

Knowledge of bulk charge density $\rho(\boldsymbol{r})$ is not enough, even in principle, to determine $\boldsymbol{P}$!

Solution:

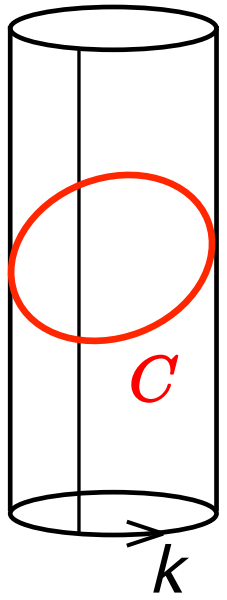
Go beyond $|\psi_{n\boldsymbol{k}}(\boldsymbol{r})|^2$ to access Berry phase information hidden in $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$

Polarization in a 1D insulator

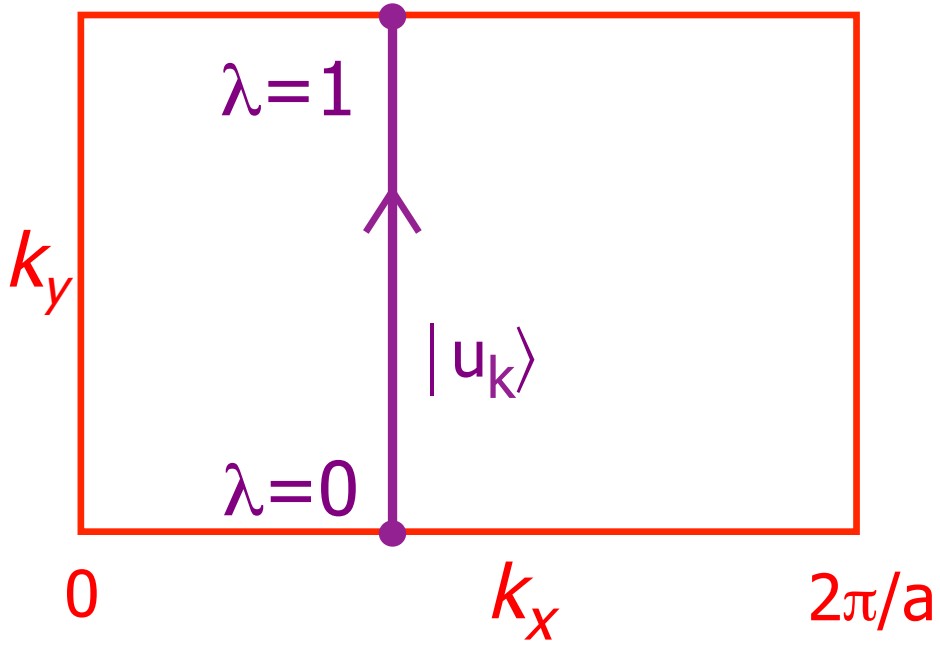
$$\mathbf{P} = \frac{-e}{2\pi} \int_{\mathrm{BZ}} dk \, \langle u_{\mathbf{k}} | i \tfrac{d}{dk} | u_{\mathbf{k}} \rangle$$

Heuristically, $x \Leftrightarrow i\frac{d}{dk}$ (Compare $p \Leftrightarrow -i\hbar\frac{d}{dx}$)

$$\mathbf{P} = -e\,\frac{\phi}{2\pi} \quad \text{where} \quad \boxed{\phi = i \oint_C dk \, \langle u_{\mathbf{k}} | \, \tfrac{d}{dk} \, | u_{\mathbf{k}} \rangle}$$



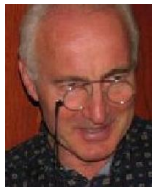
Polarization in a 2D insulator



Polarization P_y is proportional to sum of k_x-averaged Berry phases of occupied bands

$$\phi = -\mathrm{Im} \int dk_y \, \langle u_{\mathbf{k}} | \frac{d}{dk_y} | u_{\mathbf{k}} \rangle$$

Resta, Ferroelectrics 136, 51 (1992)



King-Smith and Vanderbilt, PRB 47, 1651 (1993)

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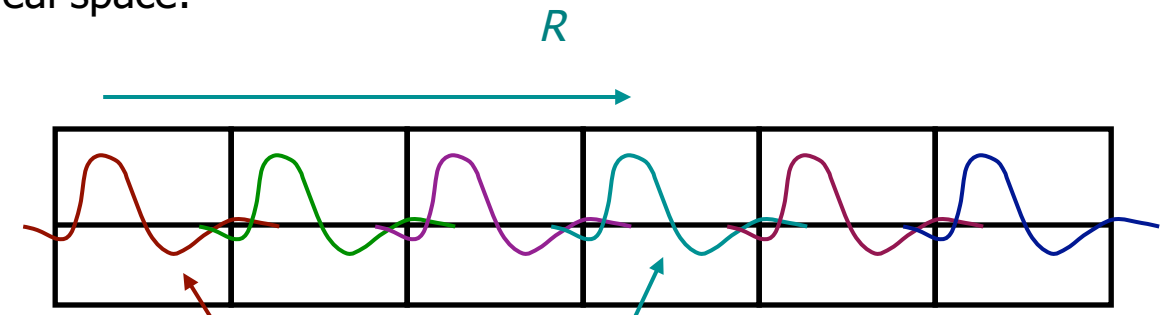
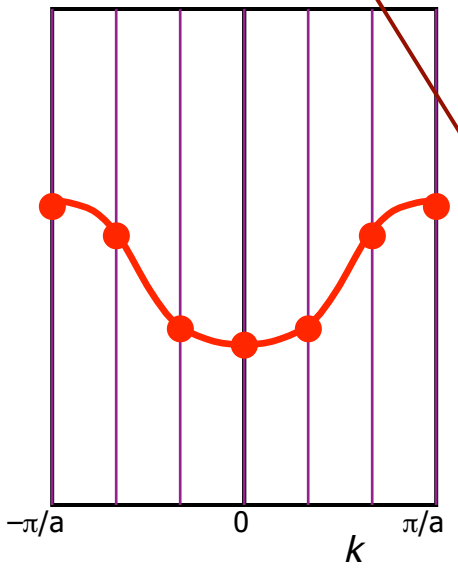
Polarization ↔ Wannier centers

Crystal in real space:



Brillouin zone in reciprocal space:



$$w_{\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

$$w_{\mathbf{0}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k}$$

Jnitary transformation

Polarization ↔ Wannier centers

Centers of Wannier functions:

$$|w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\,|\psi_{\mathbf{k}}\rangle$$

$$= \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\,e^{i\mathbf{k}\cdot\mathbf{r}}\,|u_{\mathbf{k}}\rangle$$

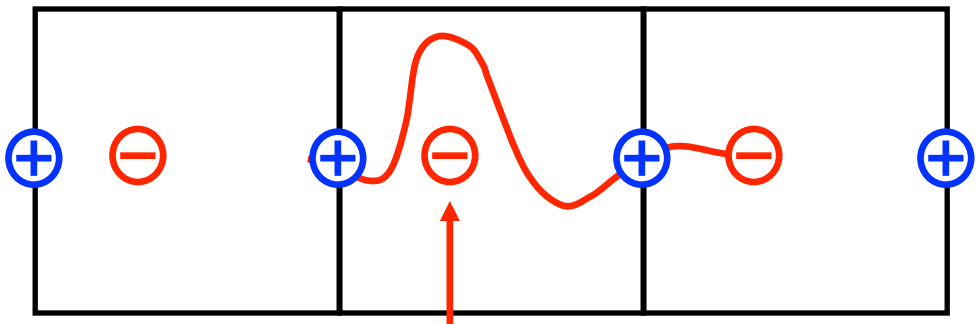
$$\mathbf{r}\,|w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\left(-i\nabla_{\mathbf{k}}\,e^{i\mathbf{k}\cdot\mathbf{r}}\right)|u_{\mathbf{k}}\rangle$$

$$= i\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\,e^{i\mathbf{k}\cdot\mathbf{r}}\left(\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle\right)$$

$$\boxed{\langle w_0\,|\,\mathbf{r}\,|\,w_0\rangle = i\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\langle u_{\mathbf{k}}|\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle}$$

Polarization ↔ Wannier centers

Centers of Wannier functions:

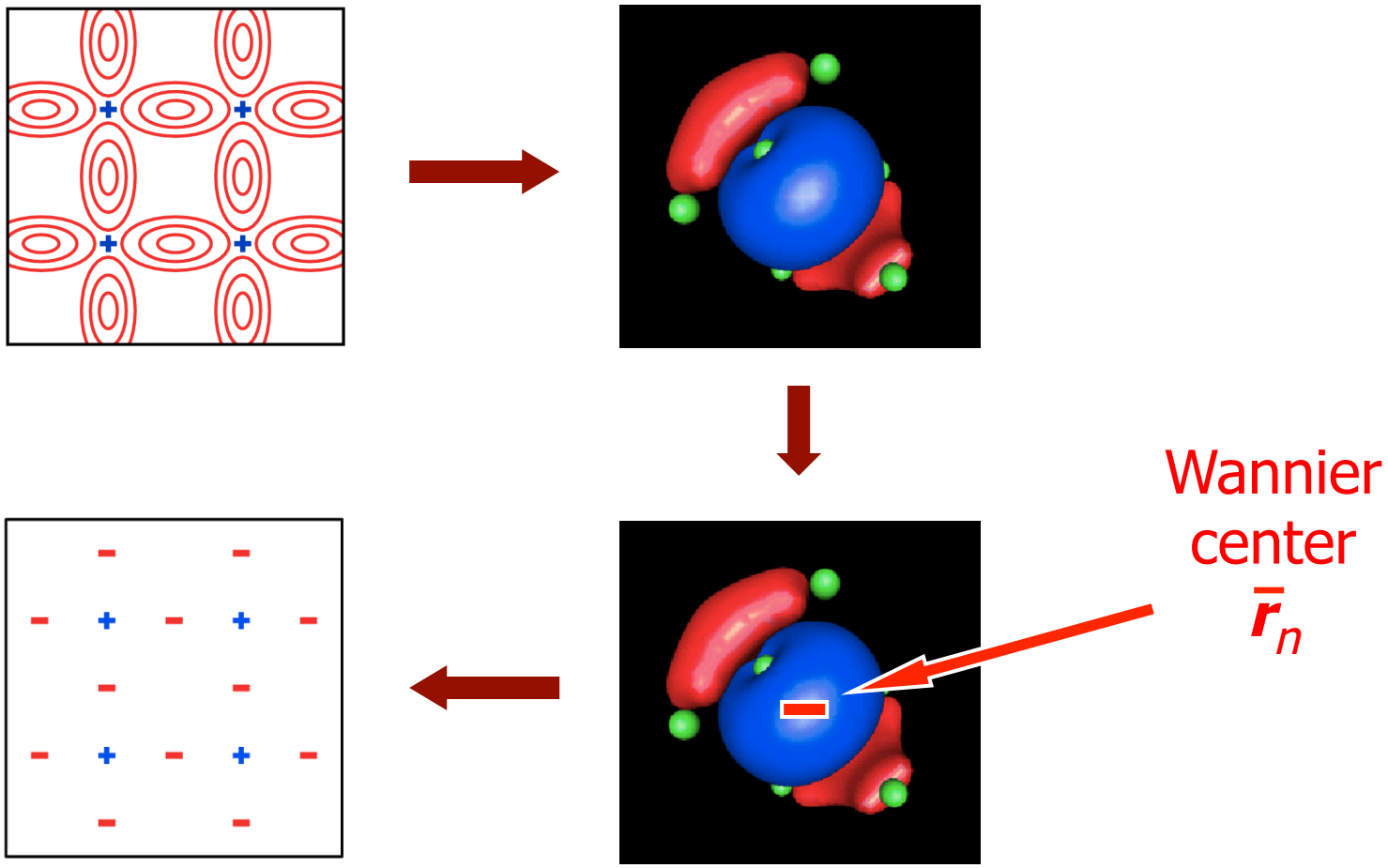


P

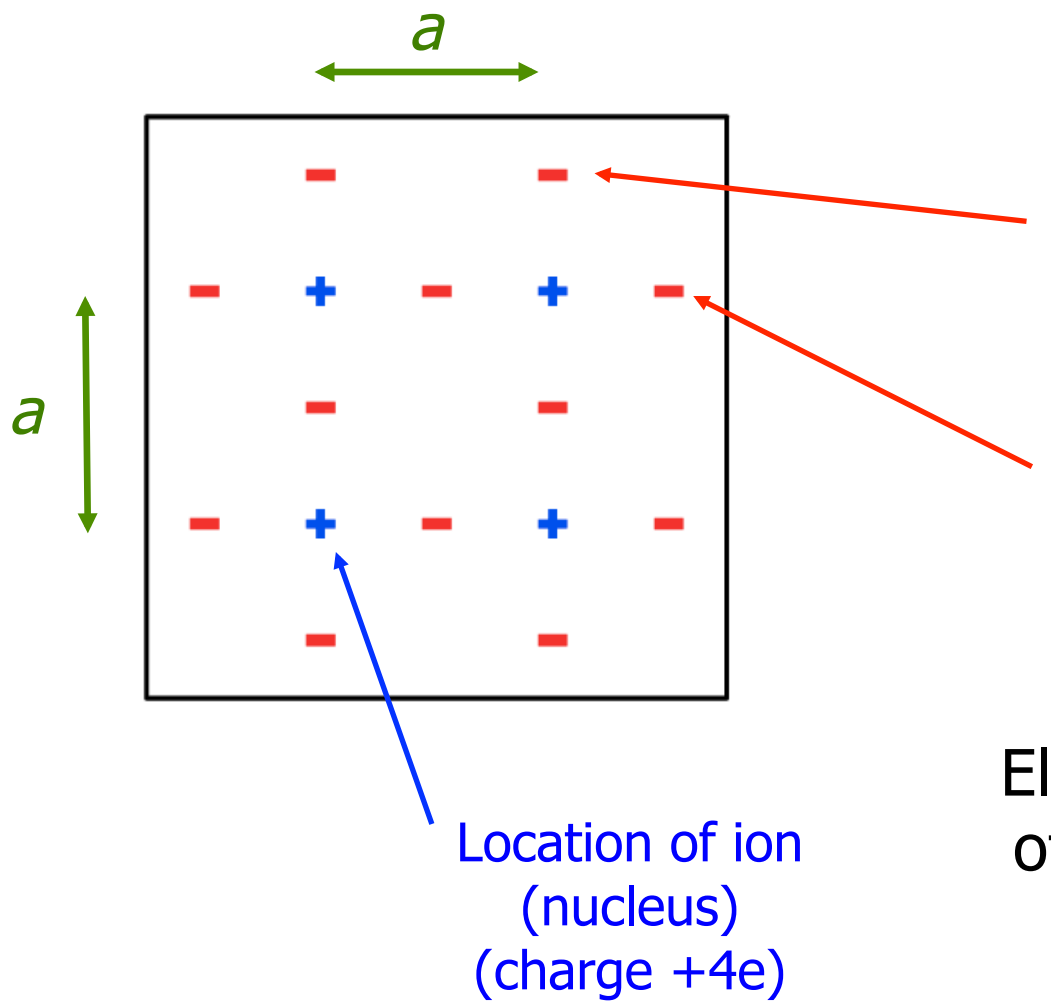
$$\langle w_0|x|w_0\rangle = i\frac{a}{2\pi}\int_{\mathrm{BZ}} dk \left\langle u_k\left|\frac{d}{dk}\right|u_k\right\rangle$$

$$= a\frac{\phi}{2\pi}$$

Mapping to Wannier centers

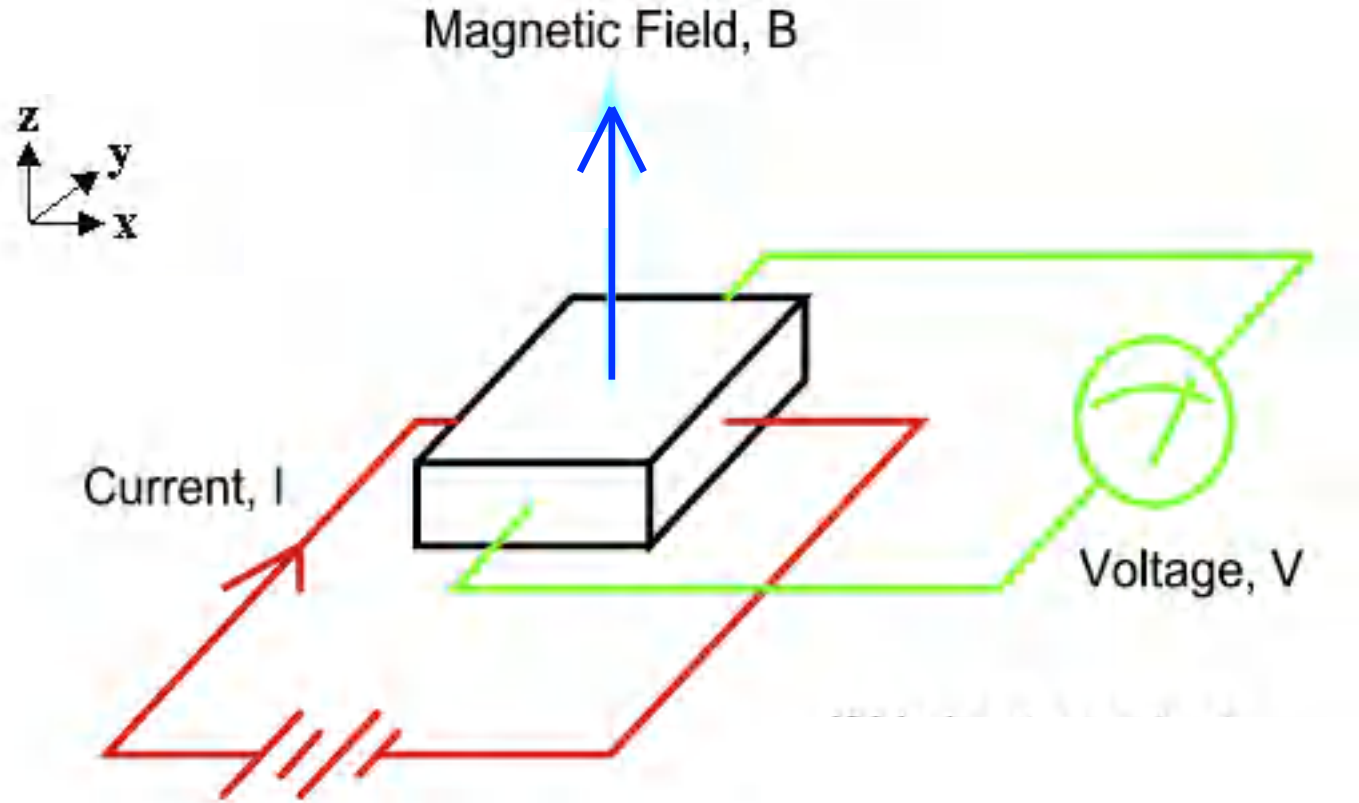


Mapping to Wannier centers



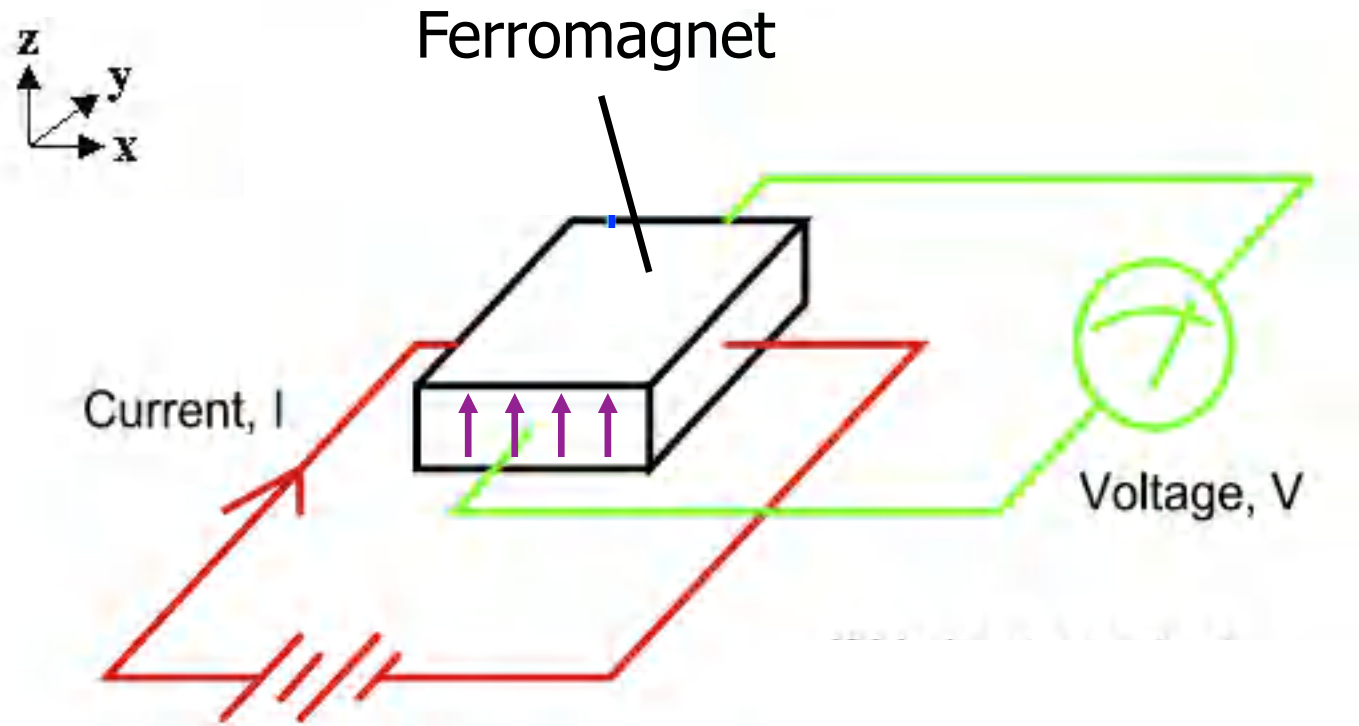
Electric polarization ***P***
of the crystal can be
deduced from
pictures like this

Ordinary Hall conductivity



$$R_H = \frac{E_y}{j_x B} = \frac{dV_H}{IB} = -\frac{1}{ne}$$

Anomalous Hall conductivity (AHC)



$$R_{AH} = \frac{E_y}{j_x}$$

Anomalous Hall conductivity (AHC)

- Karplus-Luttinger theory (1954)
  - Scattering-free, intrinsic
- Skew-scattering mechanism (1955)
  - Impurity scattering
- Side-jump mechanism (1970)
  - Impurity or phonon scattering
- Berry-phase theory (1999)
  - Restatement of Karplus-Luttinger

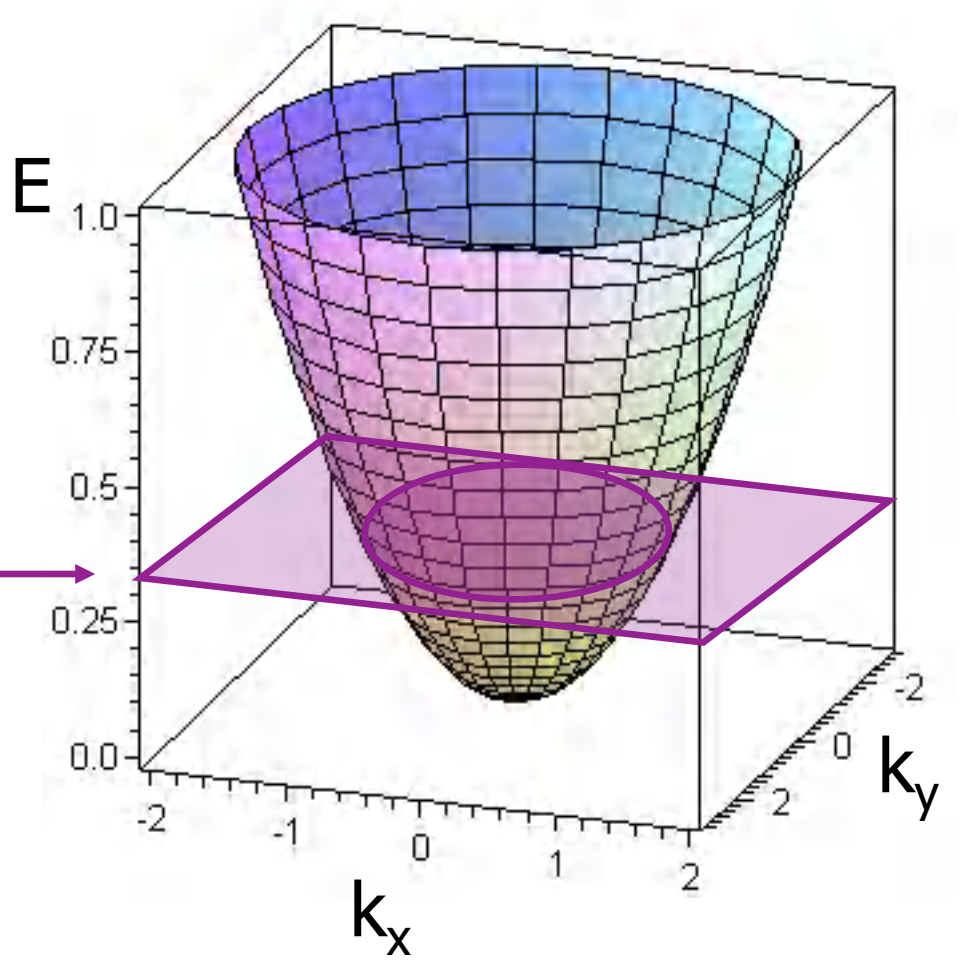
Sundaram and Niu, PRB 59, 14925 (1999).

$$\sigma_{xy}^{\mathrm{AHE}} = \frac{-e^2}{(2\pi)^3\hbar}\sum_n \int d^3k\, f_{n\mathbf{k}}\,\Omega_{n,z}(\mathbf{k})$$

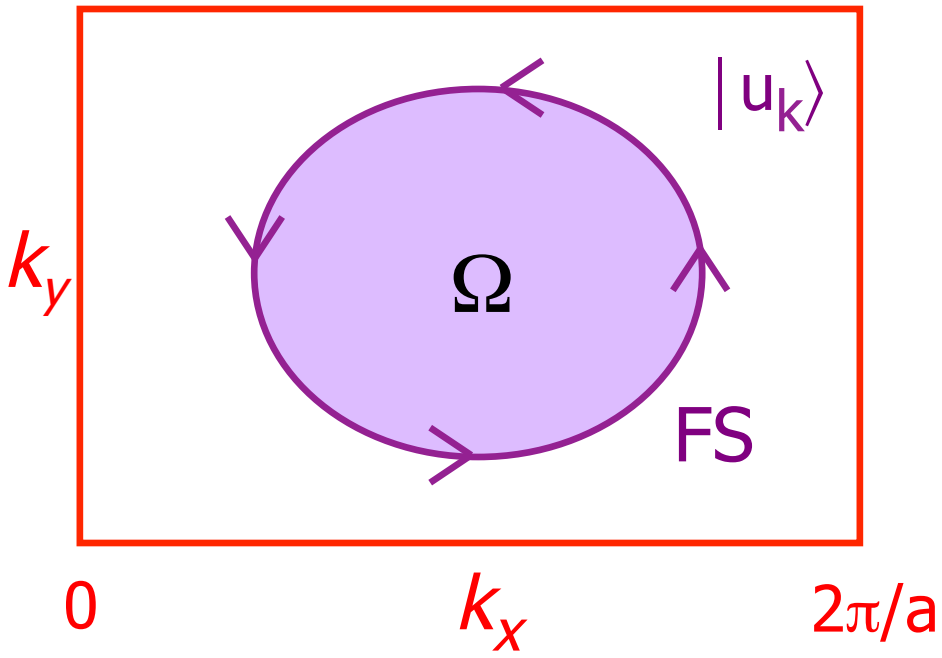
A pure bandstructure effect!

Bandstructure of a metal

Fermi Energy E_F →



Non-magnetic metal: no net Berry curvature



Time-reversal symmetry

$$\Downarrow$$

$$u(k_x, k_y) = u^*(-k_x, -k_y)$$

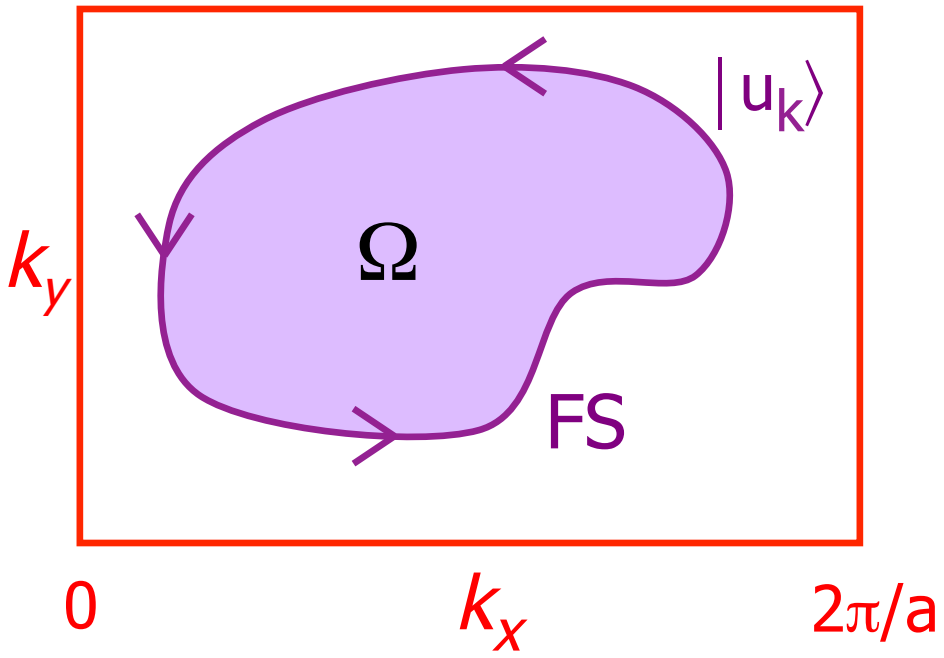
$$\Downarrow$$

$$\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$$

$$\Downarrow$$

$$\phi = 0$$

Magnetic metal: things get interesting



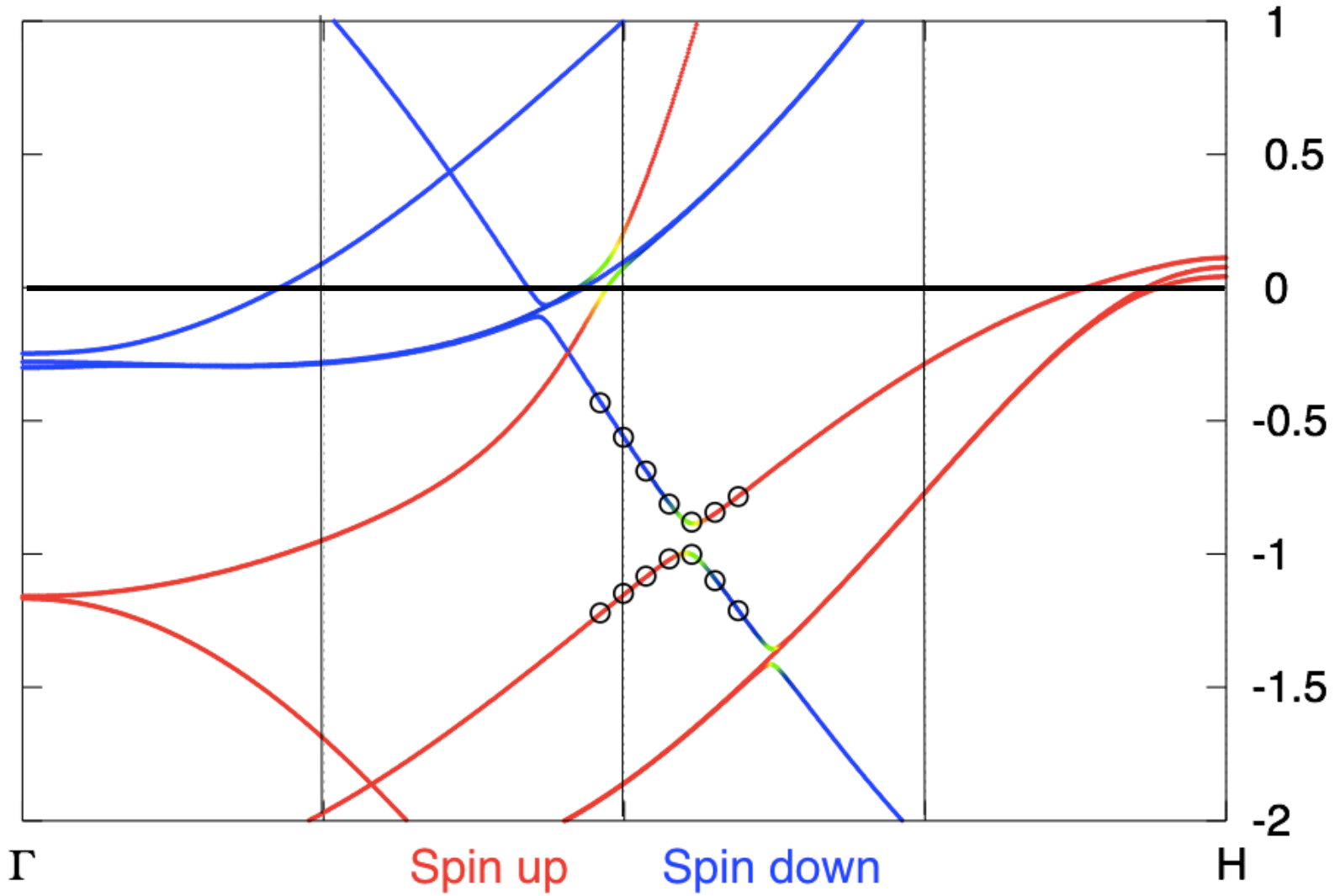
$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\phi = \int_{\mathrm{FS}} \Omega_z(\mathbf{k})\, d^2k$$

$$\sigma_{xy}^{\mathrm{AHE}} = \frac{-e^2}{(2\pi)^3\hbar} \sum_n \int d^3k\, f_{n\mathbf{k}}\, \Omega_{n,z}(\mathbf{k})$$

(3D)

Avoided Crossing in bcc Fe



Wannier interpolation of other operators

$$\mathcal{O}_{nm}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \mathbf{0}n|\hat{\mathcal{O}}|\mathbf{R}m\rangle$$

$\hat{\mathcal{O}} = H$: First-principles TB Hamiltonian

$\hat{\mathcal{O}} = \hat{X}\,,\ \hat{Y}\,,\ \hat{Z}$: Berry-related quantities

Wannier interp. of Berry properties

Berry connection

Formal: $\mathbf{A}_n(\mathbf{k}) = i\langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}}|u_{n\mathbf{k}}\rangle$

Practical: $A^{(\mathrm{W})}_{nm,\alpha}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\langle 0n|\hat{r}_\alpha|\mathbf{R}m\rangle$

Berry curvature

Formal: $\boldsymbol{\Omega}_n(\mathbf{k}) = \nabla \times \mathbf{A}_n(\mathbf{k})$

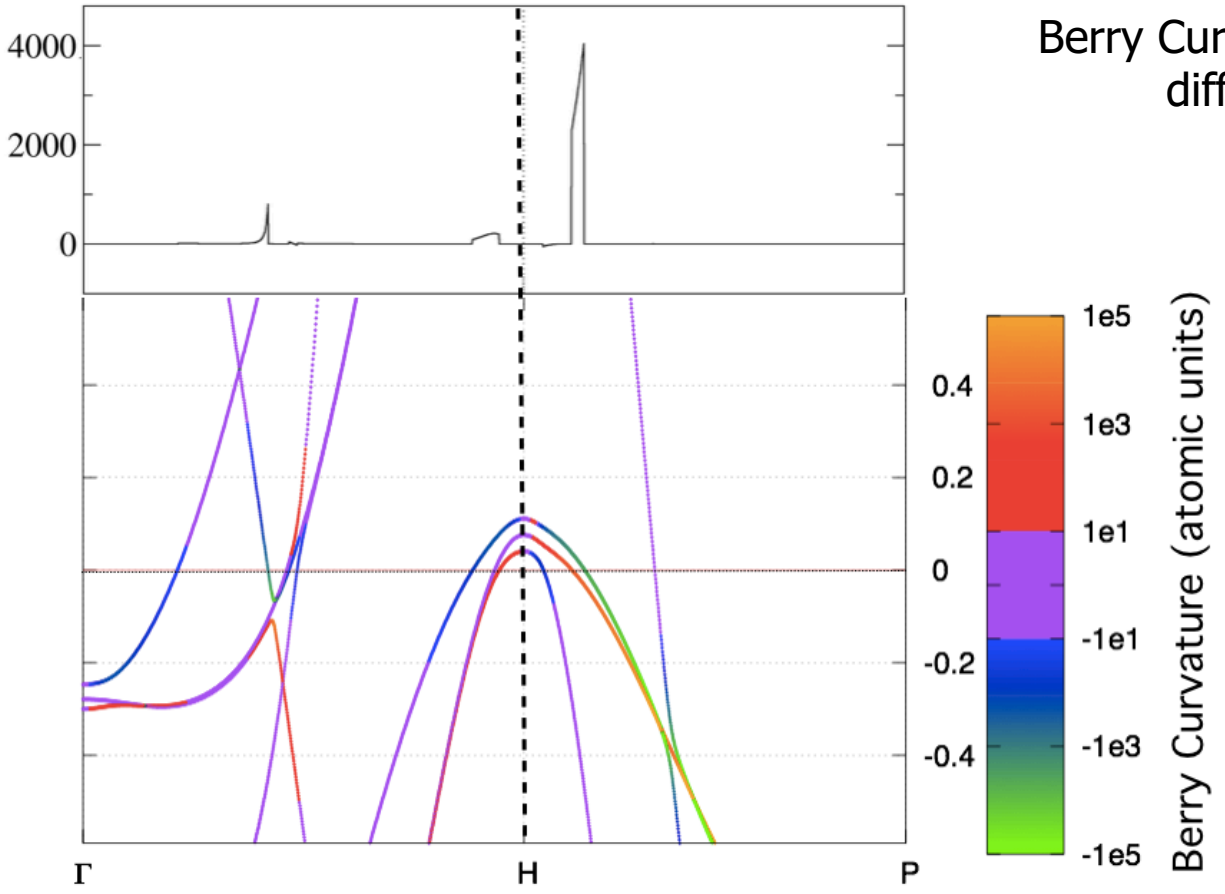
Practical $\Omega^{(\mathrm{W})}_{nm,\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}(iR_\alpha\langle 0n|\hat{r}_\beta|\mathbf{R}m\rangle - iR_\beta\langle 0n|\hat{r}_\alpha|\mathbf{R}m\rangle)$

position operator in Wannier basis is well defined!

Anomalous Hall Conductivity

$$\sigma_{xy} = \frac{-e^2}{(2\pi)^2 h} \sum_n \int_{\mathrm{BZ}} d\mathbf{k}\, f_n(\mathbf{k})\, \Omega_{n,z}(\mathbf{k})$$

$$\Omega_n(\mathbf{k}) = -Im\langle \nabla_{\mathbf{k}} u_{n,\mathbf{k}}| \times |\nabla_{\mathbf{k}} u_{n,\mathbf{k}}\rangle$$



Berry Curvature - example of a difficult BZ integral

Outline

- Wannier interpolation
- Electric polarization and anomalous Hall
- Chemical bonding and polar properties
  - Covalent semiconductors and polymers
  - Perovskites
  - Liquid water
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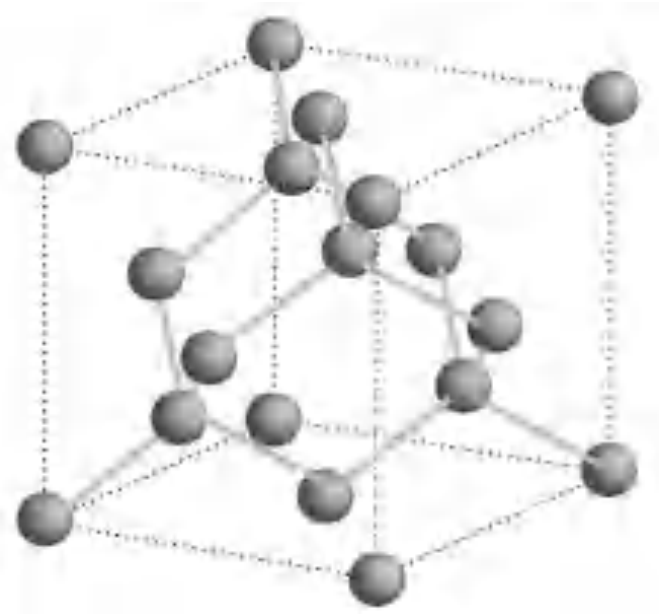
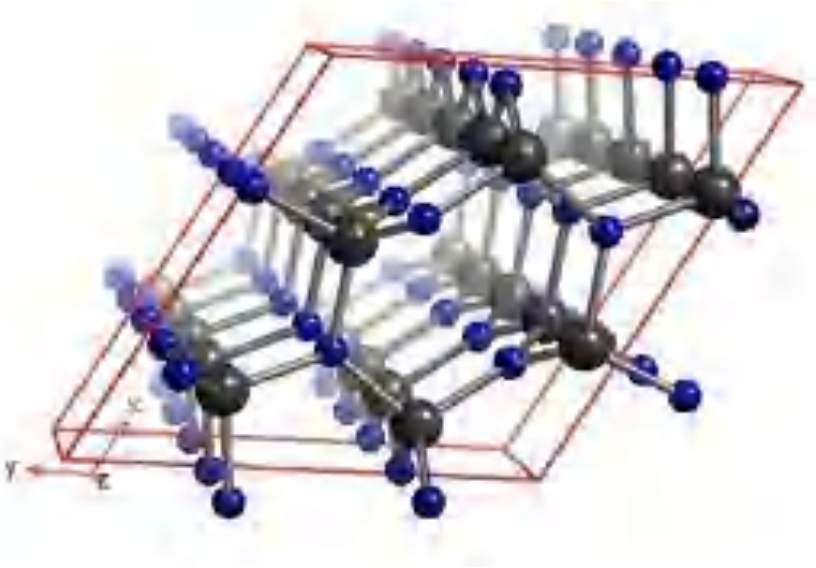
- Summary and Conclusions

RUTGERS

Diamond and zincblende structures





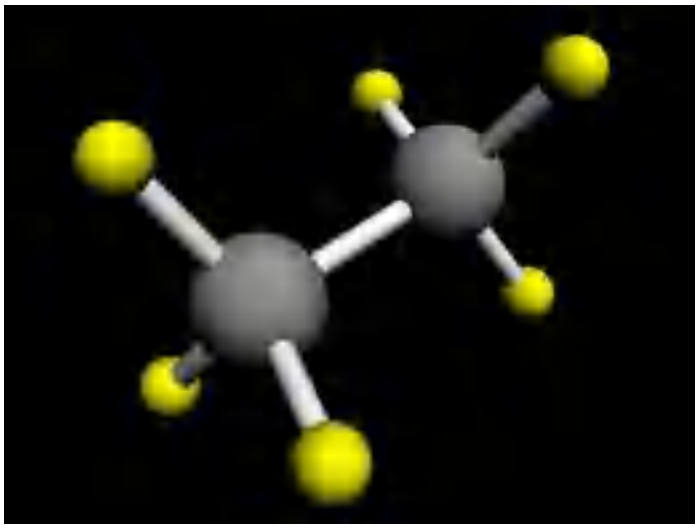
Si

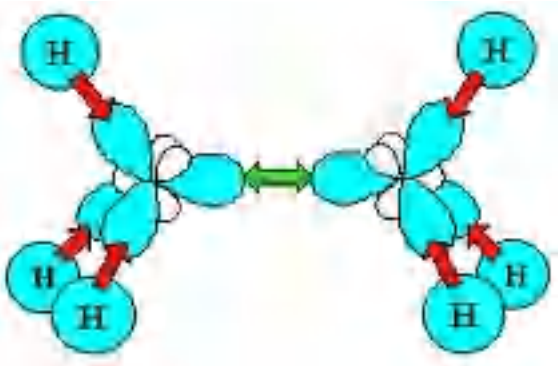
(diamond)

GaAs

(zincblende)

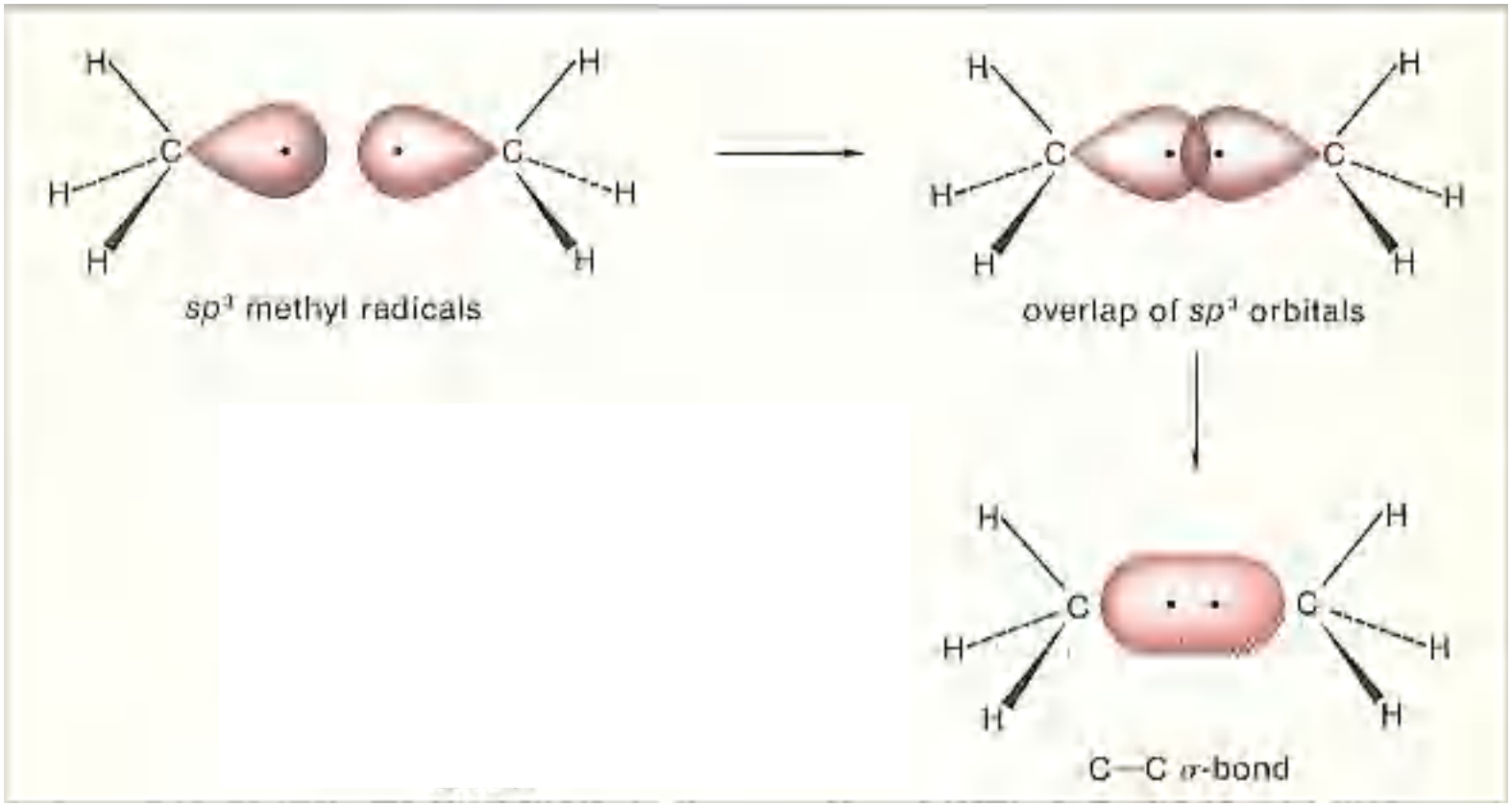
sp_3 - sp_3 bond orbitals



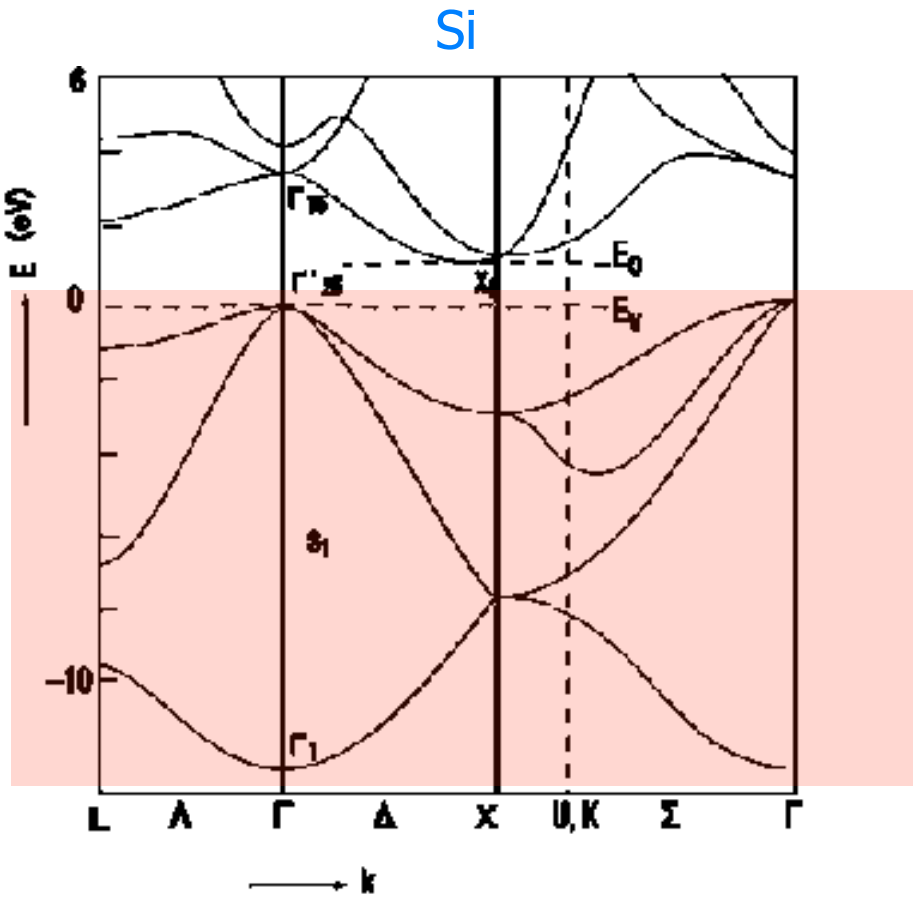


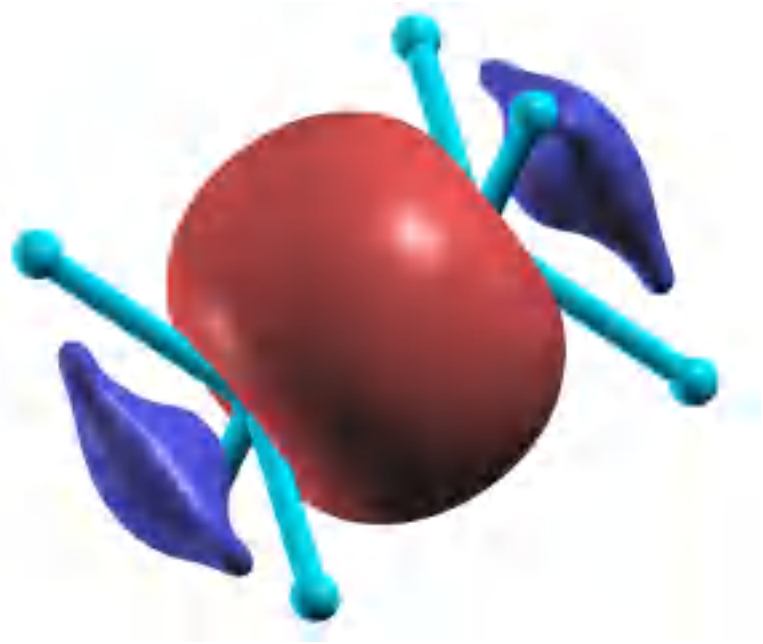
Ethane, C_2H_6

sp_3 - sp_3 bond orbitals



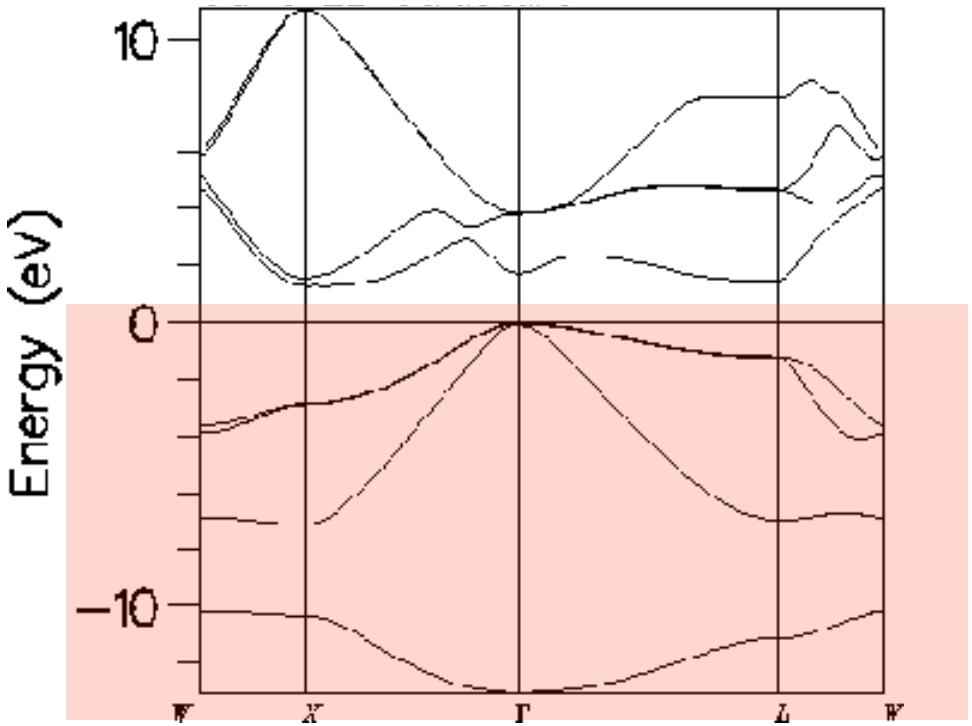
Wannier functions: Si

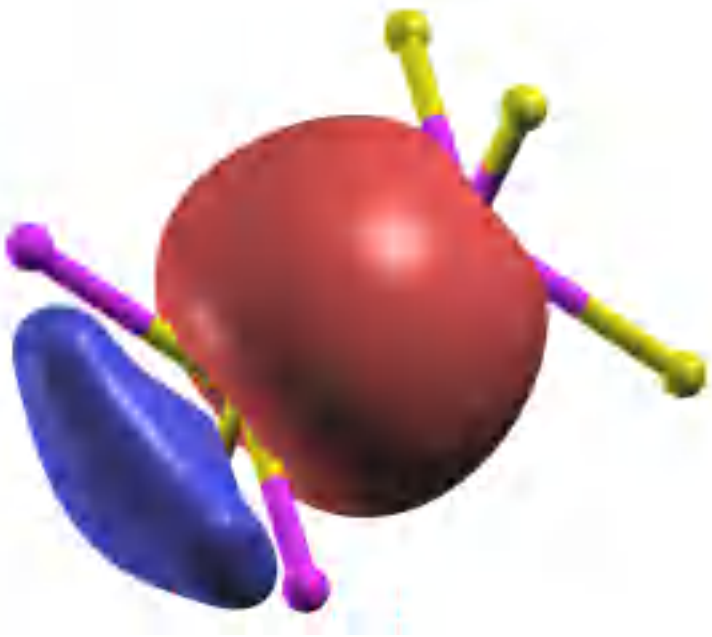




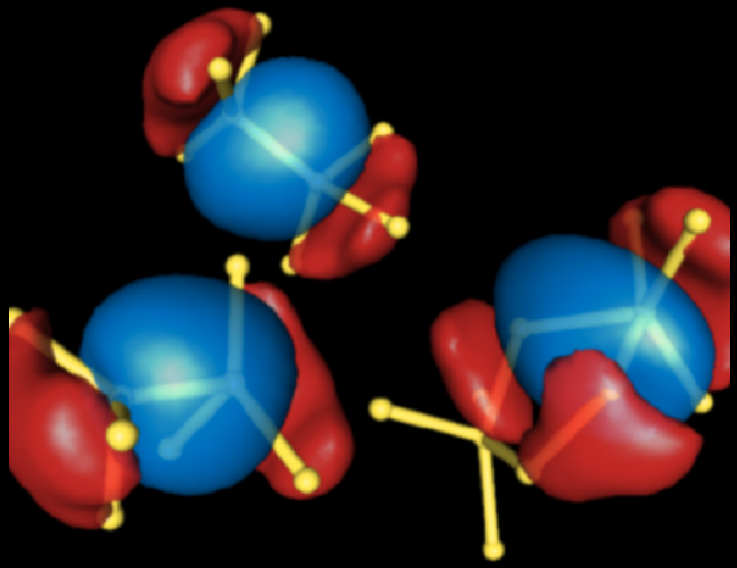
Wannier functions: GaAs

GaAs



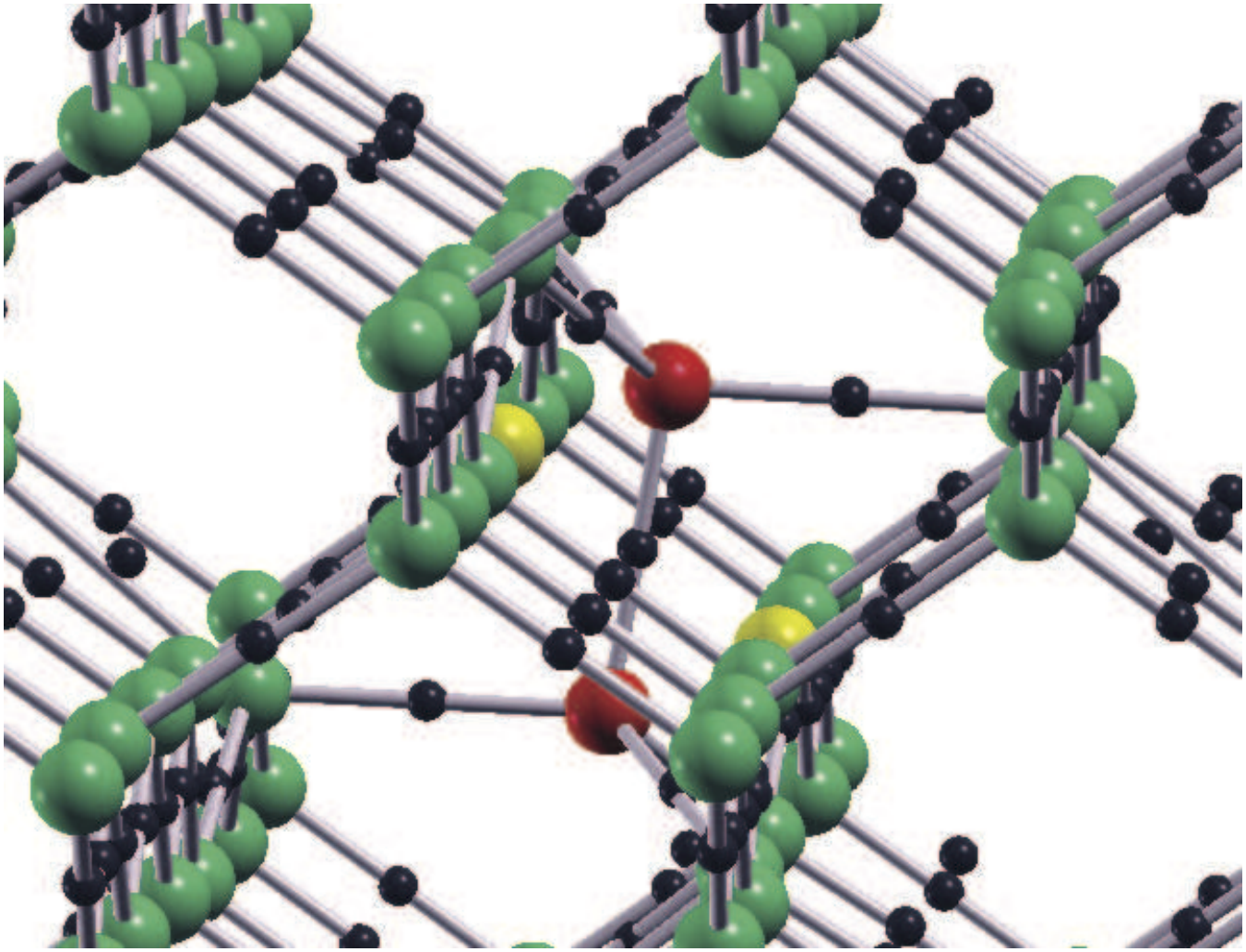


Wannier functions in *a-Si*

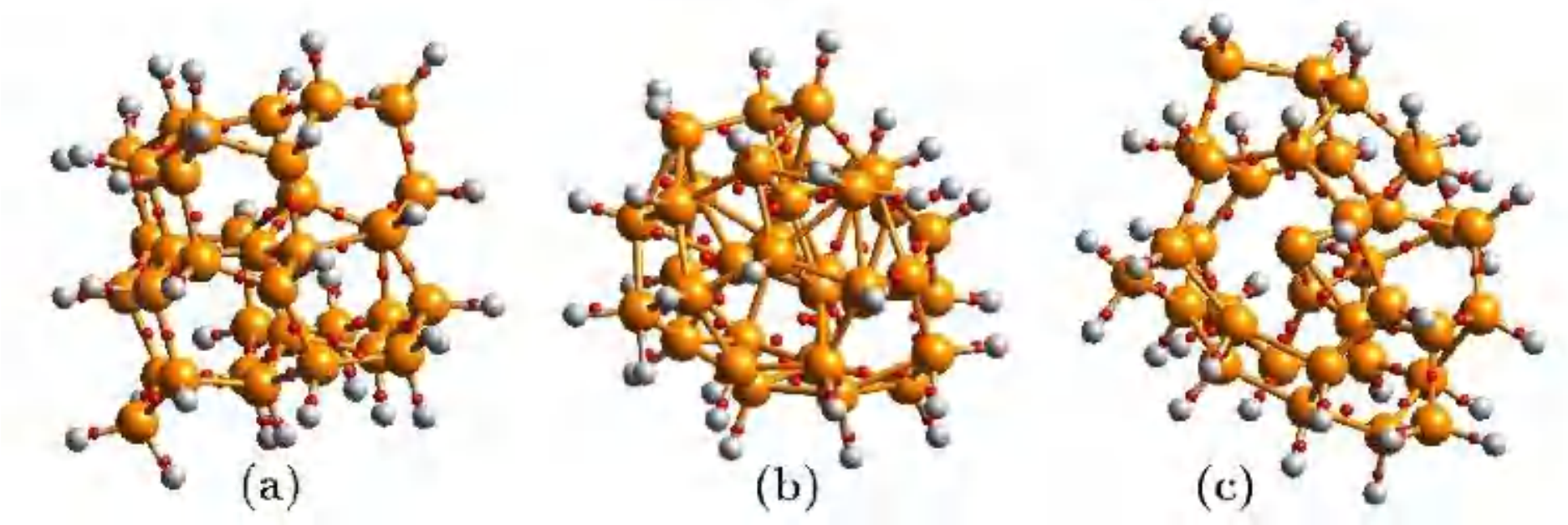


Fornari et al.

Buckled dimer defect in Si



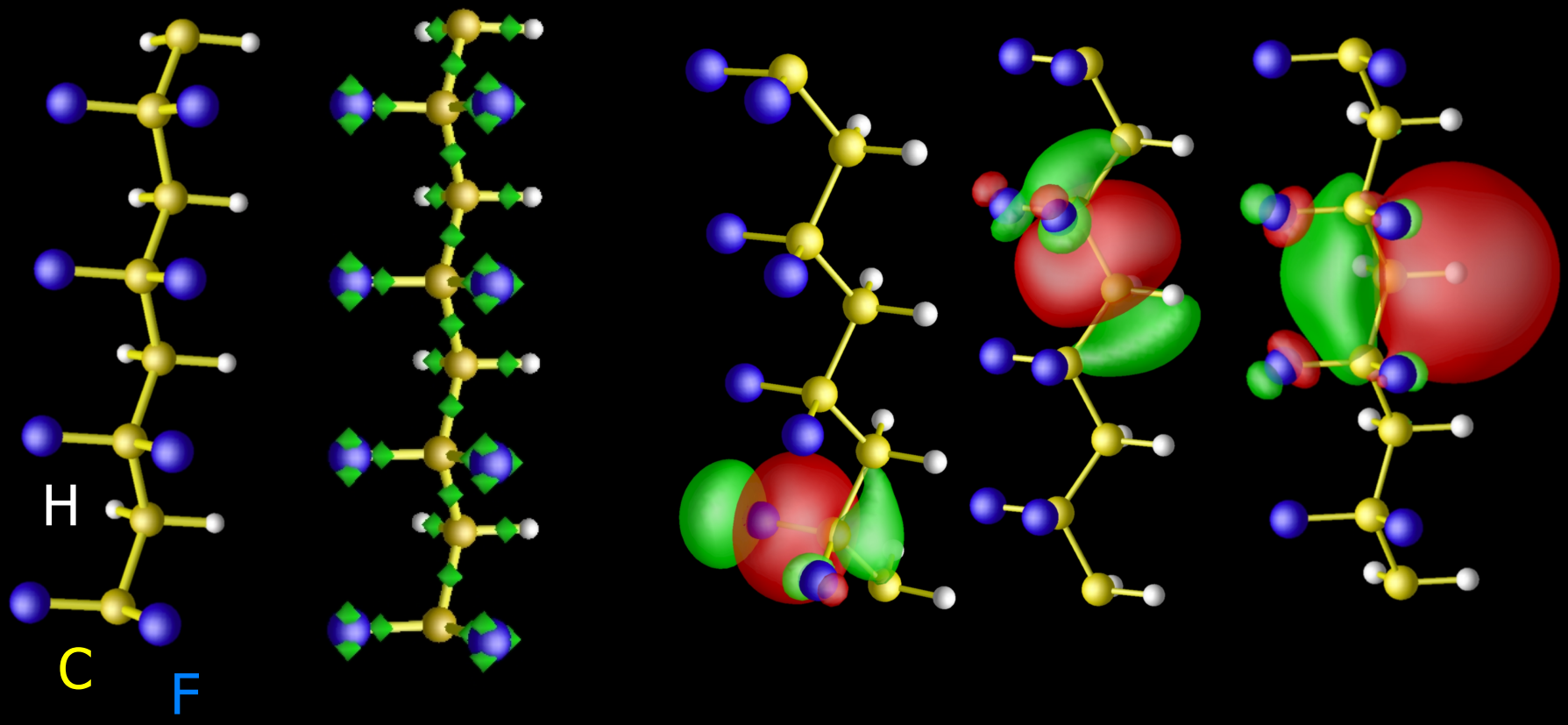
Collapse and amorphization of a Si cluster under pressure



Pressure: 25 GPa (a), 35 GPa (b) and back to 5 GPa (c).
Small red "atoms" are the Wannier centers.

(Martonak et al., 2001)

Wannier analysis of PVDF polymers and copolymers



… - CH_2 - CF_2 - CH_2 - CF_2 - …

Courtesy S. Nakhmanson

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- Wannier interpolation
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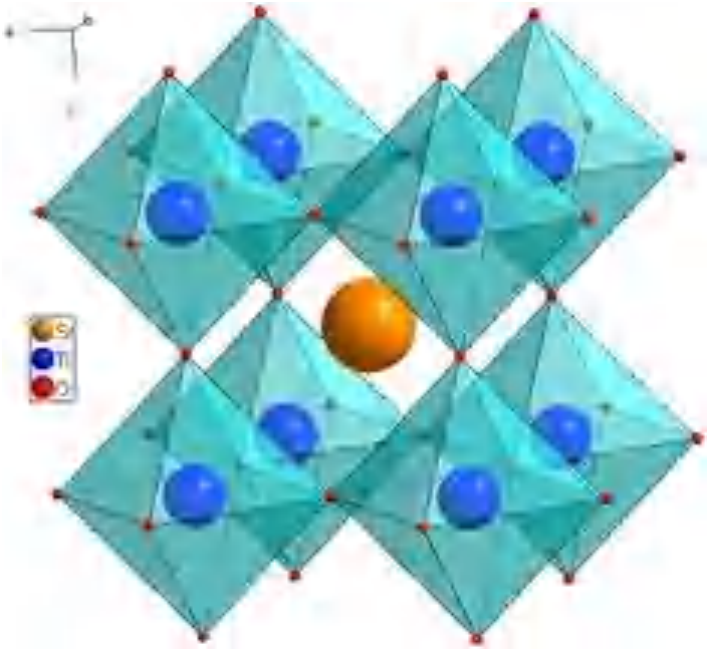
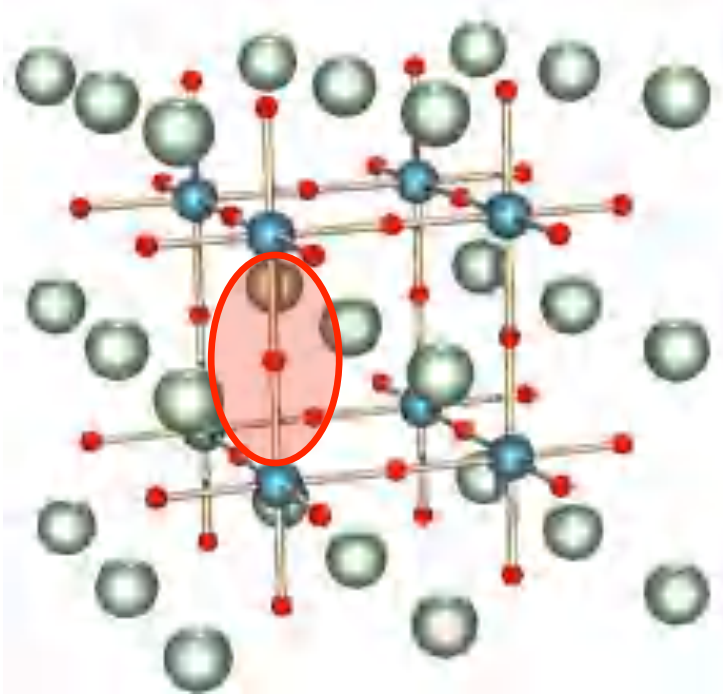
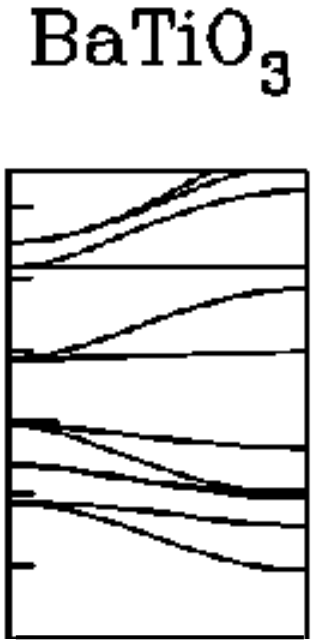
Perovskite crystal structure



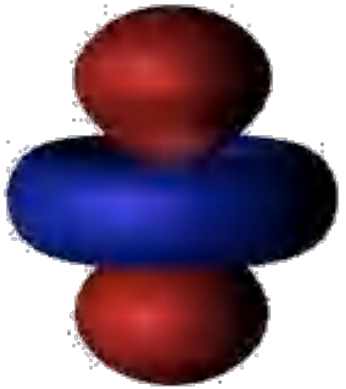


Example: Wannier functions in $BaTiO_3$

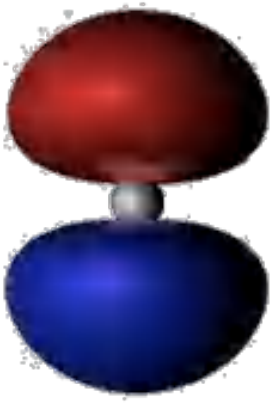


Mainly Ti *3d*
(also some O *2p*)

Mainly O *2p*
(also some Ti *3d*)

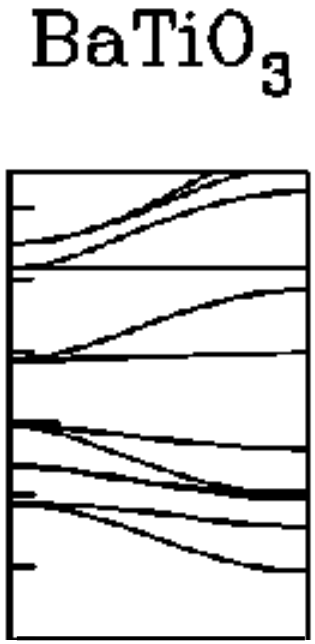


Ti *3d*

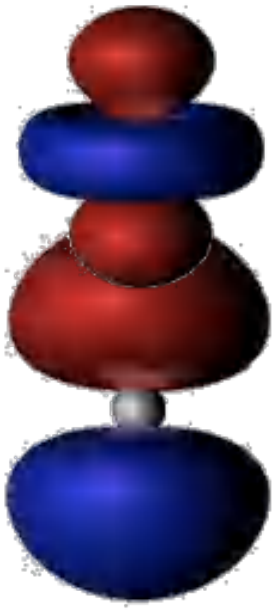


O *2p*

Example: Wannier functions in $BaTiO_3$

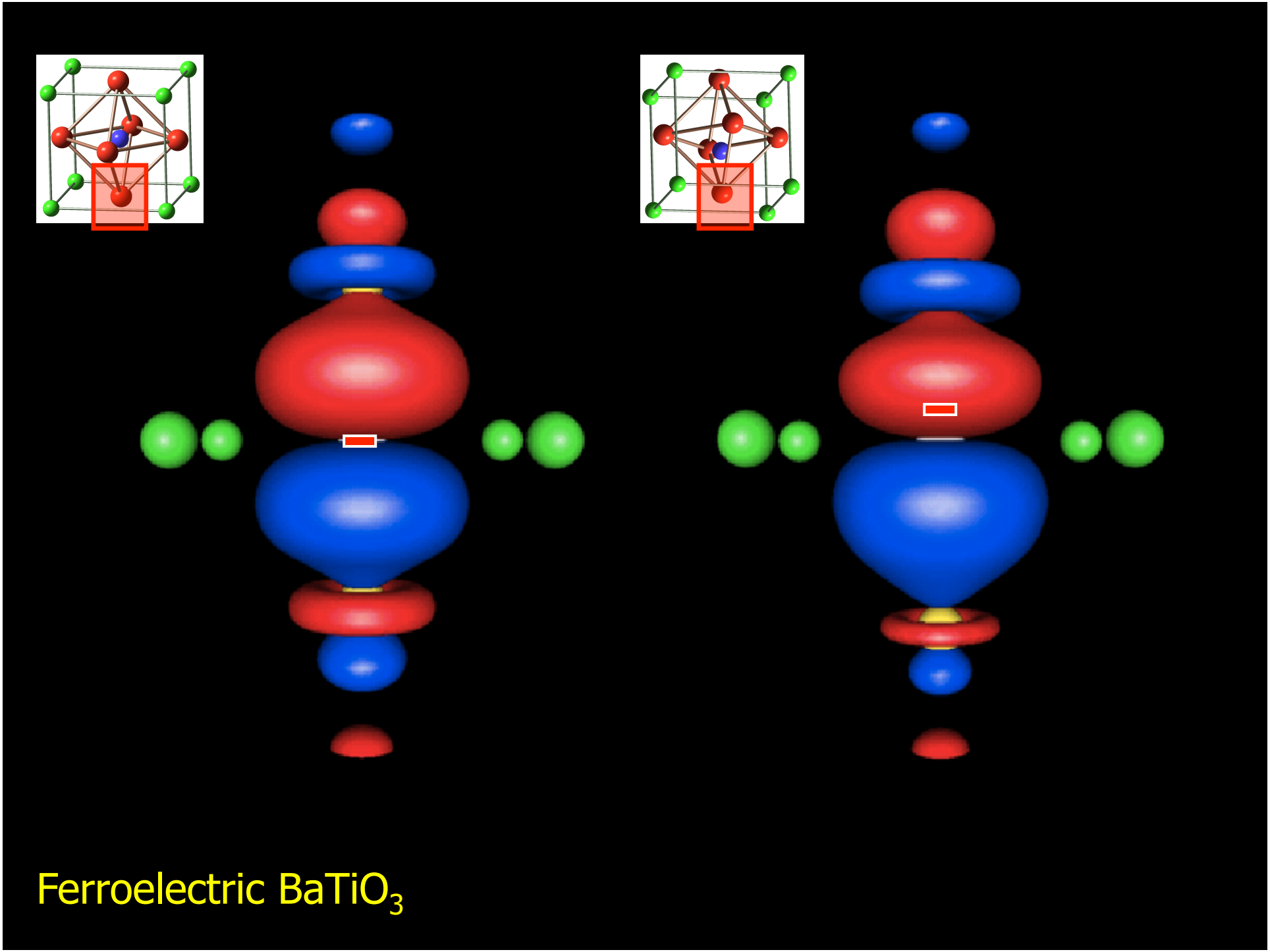


Mainly O *2p*
(also some Ti *3d*)

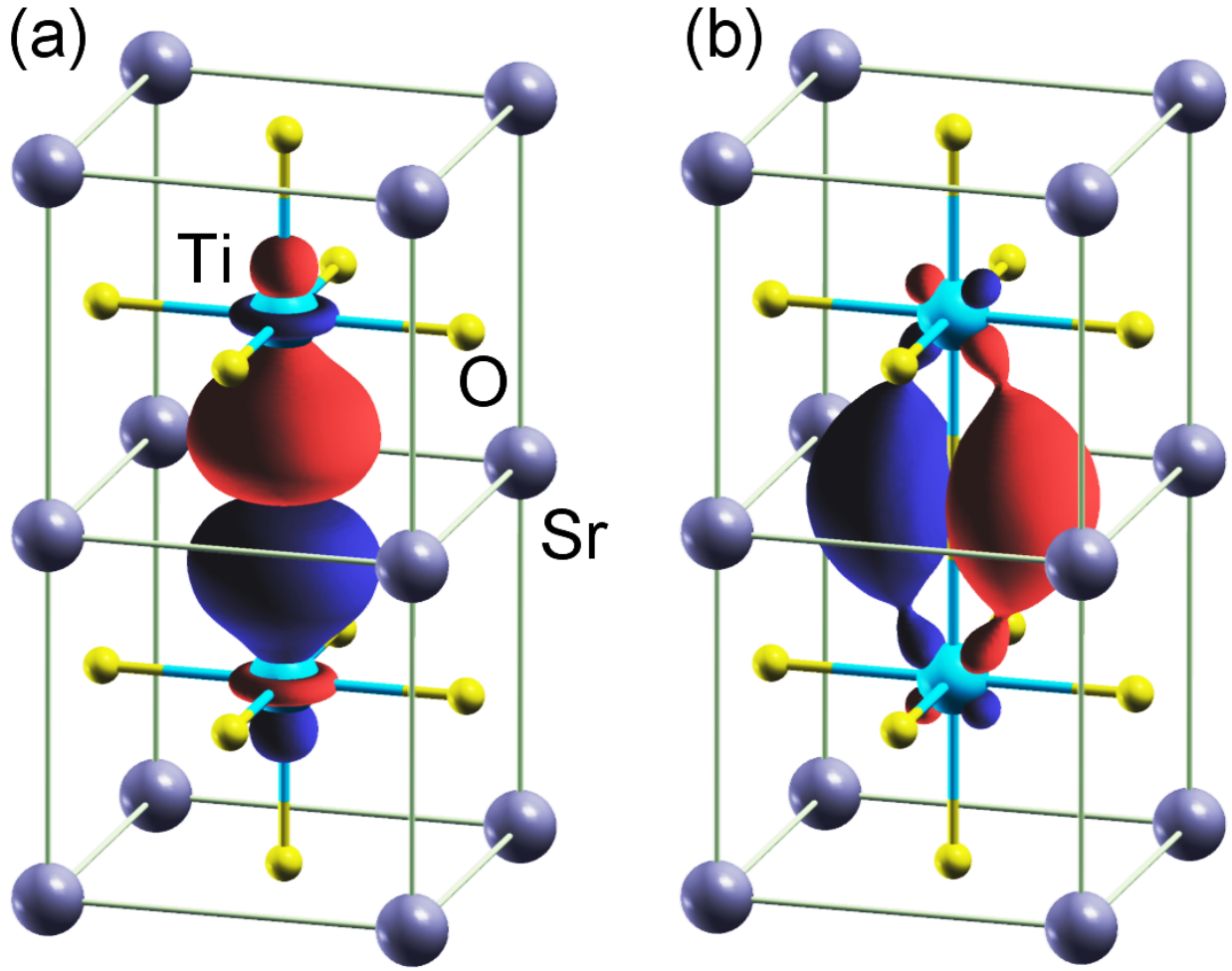


Ti *3d*

O *2p*


Ferroelectric $BaTiO_3$

WFs in $SrTiO_3$



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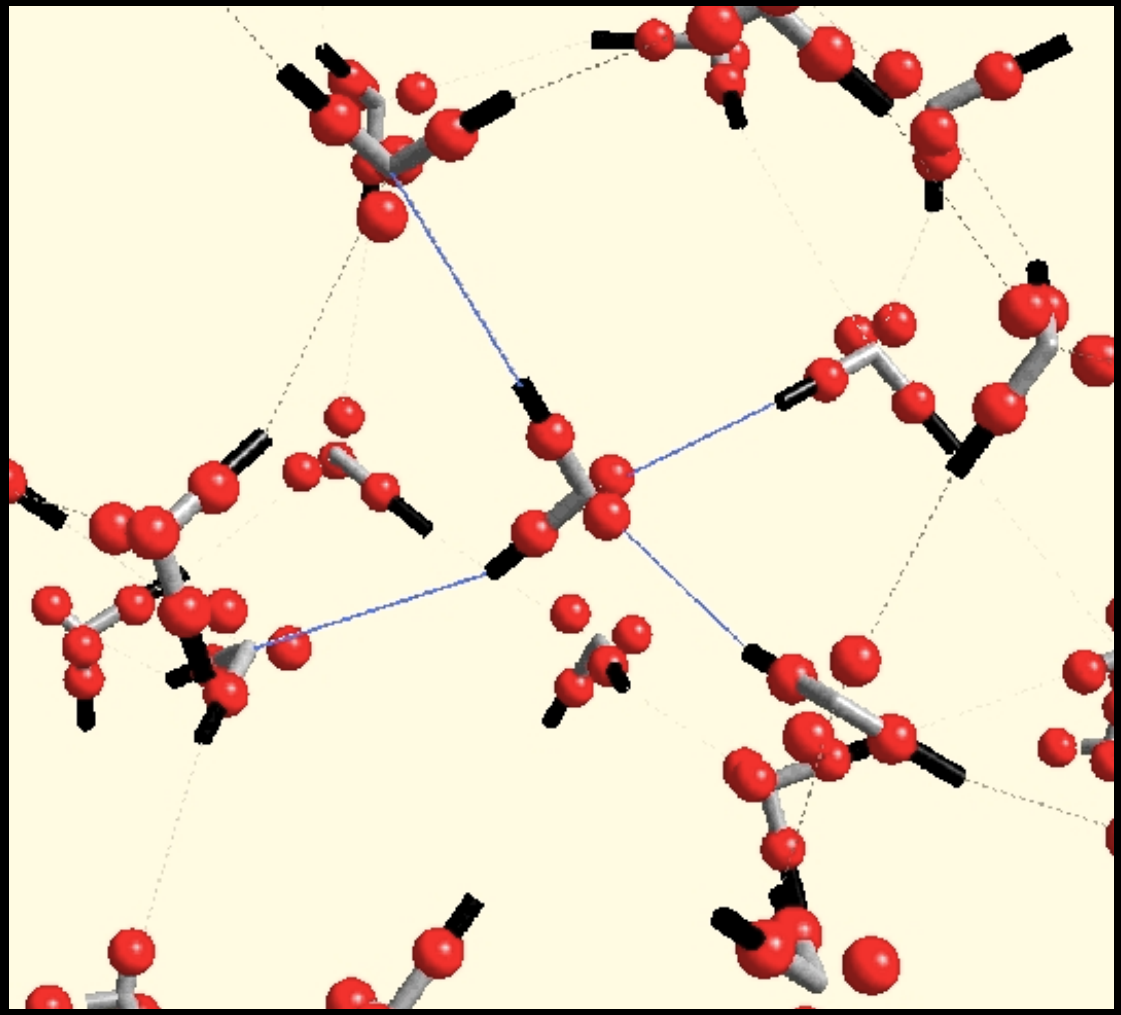
Wannier centers in *l-H_2O*



Silvestrelli et al.

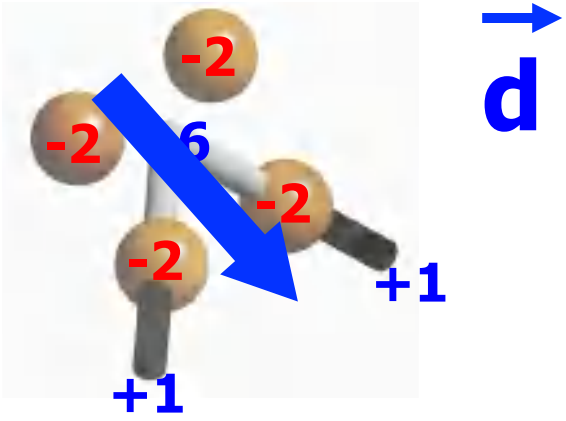
WFs define molecular dipoles

VOLUME 82, NUMBER 16 PHYSICAL REVIEW LETTERS 19 APRIL 1999

Water Molecule Dipole in the Gas and in the Liquid Phase

Pier Luigi Silvestrelli* and Michele Parrinello
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany
(Received 30 November 1998)

We study with *ab initio* molecular dynamics the change that the electric dipole moment of water molecules undergoes in passing from the gas to the liquid phase. Our analysis is based on the recently introduced maximally localized Wannier functions and is devoid of the ambiguities that have affected previous attempts. We find that in the liquid the dipole moment has an average value of about 3 D, 60% higher than in the gas phase. This value is much larger than is currently assumed (2.6 D). Furthermore, a broad distribution around this average value is observed. The relevance of these results for current modeling of water is discussed. [S0031-9007(99)08956-5]



Dipole moments in liquid phase

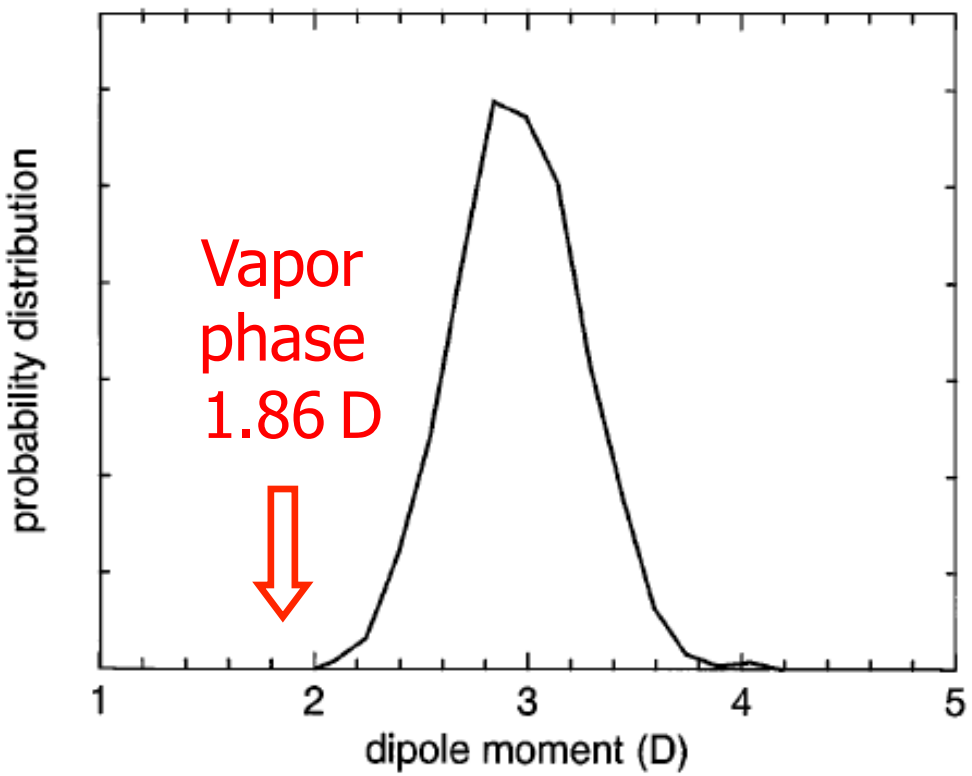
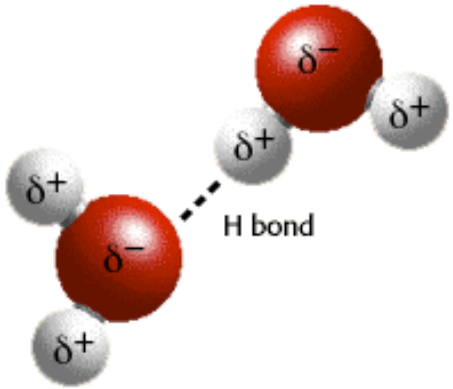
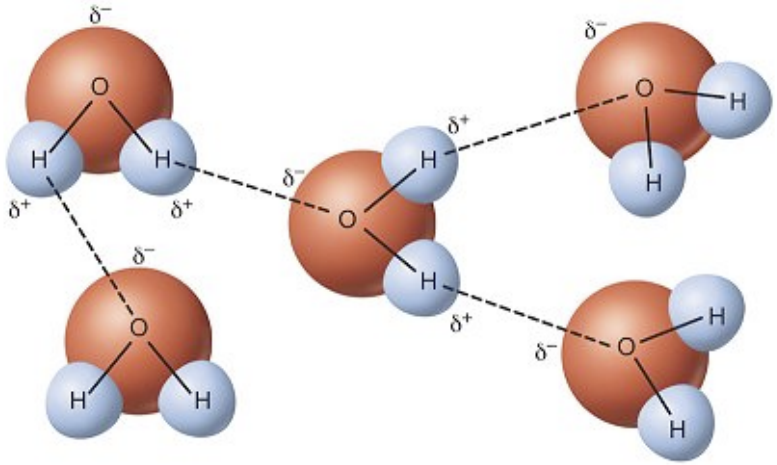


FIG. 4. Distribution of the modulus of the water molecule dipole moment in liquid water, by considering 12 molecular dynamics configurations.

Hydrogen bonds in water





H bonds enhance dipole moments of molecules

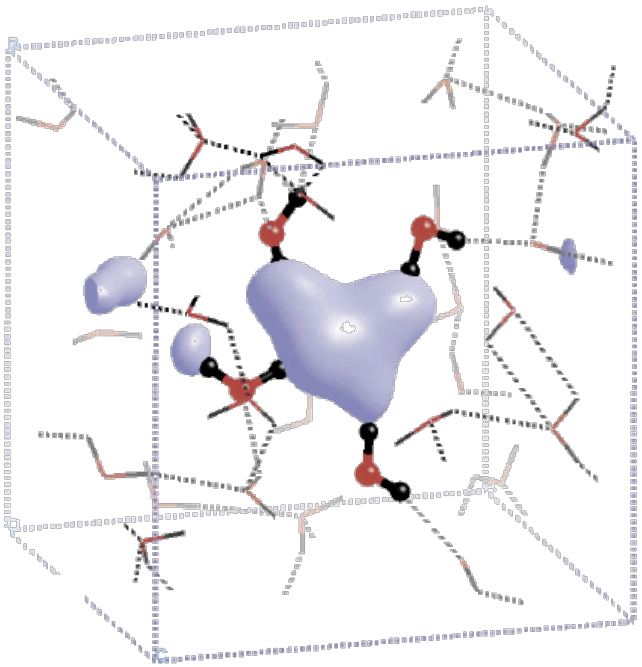
Wannier function of hydrated electron

VOLUME 90, NUMBER 22 PHYSICAL REVIEW LETTERS week ending 6 JUNE 2003

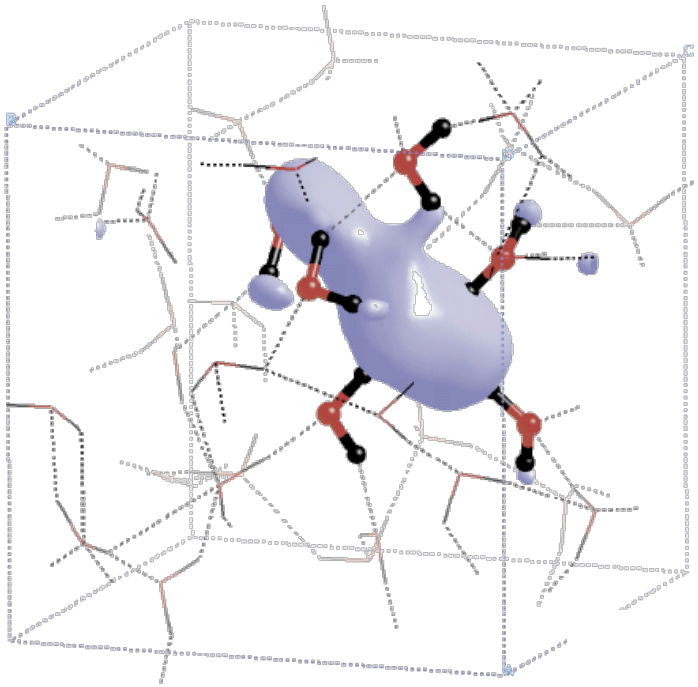
First-Principles Molecular-Dynamics Simulations of a Hydrated Electron in Normal and Supercritical Water

Mauro Boero,[1,2] Michele Parrinello,[3] Kiyoyuki Terakura,[2] Tamio Ikeshoji,[2] and Chee Chin Liew[2]

Supercritical water



Normal water



RUTGERS

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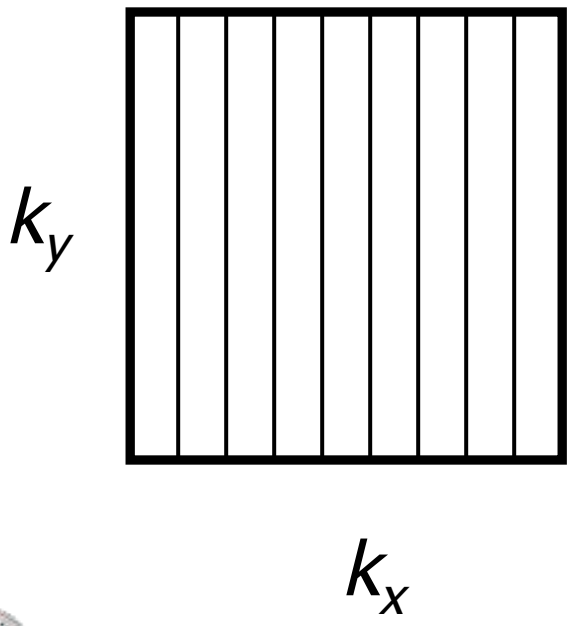
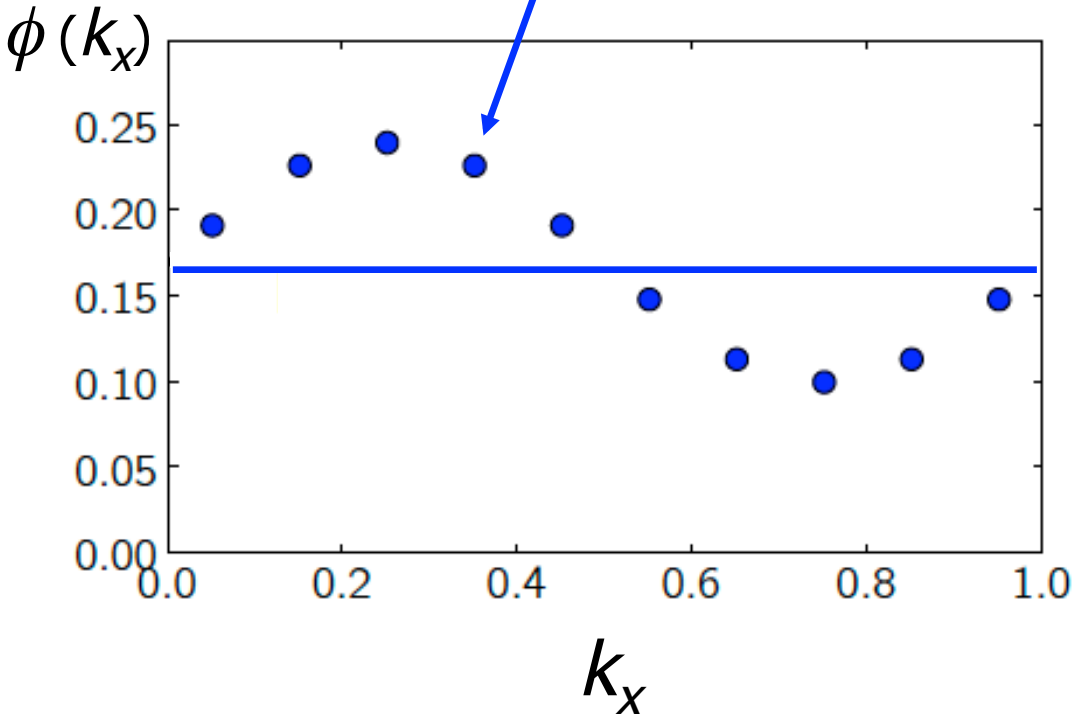
Polarization in a 2D insulator

$\phi(k_x)$ = Berry phase along y at given k_x

= "Hybrid Wannier centers"



$P_y(k_x) \propto \phi(k_x)$



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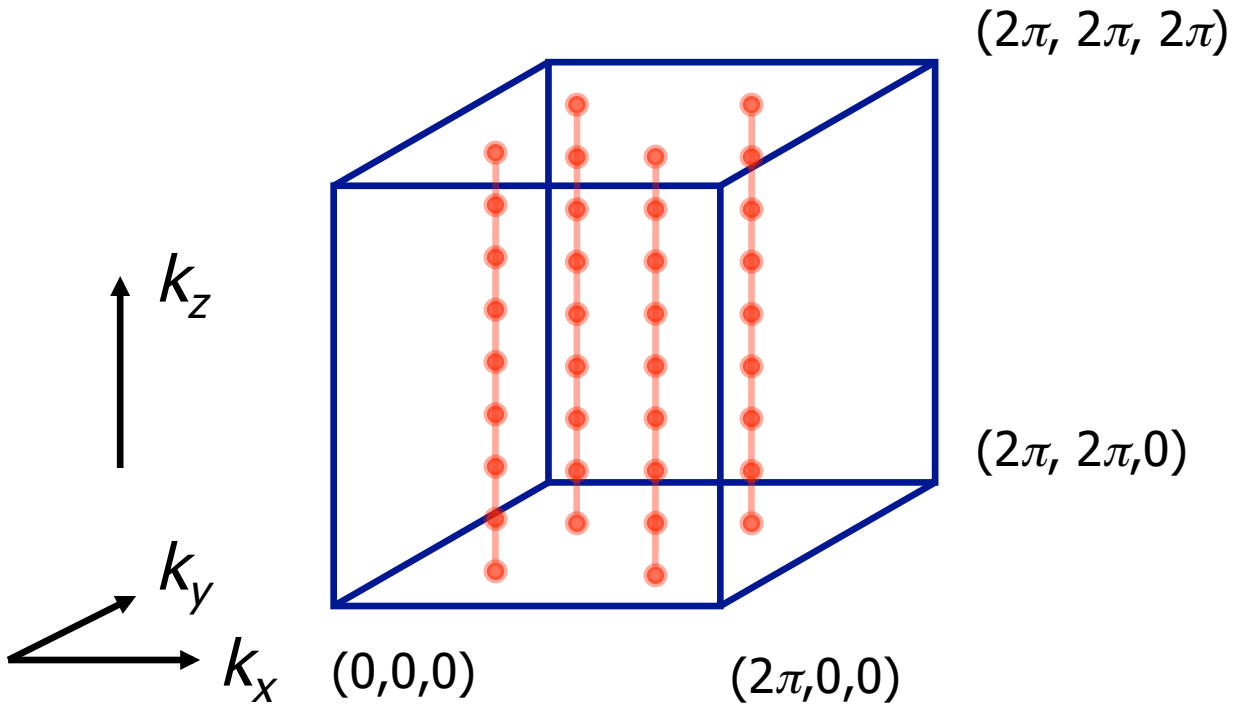
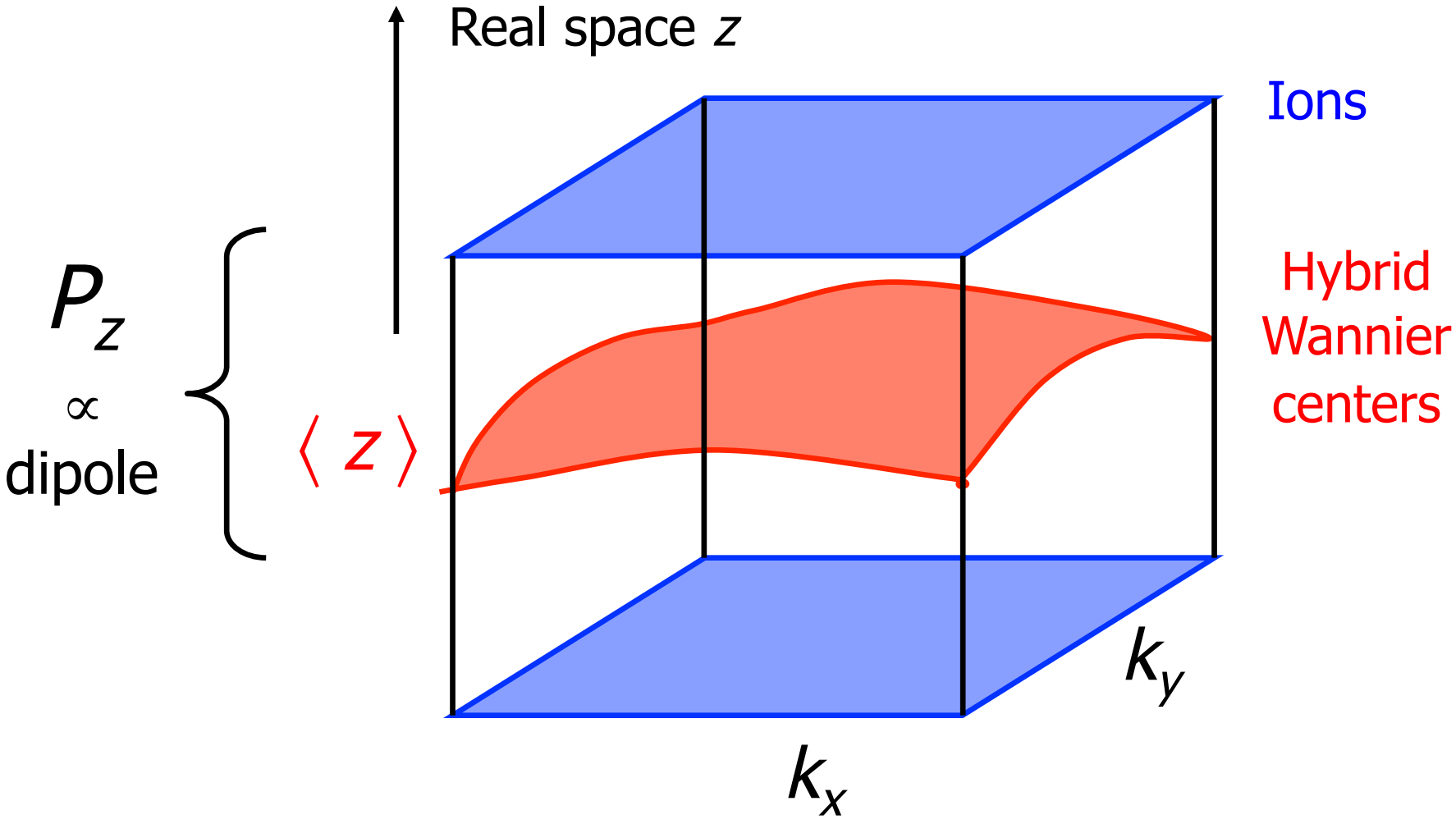
Polarization in 3D: Hybrid WFs again

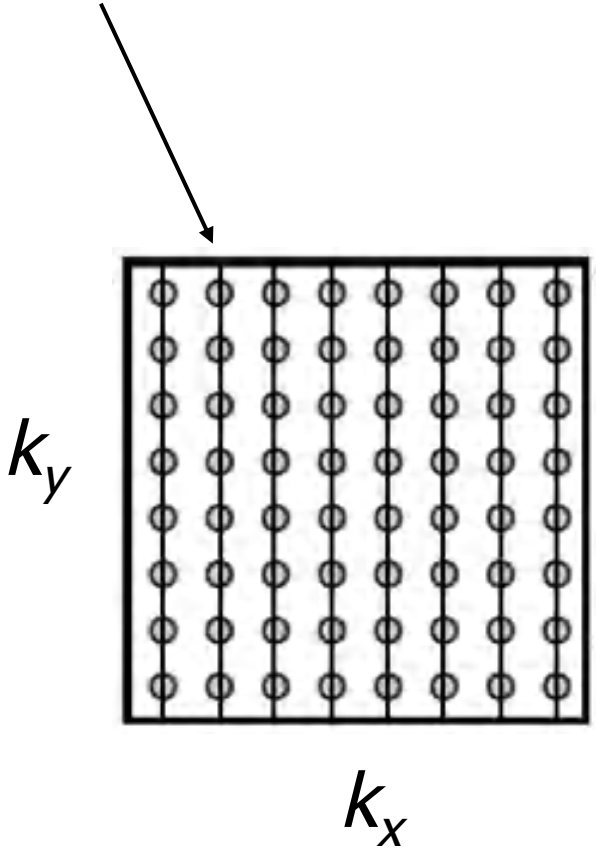


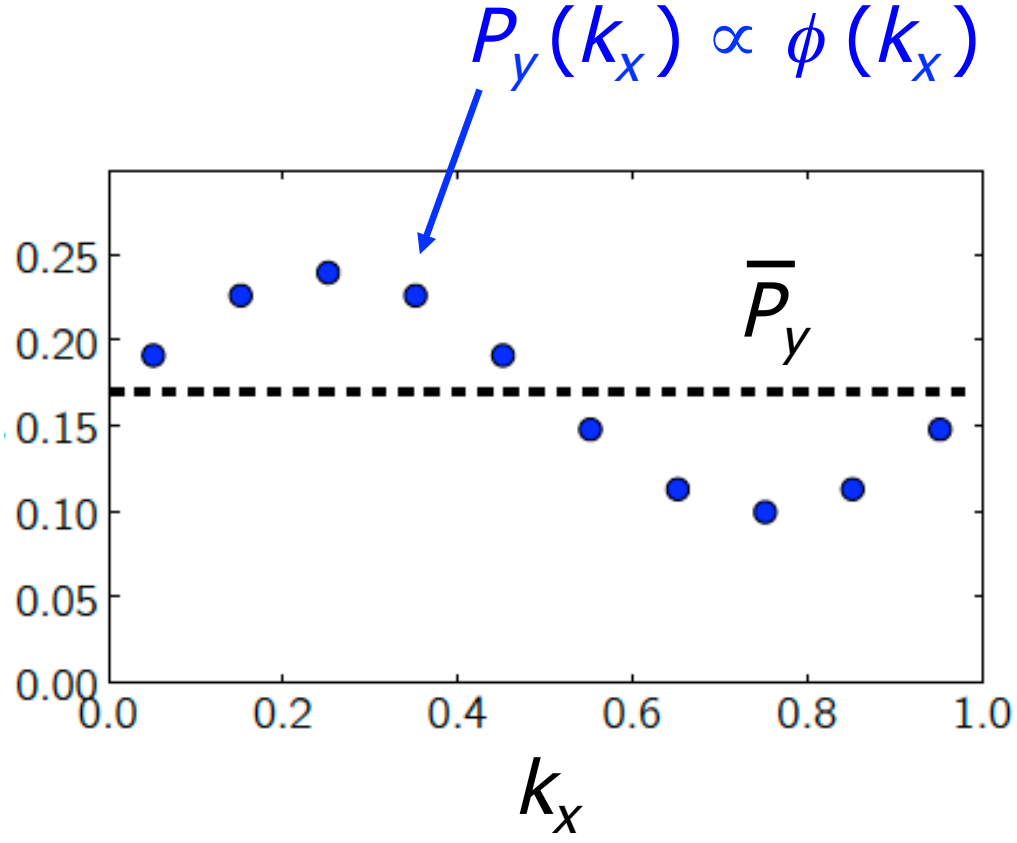
Polarization in a 3D insulator



Hybrid Wannier centers for normal band

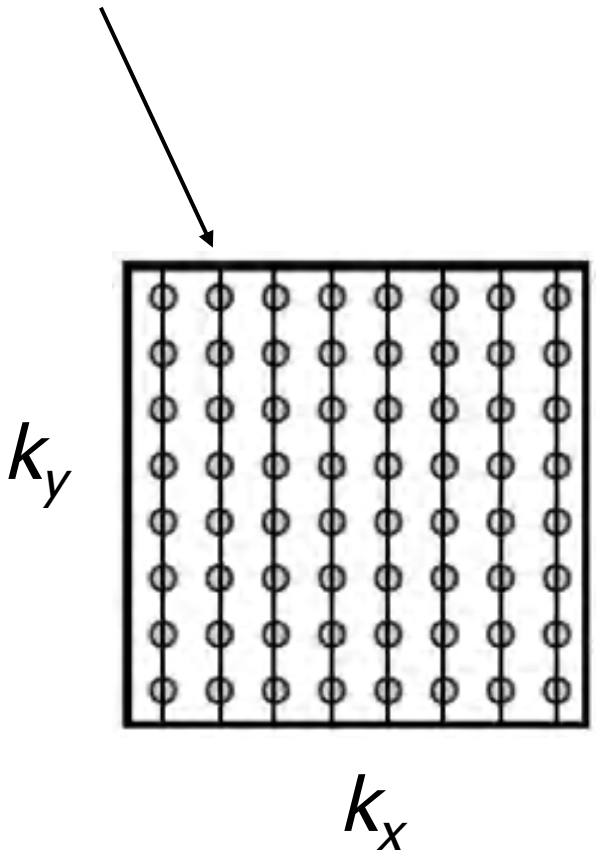
$\phi(k_x)$ $\quad -\mathrm{Im}\ \ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n\ \ 1}|u_n\rangle\right]$

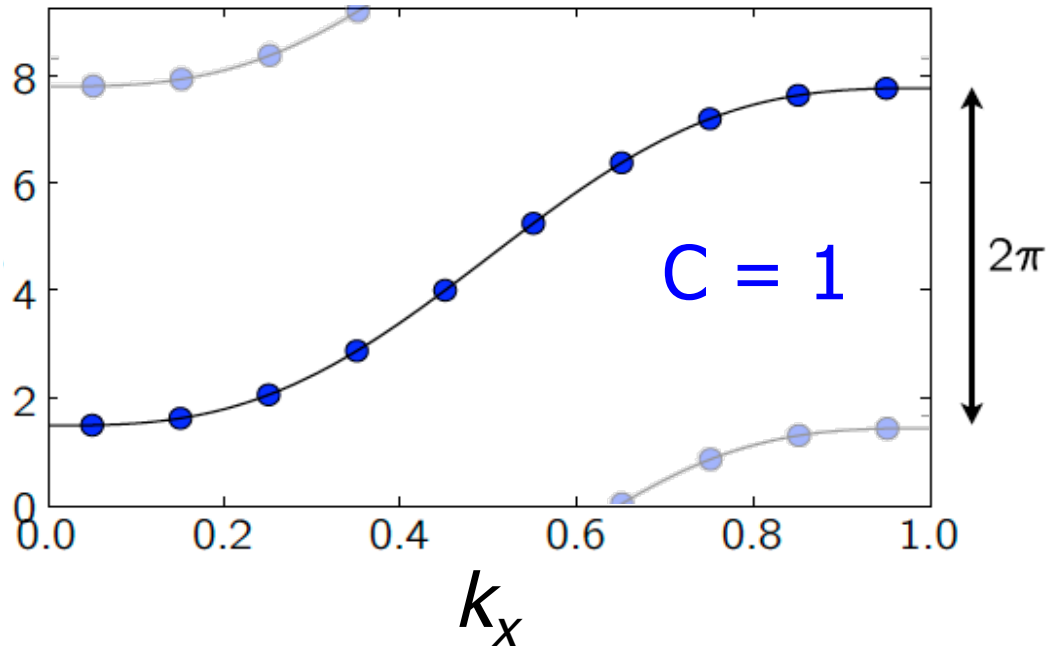




Hybrid Wannier centers for QAH band

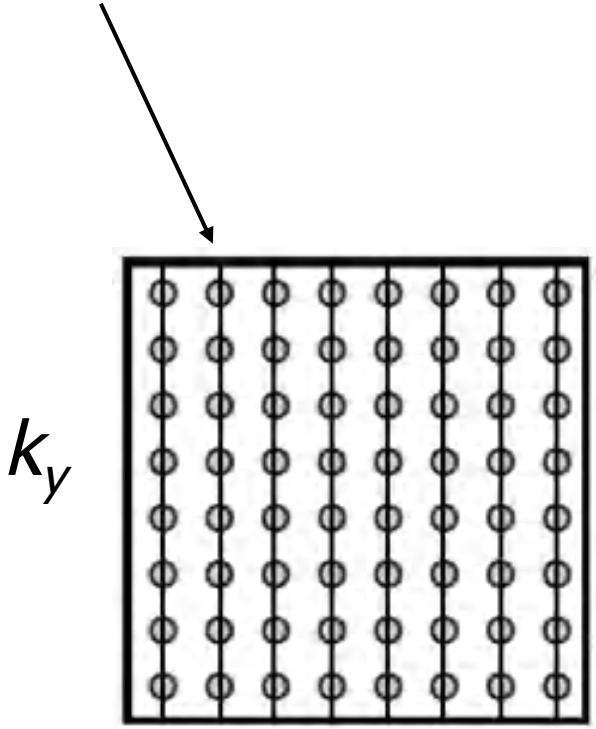
$\phi(k_x)$ $\quad -\mathrm{Im}\ \ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle \ldots \langle u_{n\ \ 1}|u_n\rangle\right]$

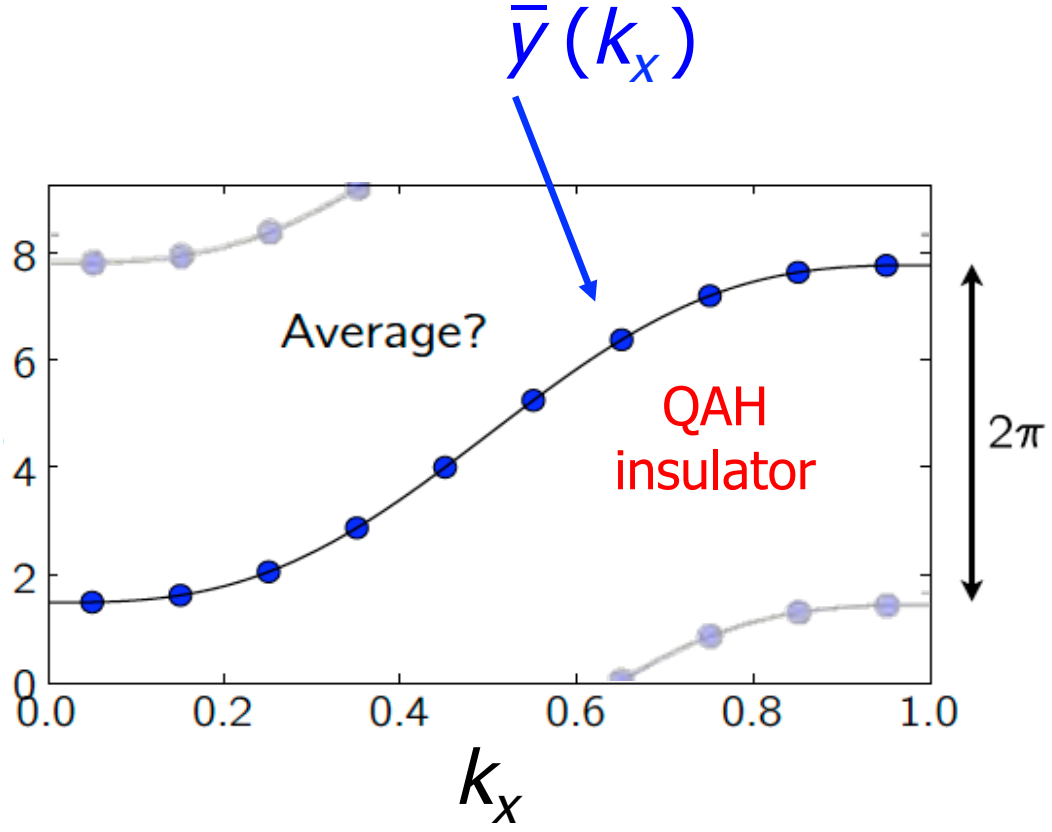




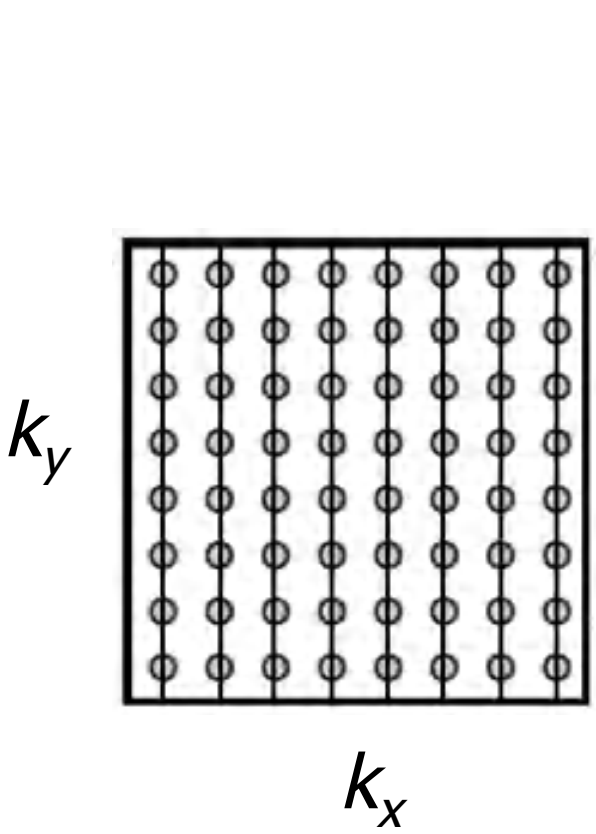
QAH: Hybrid WF centers $\bar{y}(k_x)$

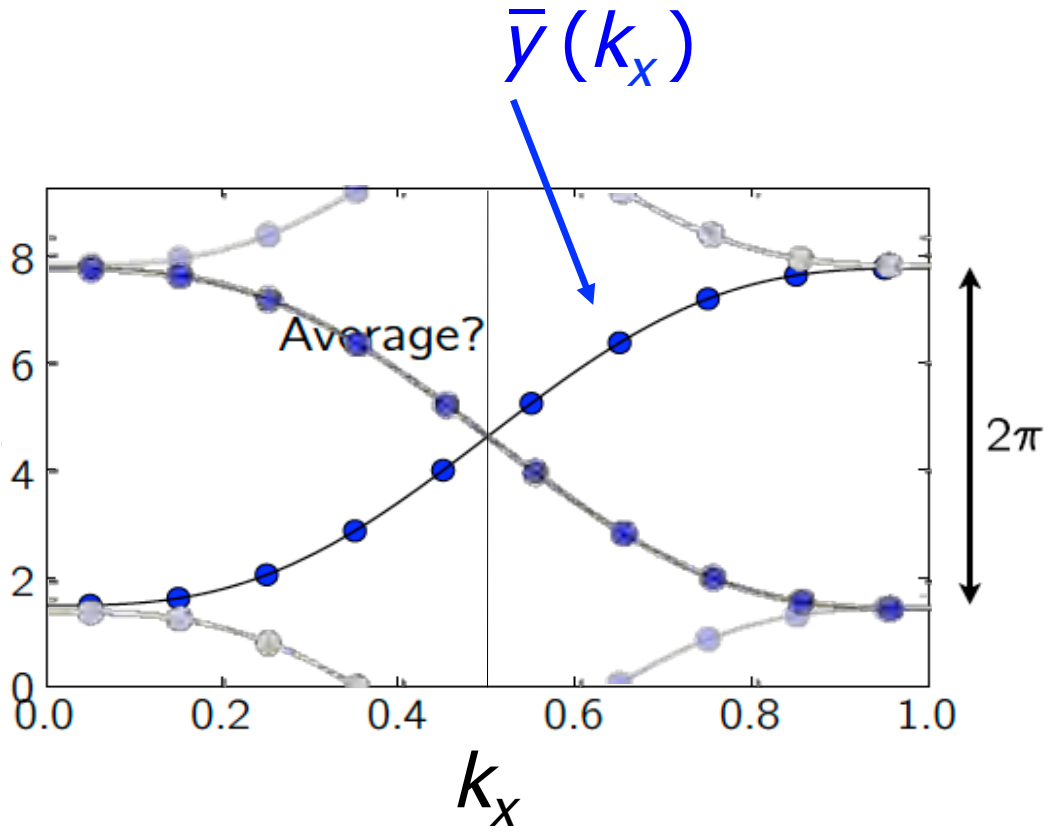
$\phi(k_x)$ $\quad -\mathrm{Im}\ \ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n\ \ 1}|u_n\rangle\right]$



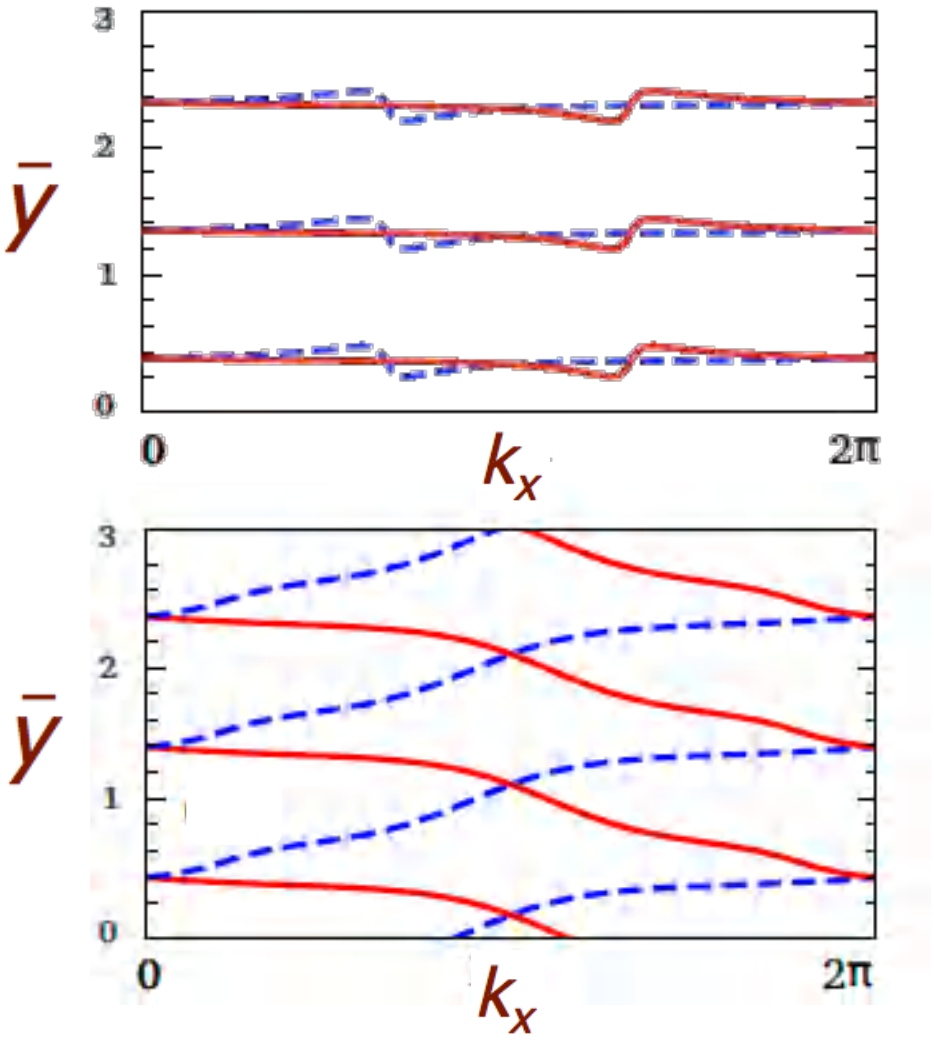


Z_2 insulator: Hybrid WF centers $\bar{y}(k_x)$





Z_2 insulator: Hybrid WF centers $\bar{y}(k_x)$

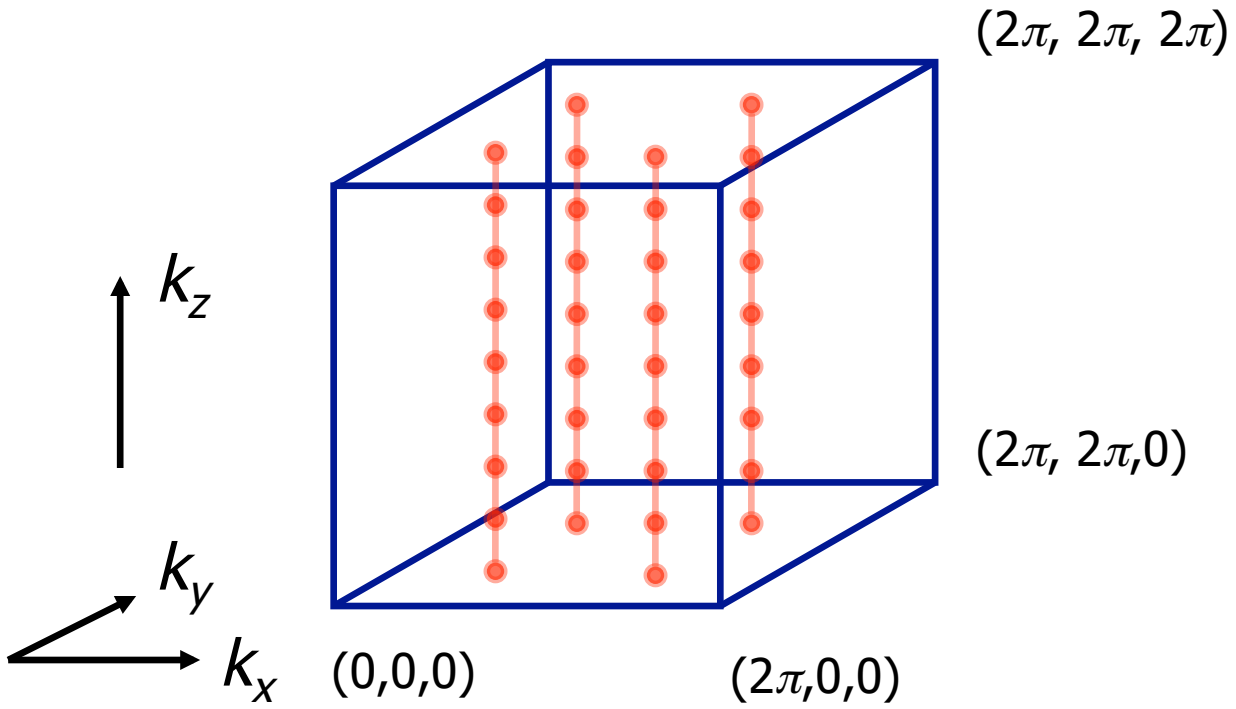


Normal

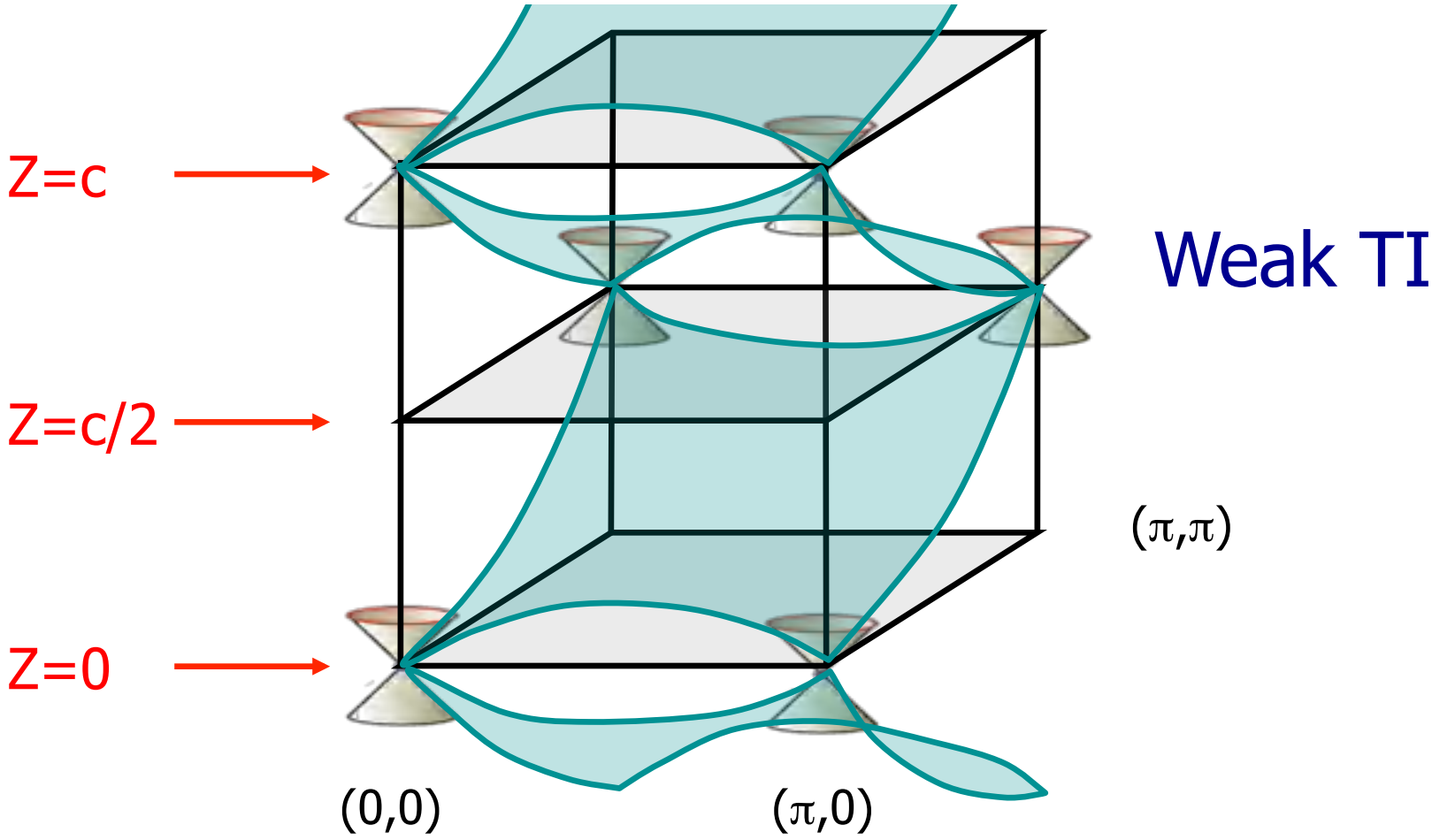
Kane-Mele tight-binding model

Z_2-odd

Polarization in 3D: Hybrid WFs again



Hybrid WF sheets



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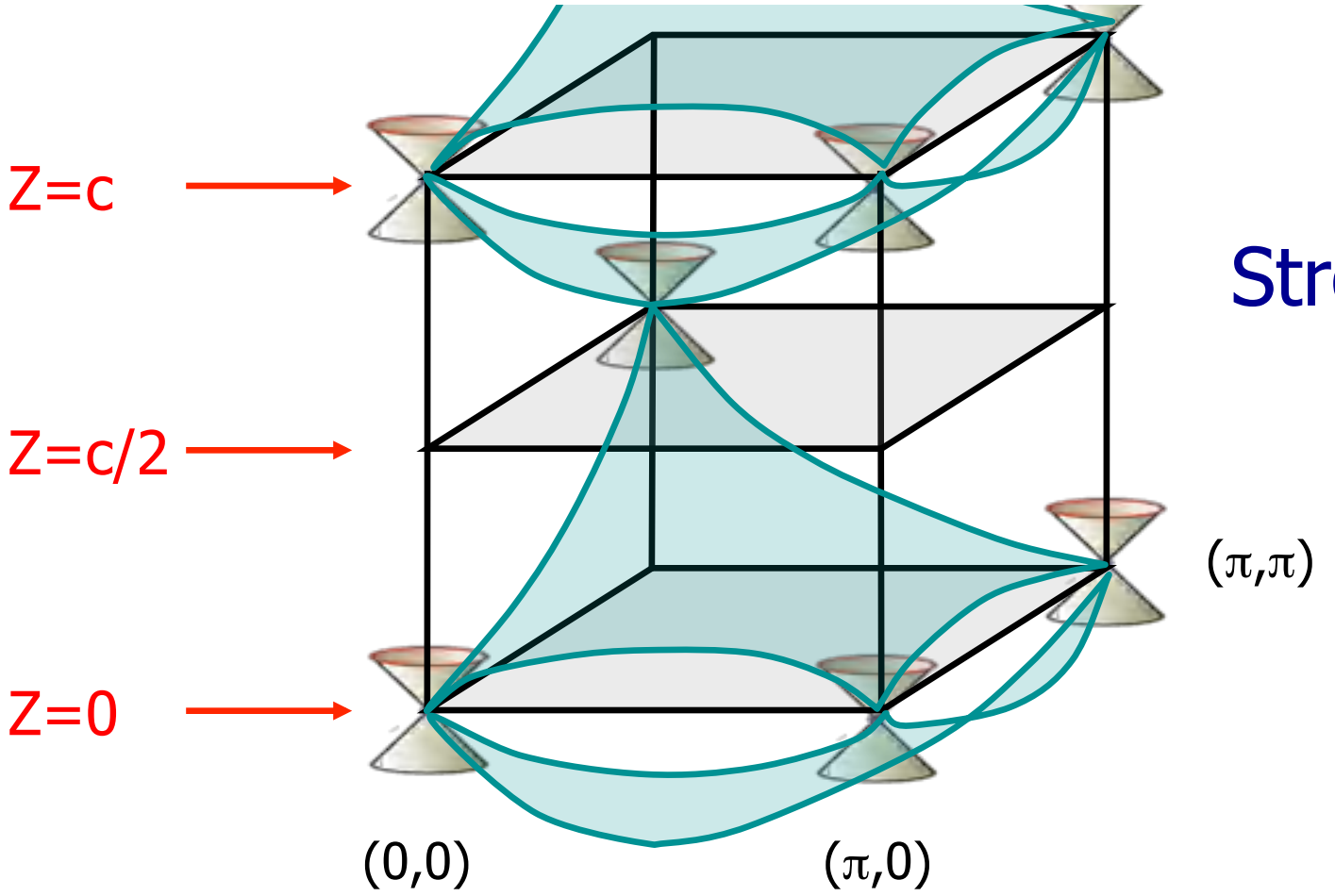
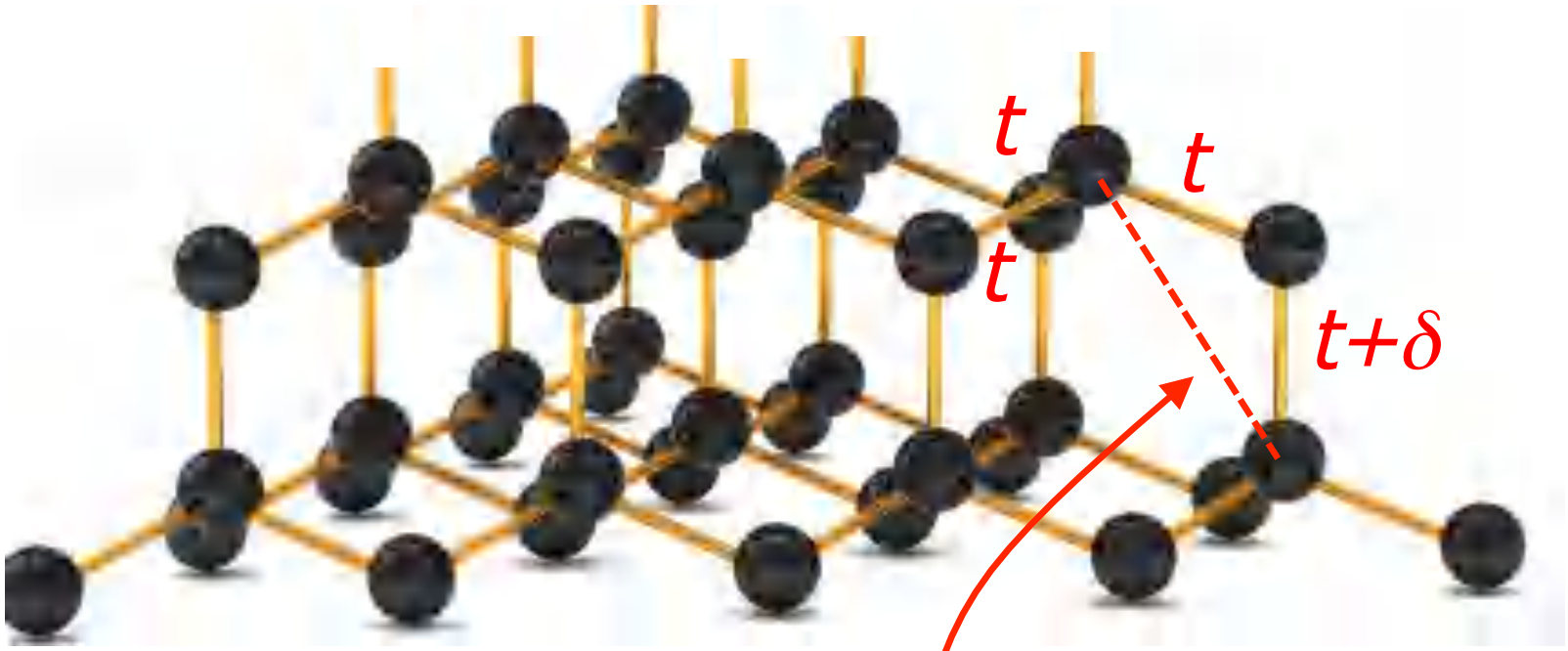


Strong TI

3D Kane-Mele model



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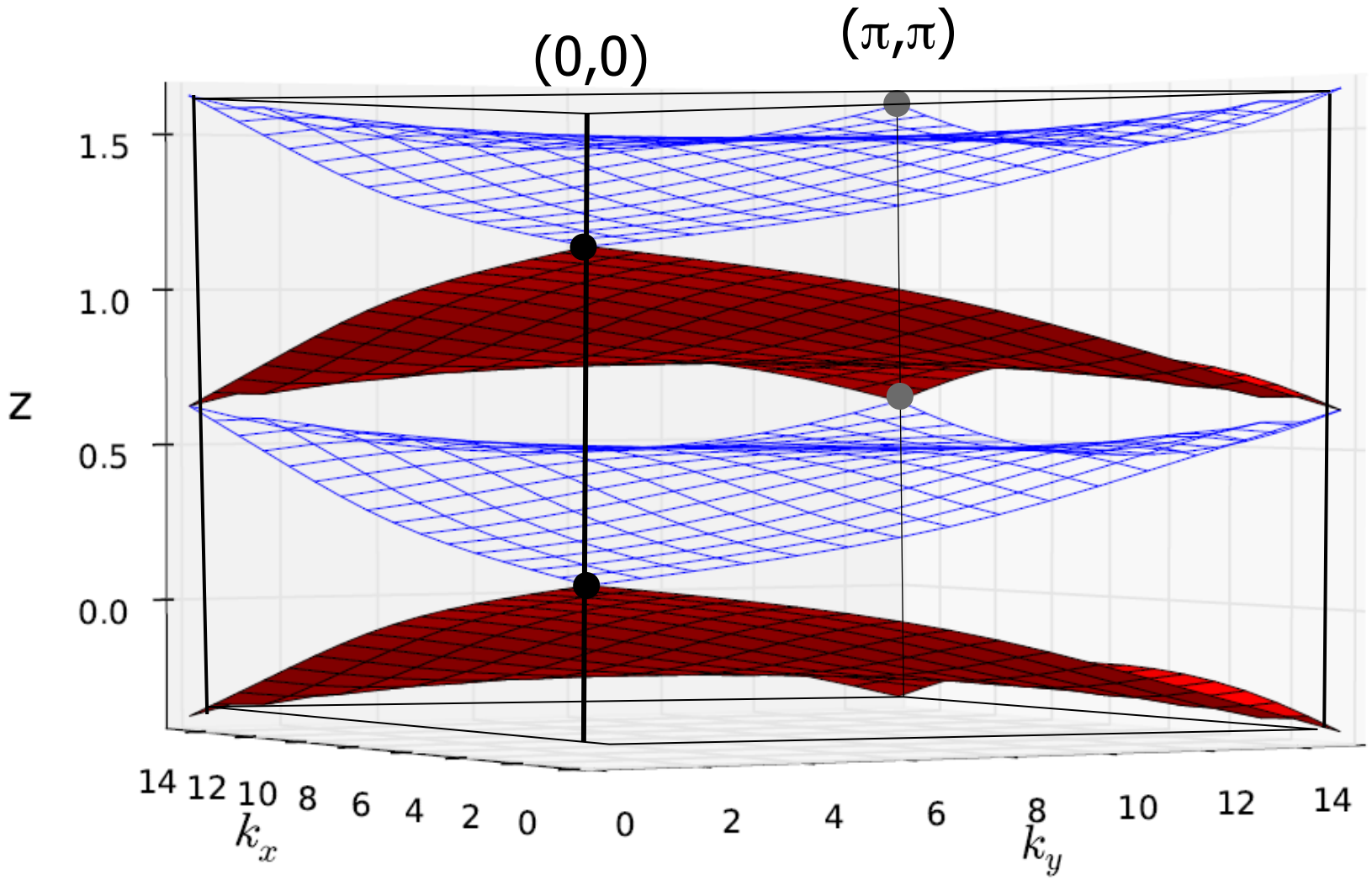
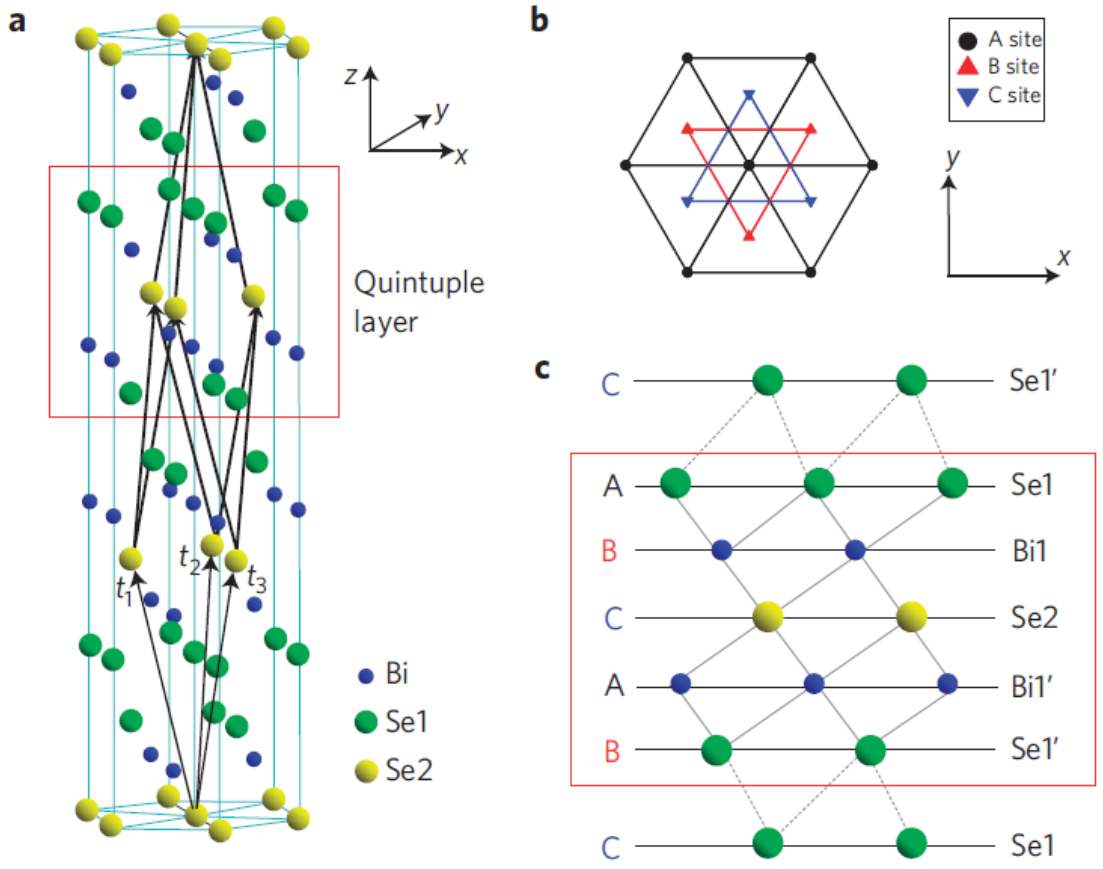


First-principles calculation: Bi_2Se_3



H. Zhang et al., Nature Physics **5**, 2009

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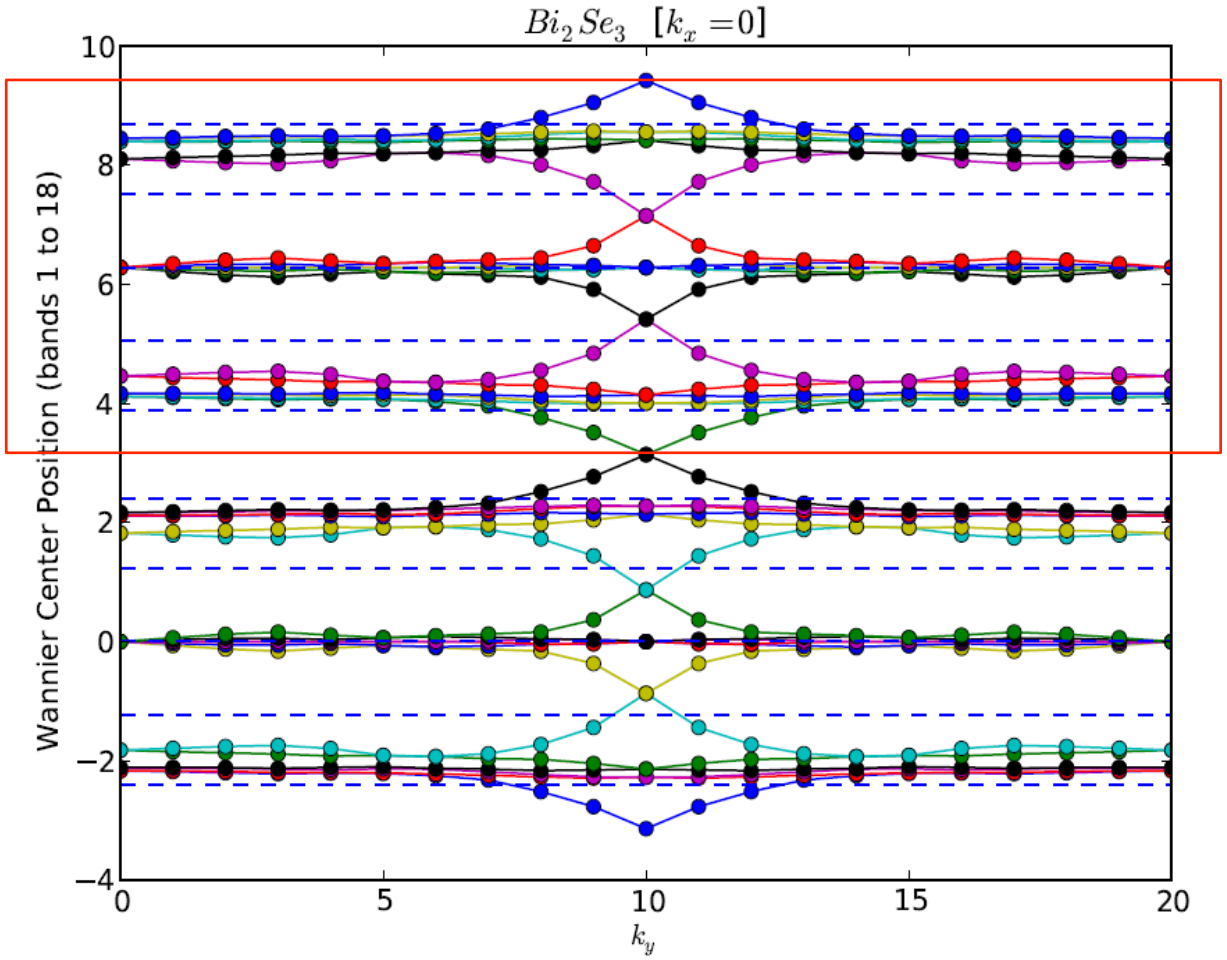
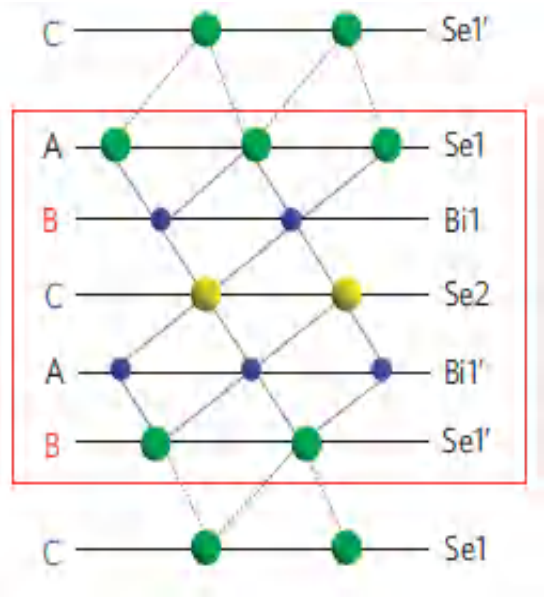
First-principles Bi_2Se_3 Wannier centers





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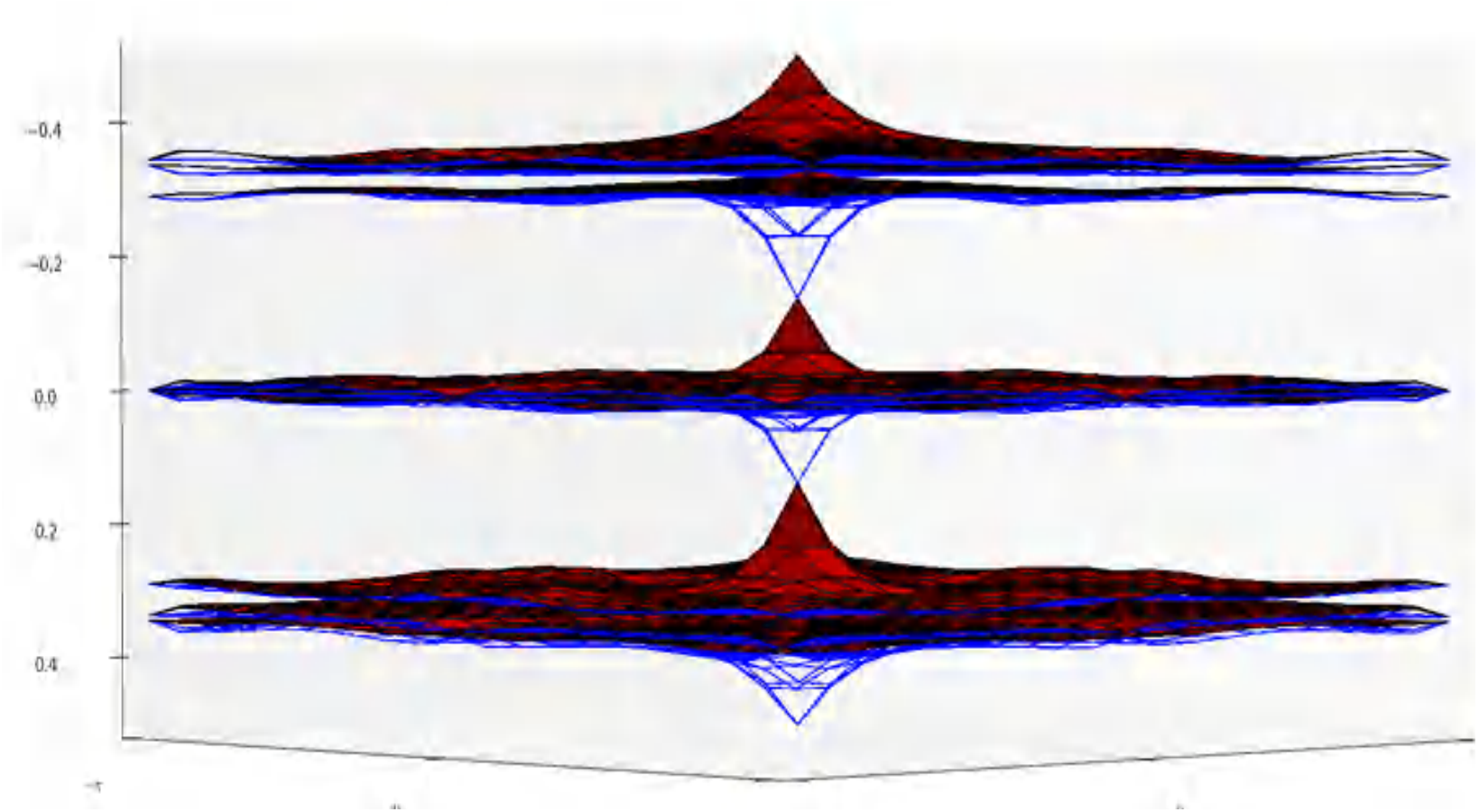
First-principles Bi_2Se_3 Wannier centers



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Summary

- Wannier interpolation
- Electric polarization and anomalous Hall
- Chemical bonding and polar properties
  - Covalent semiconductors and polymers
  - Perovskites
  - Liquid water
- Hybrid Wannier functions and centers

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Wannier90 code

Authors

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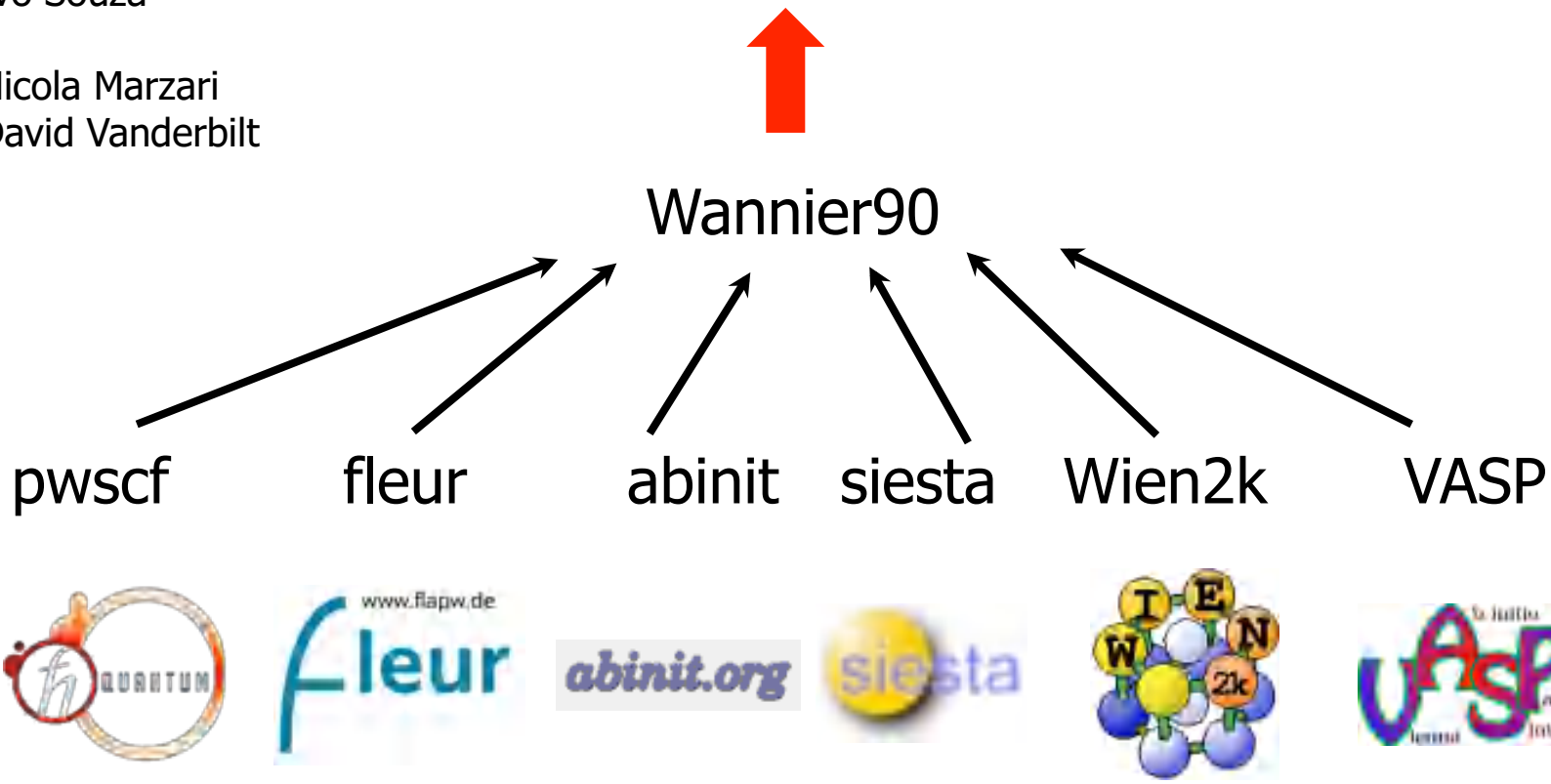
David Vanderbilt

Wannier interpolation, transport, etc.



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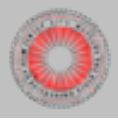
EXTRAS



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