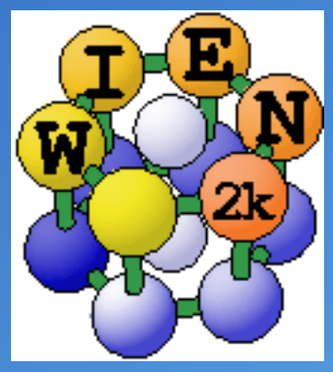
Effective band structure of supercells

Wannier functions

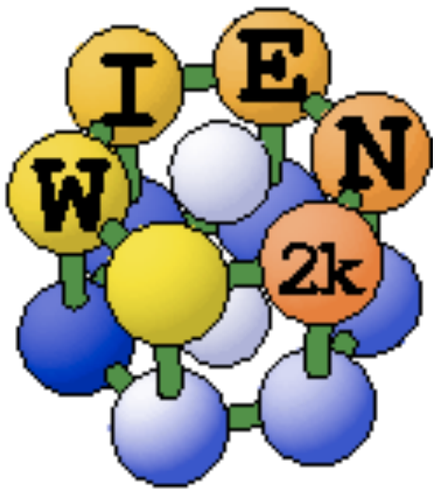
Oleg Rubel

Department of Materials Science and Engineering



McMaster University

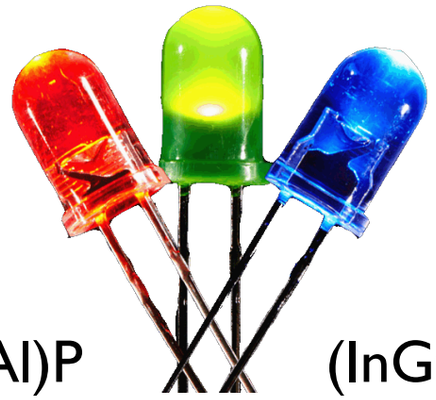
Effective band structure of supercells



+ fold2Bloch

https://github.com/rubel75/fold2Bloch-Wien2k

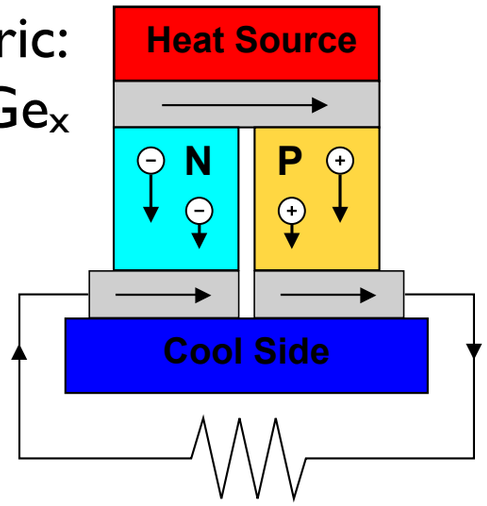
Semiconductor alloys

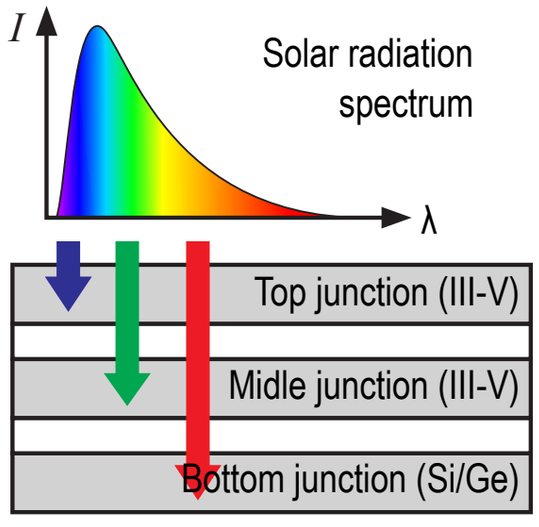


(InGaAl)P (InGa)N

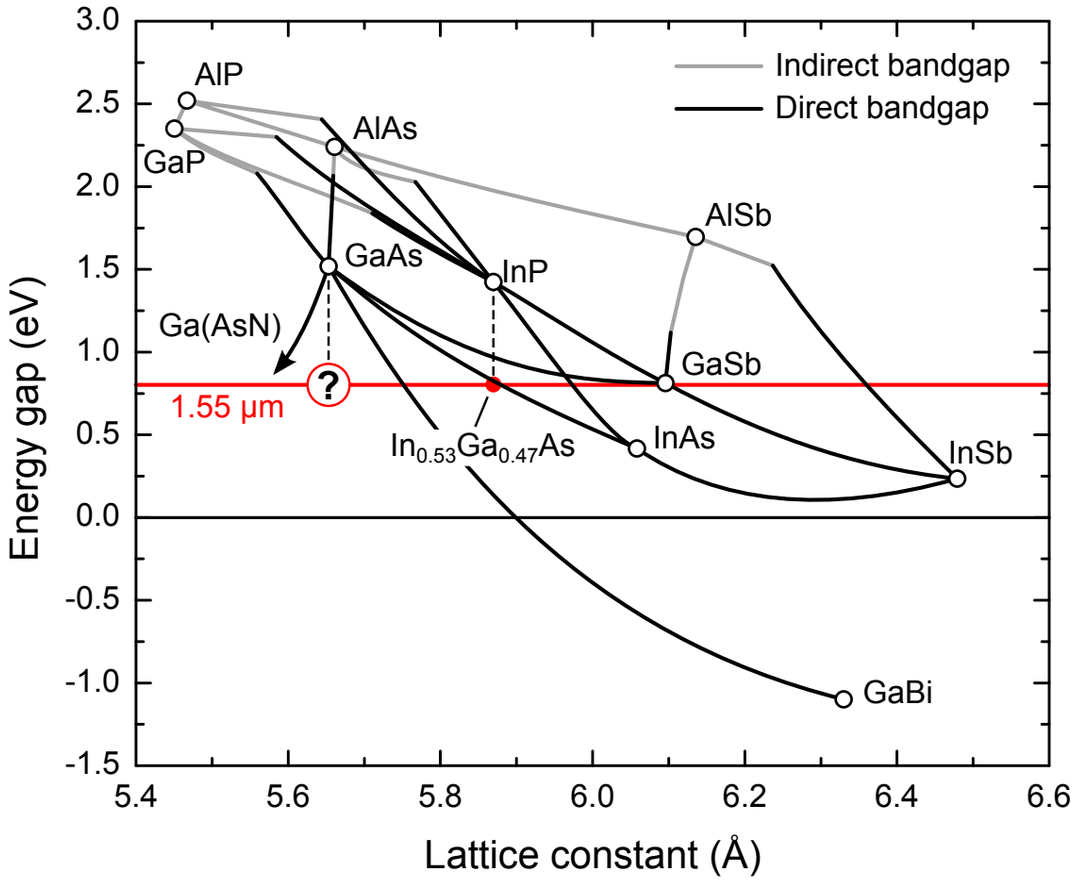
IR detector:
(HgCd)Te

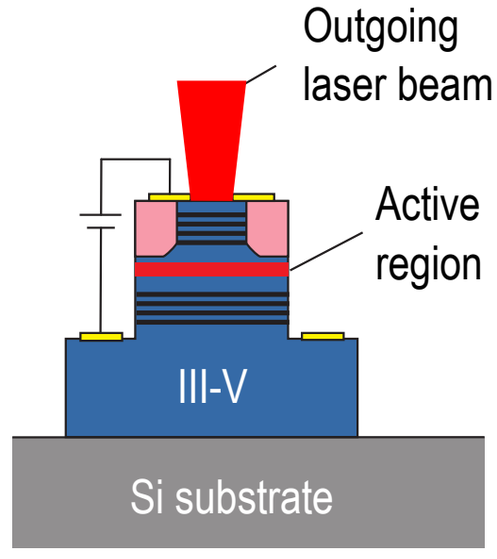
Thermoelectric:
$Si_{1-x}Ge_x$





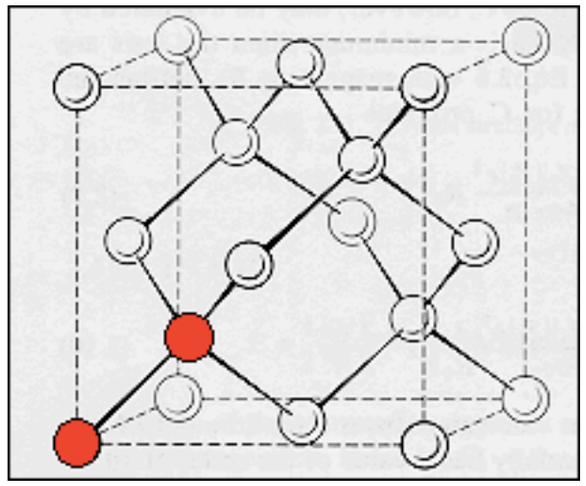
Eg = 1 eV junction:
(InGa)(NAs)





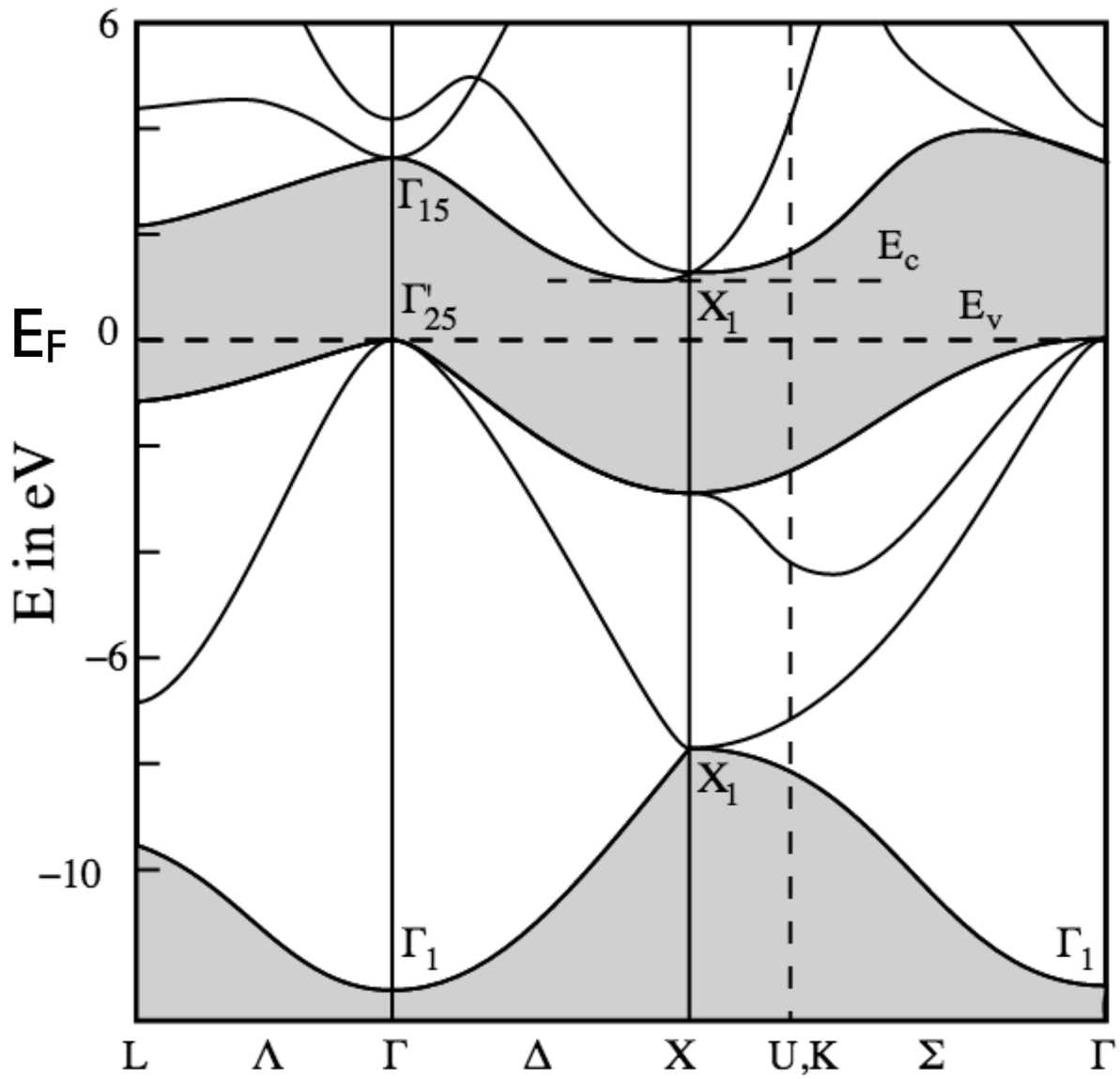
1.55 μm lasers:
(InGa)As
(InGa)(NAsSb)
Ga(AsBi)

Band structure



Silicon

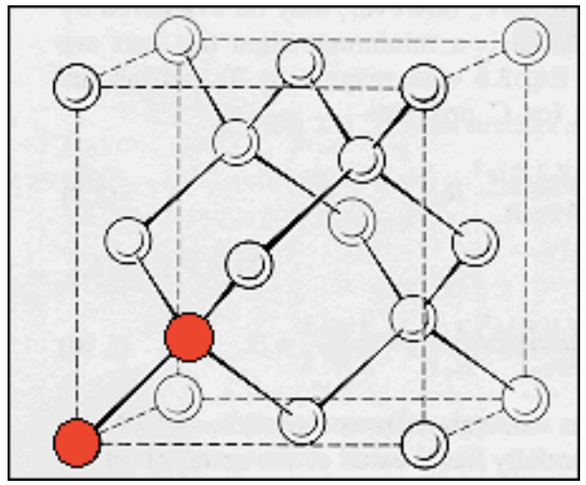
2-atom basis



Si

Bloch wave vector

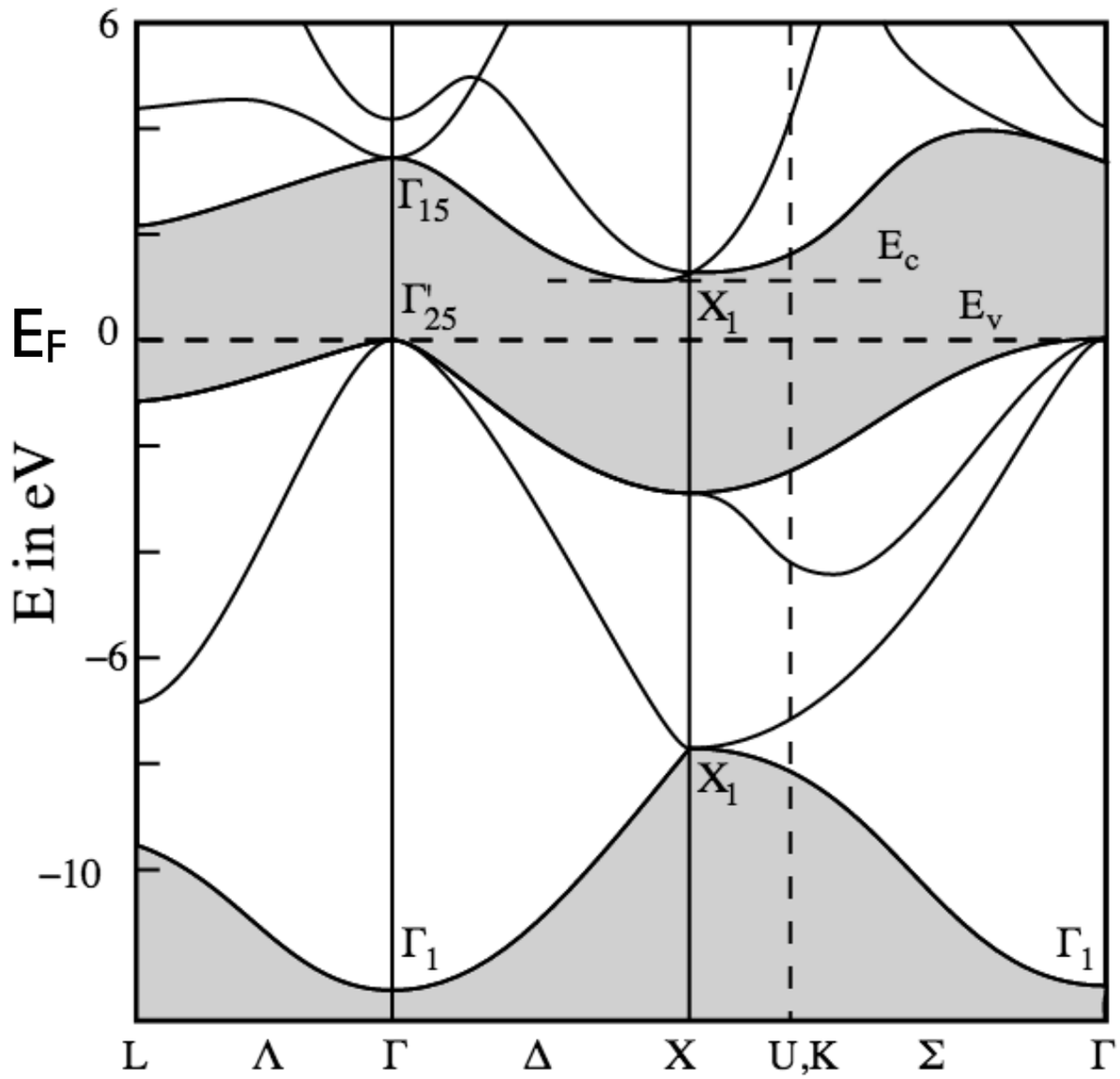
Band structure



Silicon

2-atom basis

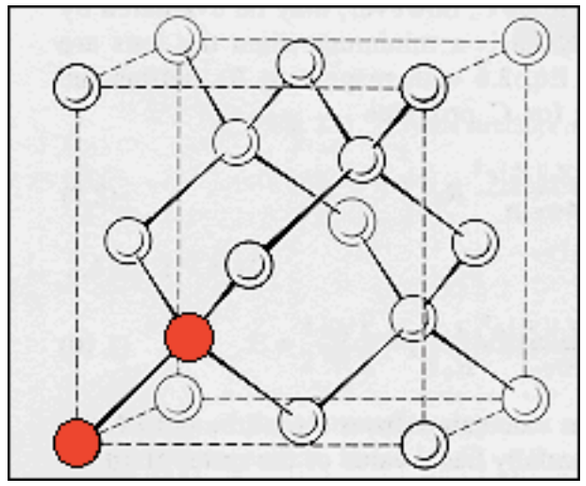
Energy gap



Si

Bloch wave vector

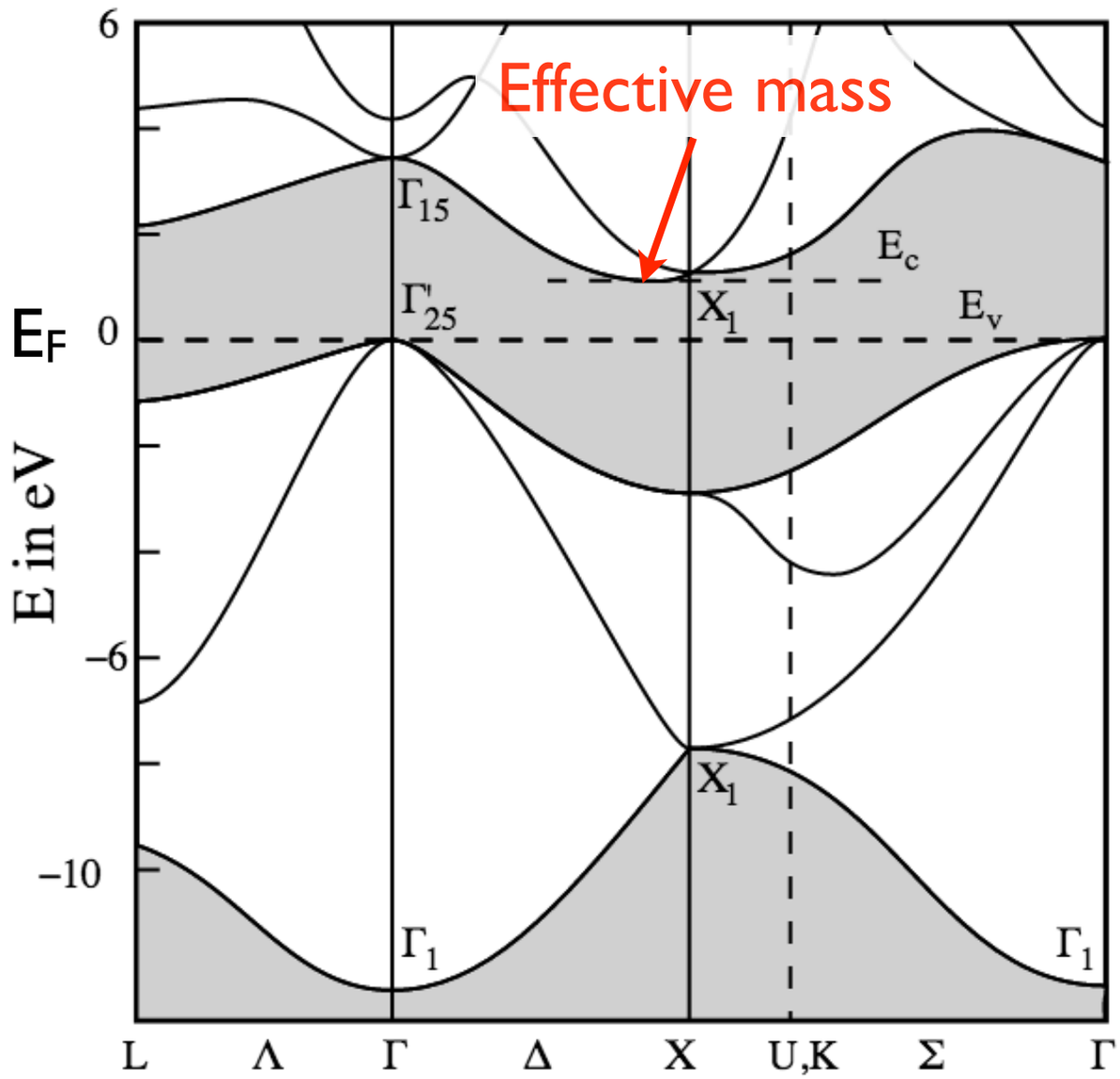
Band structure



Silicon

2-atom basis

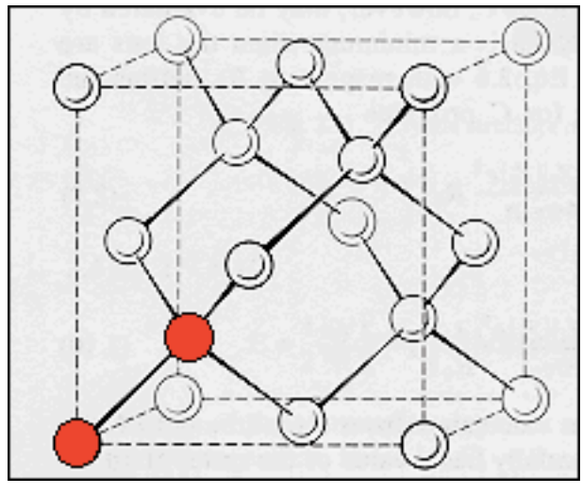
Energy gap



Si

Bloch wave vector

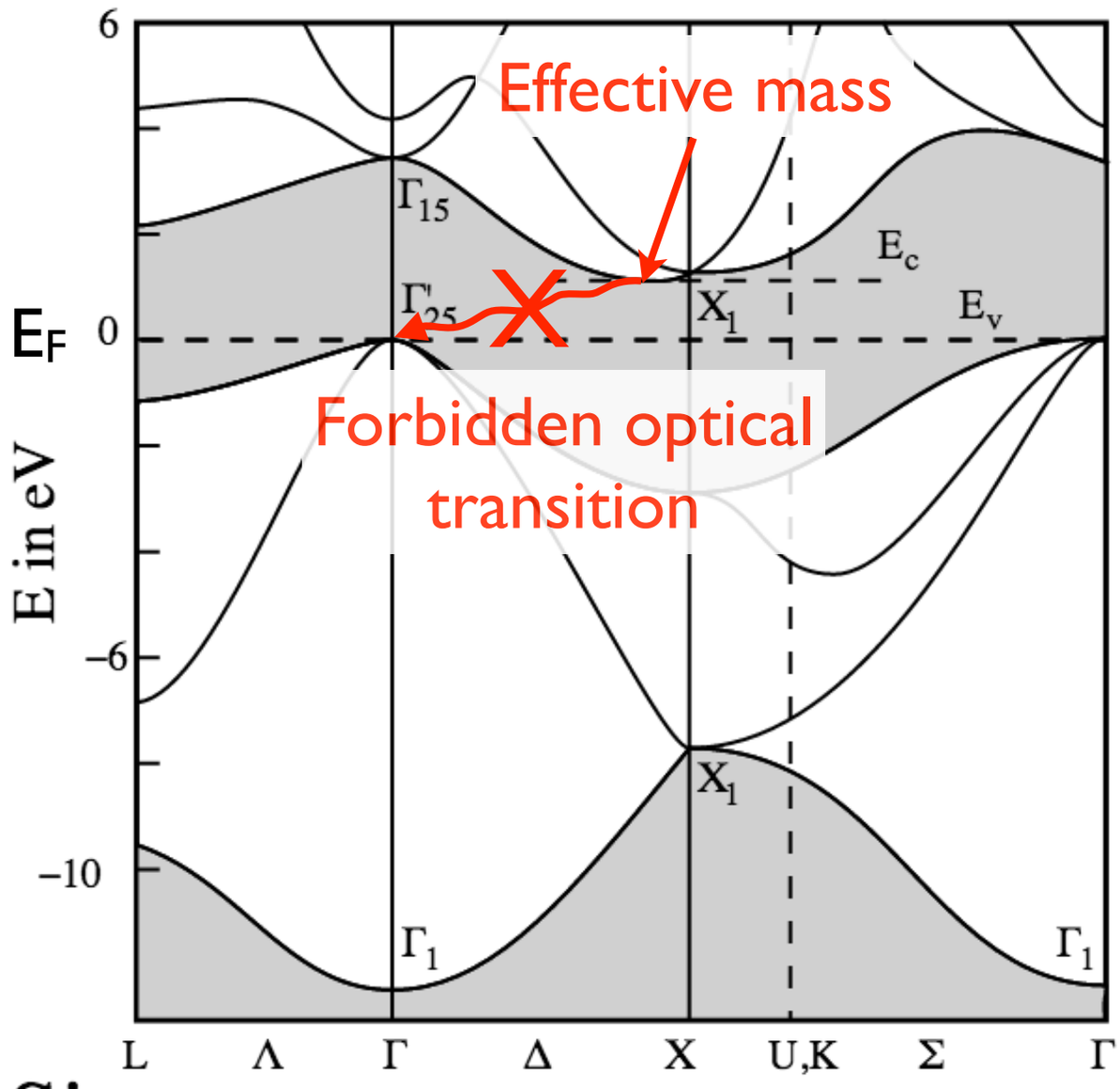
Band structure



Energy gap

Silicon

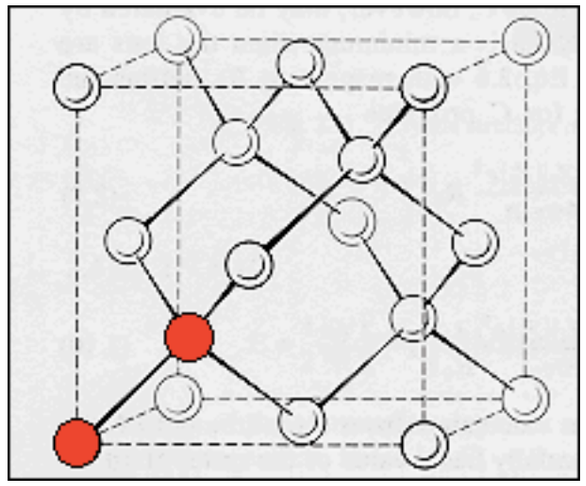
2-atom basis



Si

Bloch wave vector

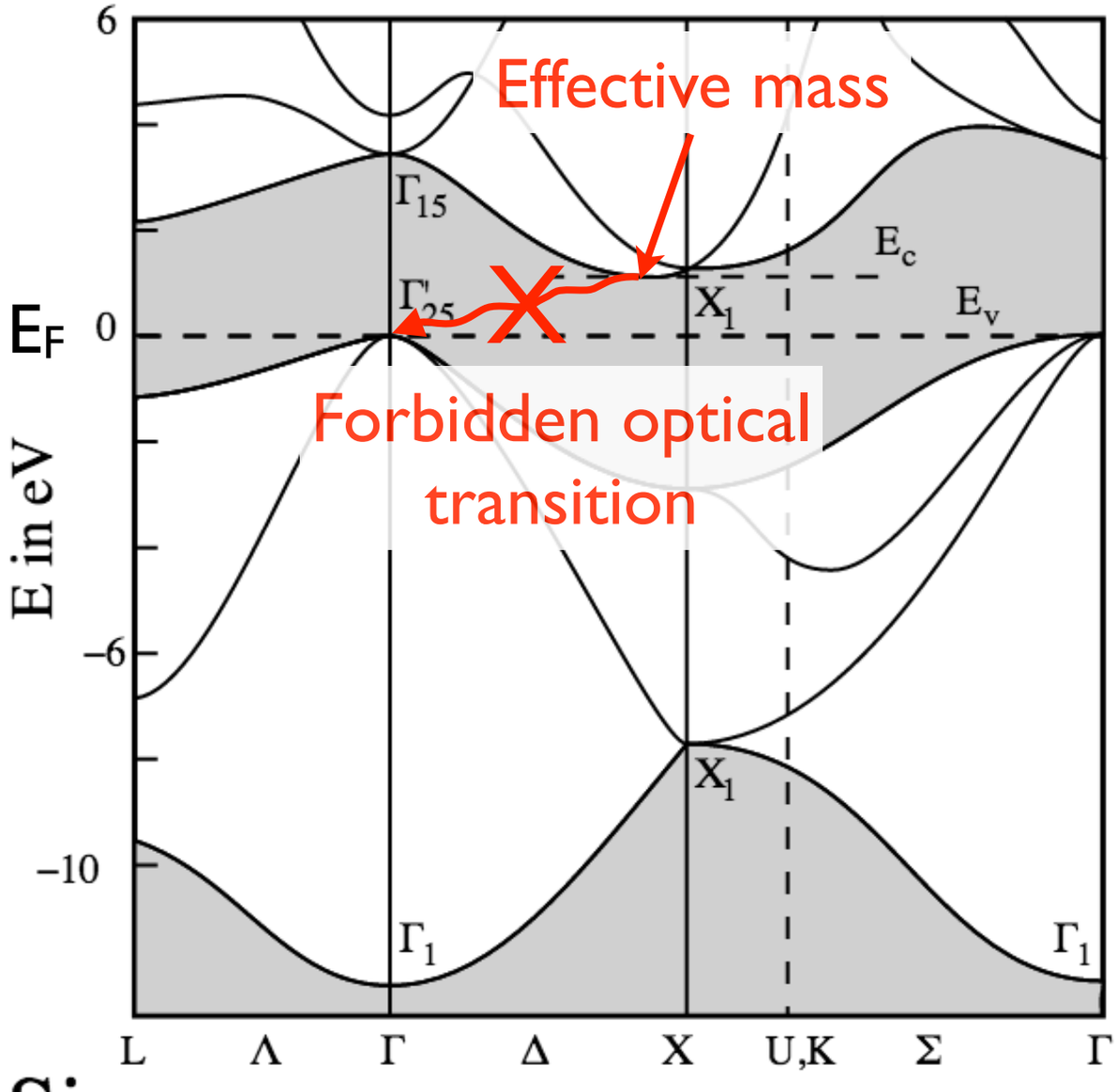
Band structure

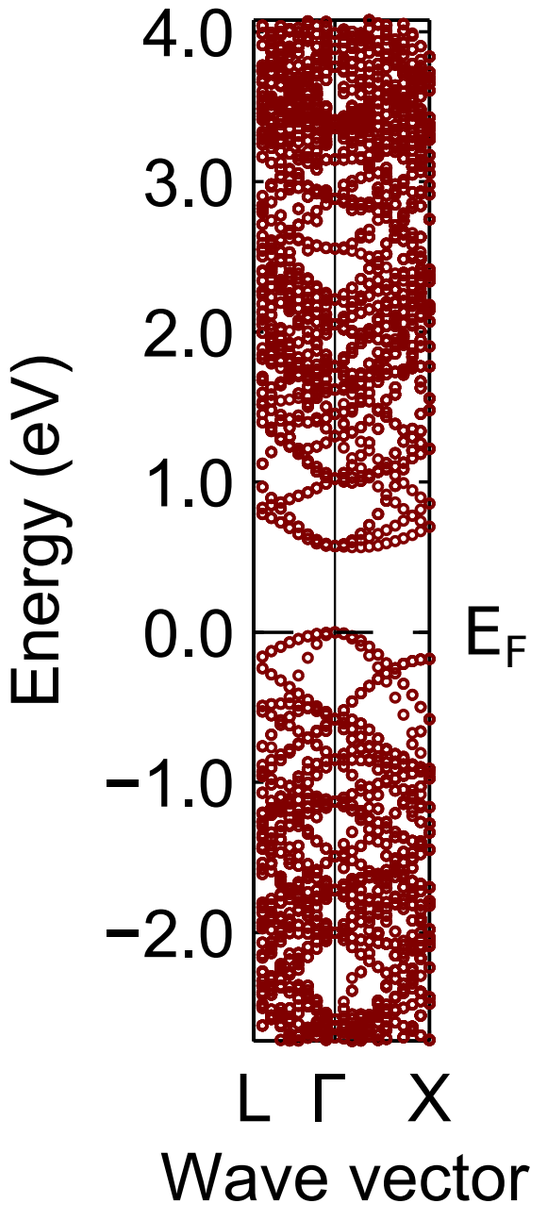


Energy gap

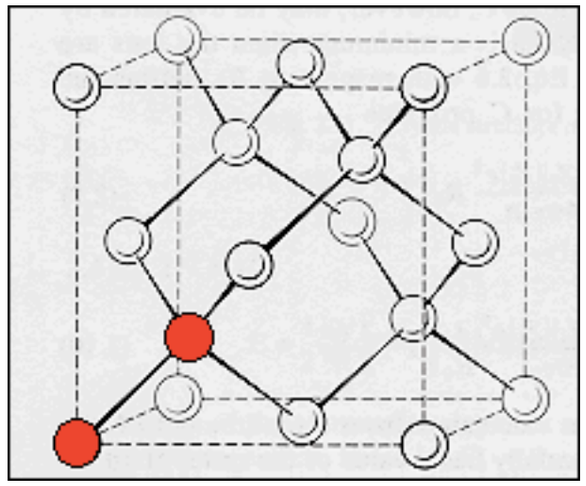
Silicon

2-atom basis



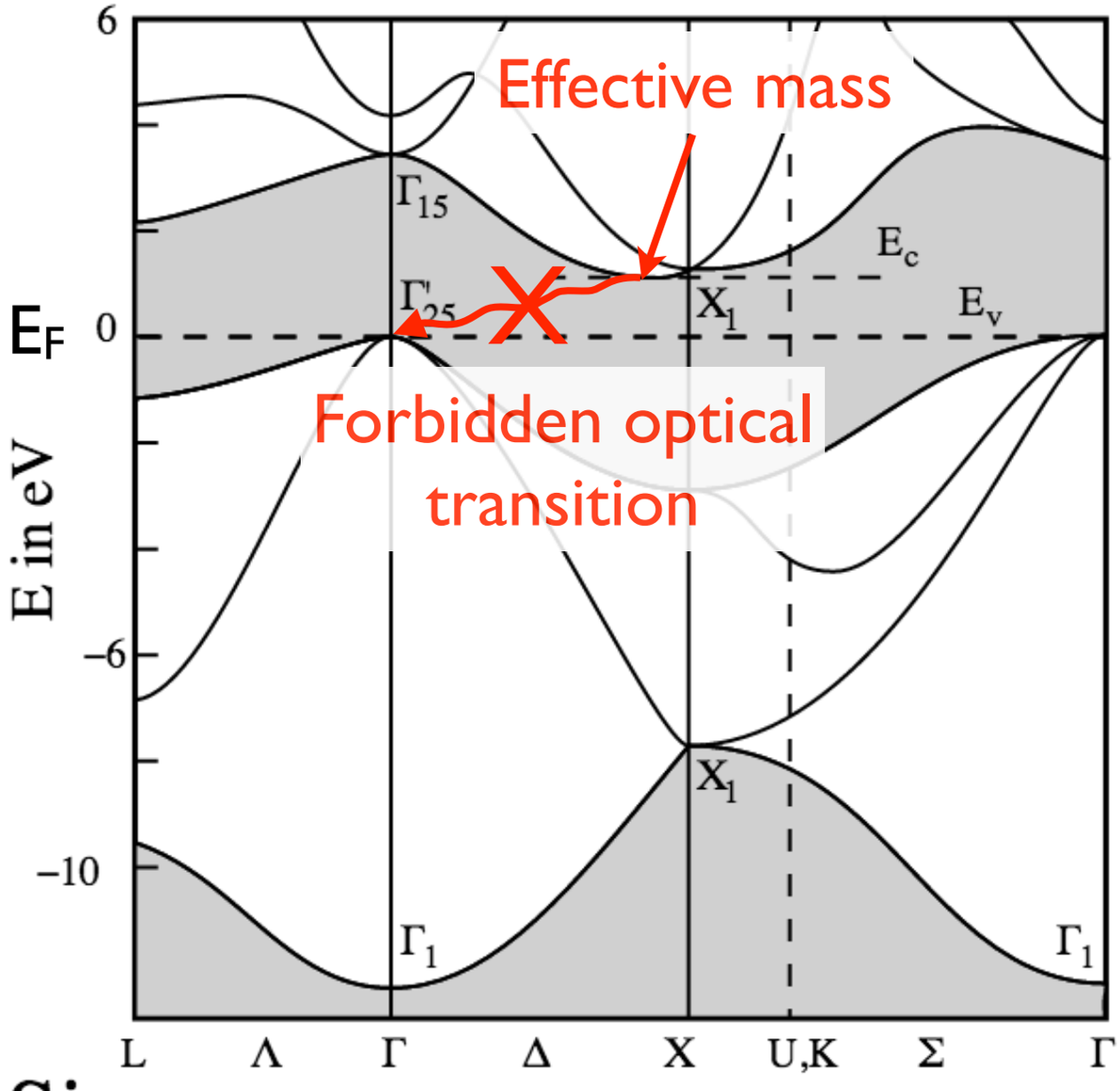


Band structure



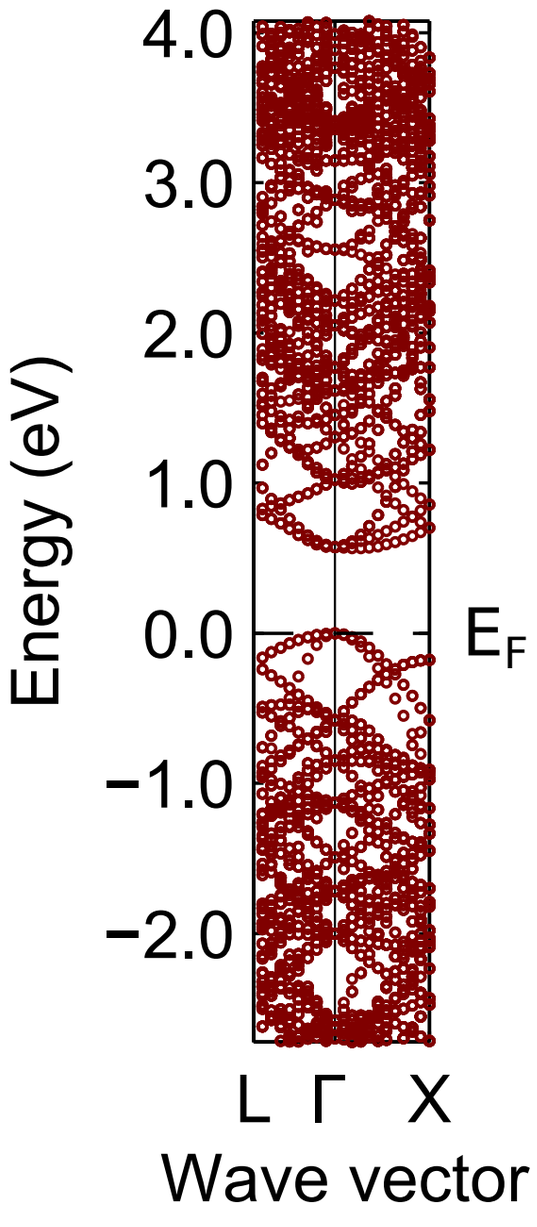
Energy gap

Silicon
2-atom basis



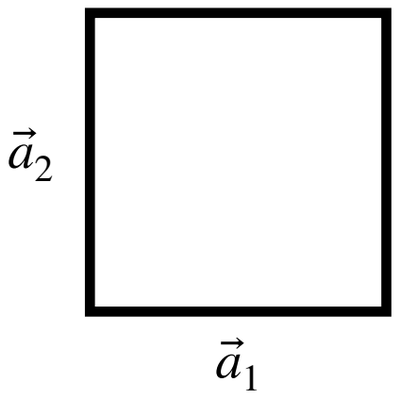
Si

Silicon
250-atom supercell



Band folding and unfolding

Primitive

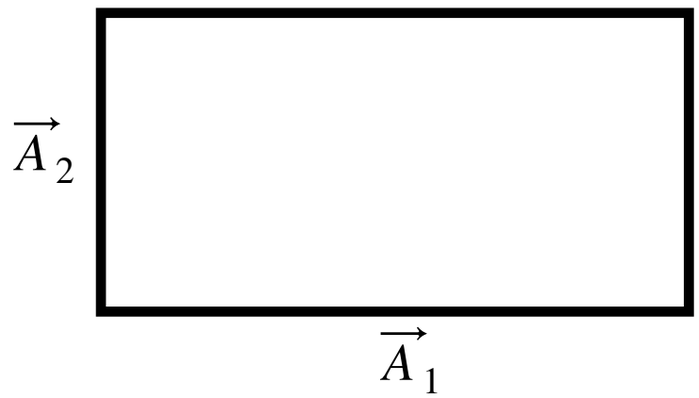


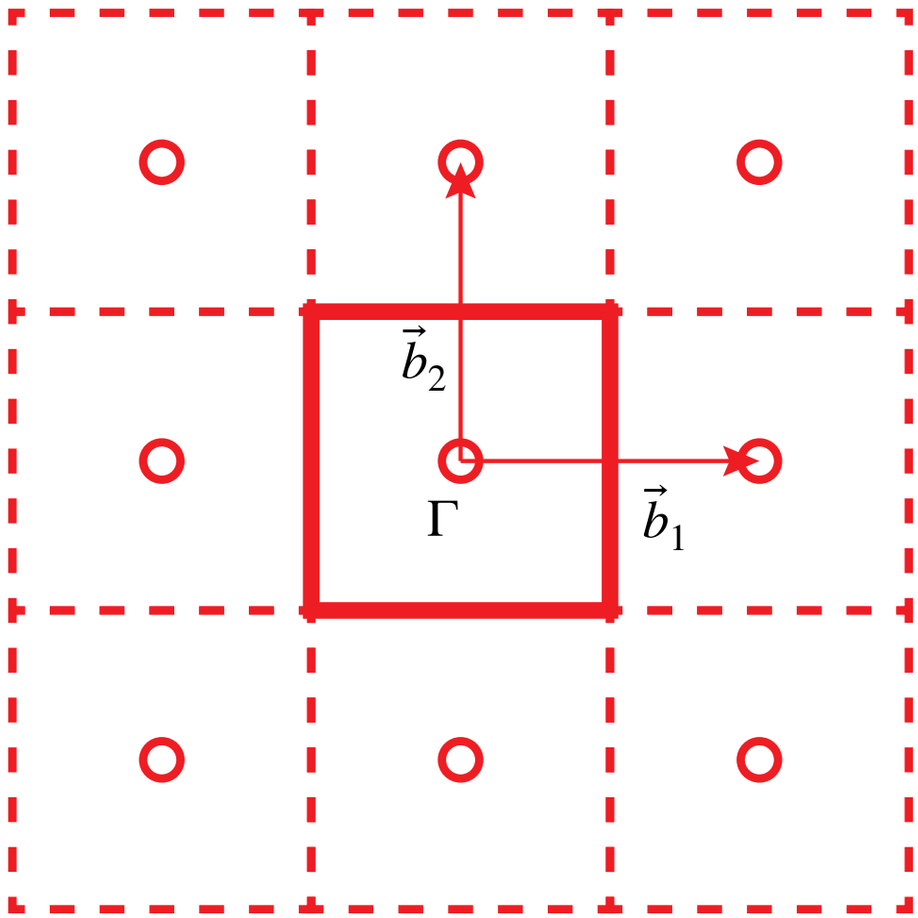
Transformation matrix P
(also in Vesta)

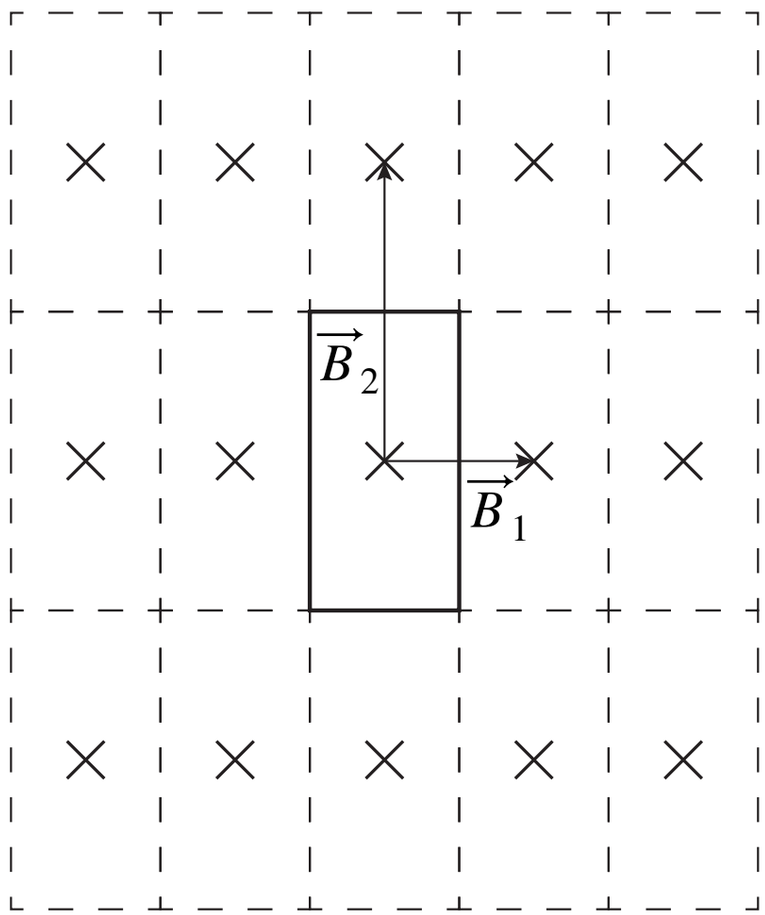
$$\overrightarrow{A}_i = \sum_{j=1}^{3} P_{ji}\,\vec{a}_j$$

$$P = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Supercell

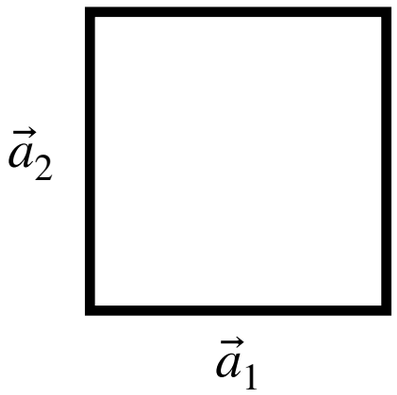






Band folding and unfolding

Primitive



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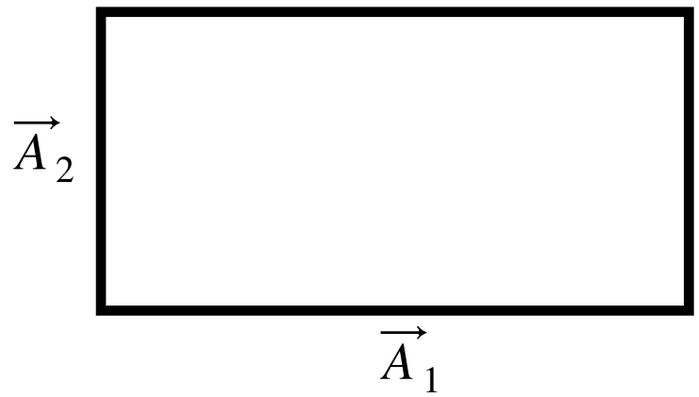
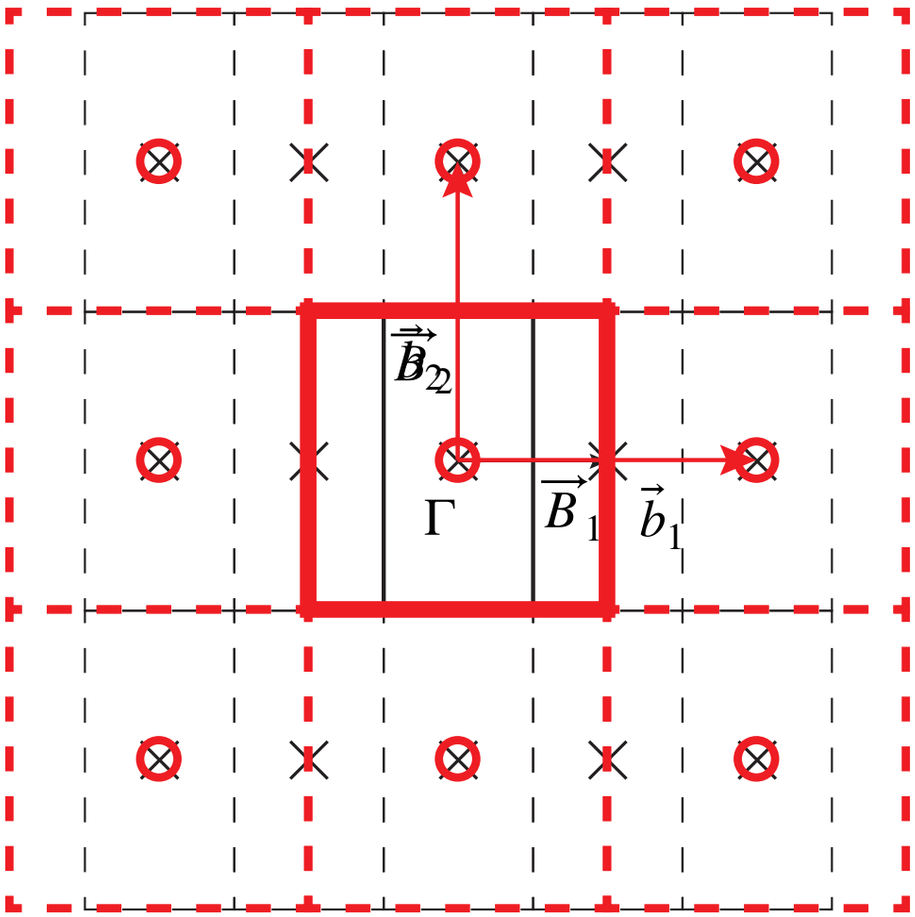
Supercell





Unfolding the first-principle band structure

Plane wave expansion

$$\Psi_{n,\mathbf{K}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{n,\mathbf{K}}(\mathbf{G})\, \mathrm{e}^{i(\mathbf{K}+\mathbf{G})\cdot\mathbf{r}}$$

Bloch spectral weight

$$w_n(\mathbf{k}) = \sum_{\mathbf{g}} |C_{n,\mathbf{K}}(\mathbf{k}+\mathbf{g})|^2$$

Popescu & Zunger:
Phys. Rev. Lett. **104**, 236403 (2010)

Rubel *et al.*
Phys. Rev. B **90**, 115202 (2014)
Comput. Phys. Commun. **291**, 108800 (2023)

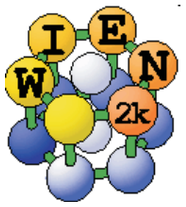
README.md

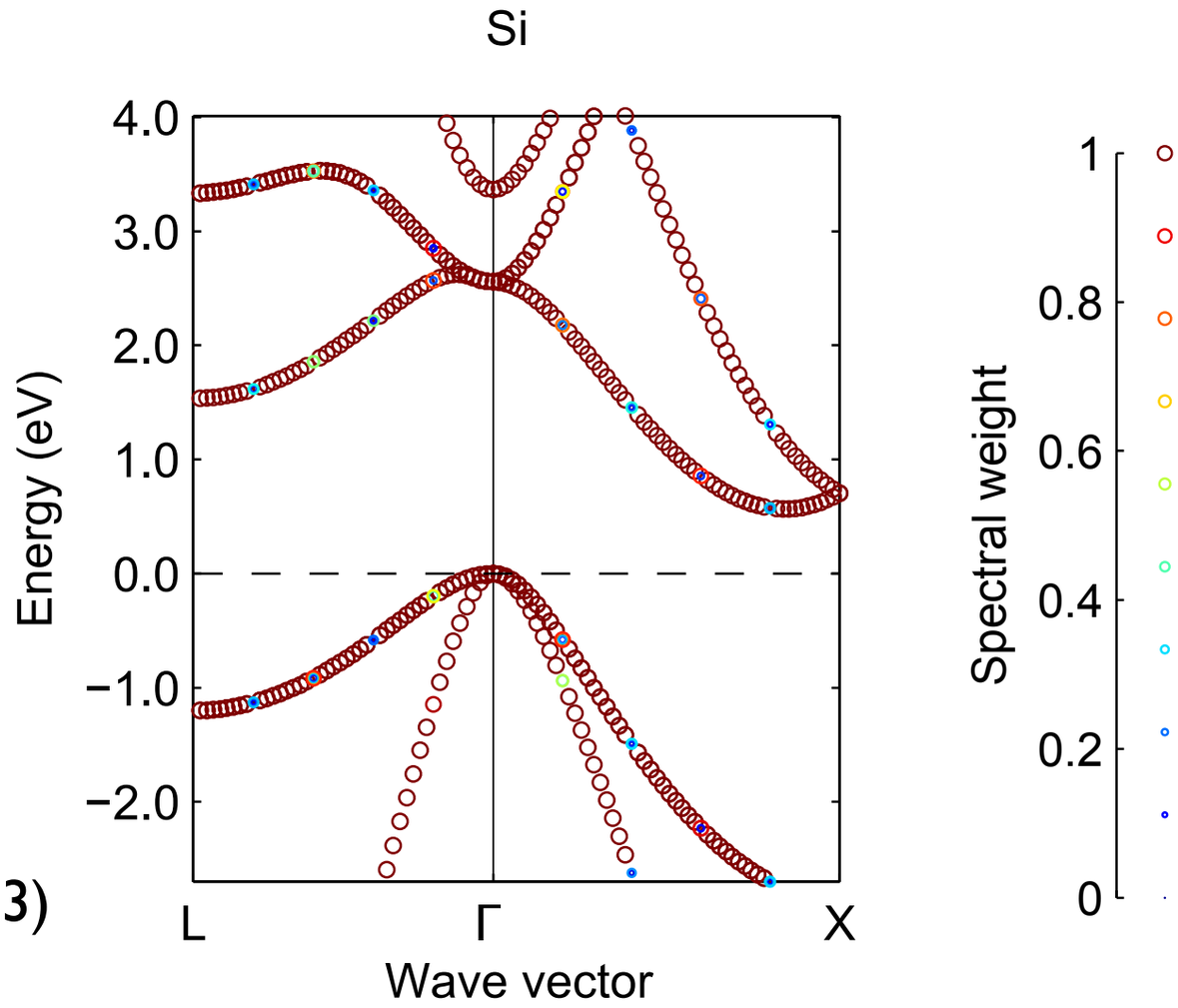
fold2Bloch

Unfolding of first-principle electronic band structure obtained with WIEN2k DFT-(L)APW code

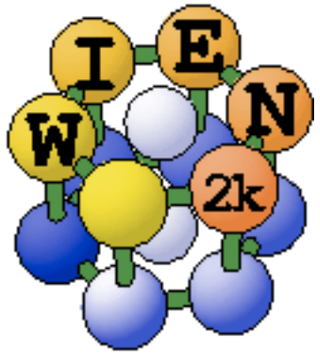
Contributors:

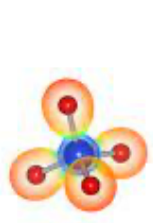
- Anton Bokhanchuk
- Elias Assmann
- Sheikh Jamil Ahmed
- Oleg Rubel





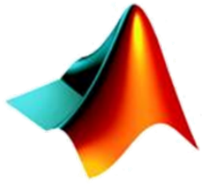
Effective band structure: Workflow





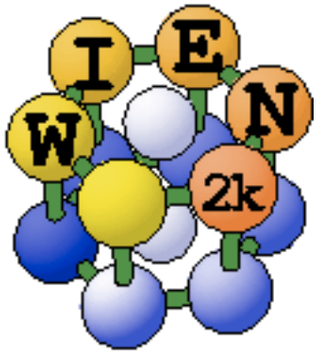
VESTA
Visualization for Electronic and STructural Analysis

- Construct primitive unit cell
- Make supercell (`supercell`)
- Create perturbation(s)
- Run SCF calculation



MATLAB

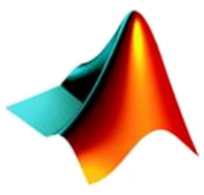
- Create k-path (`case.klist_band` file) using `fold.m`



- Compute wave functions (`case.vector[so]` file) for the selected k-path:
  - `x lapw1 -band [-p]`
  - `x lapwso [-p]` (in the case of spin-orbit coupling)

fold2Bloch

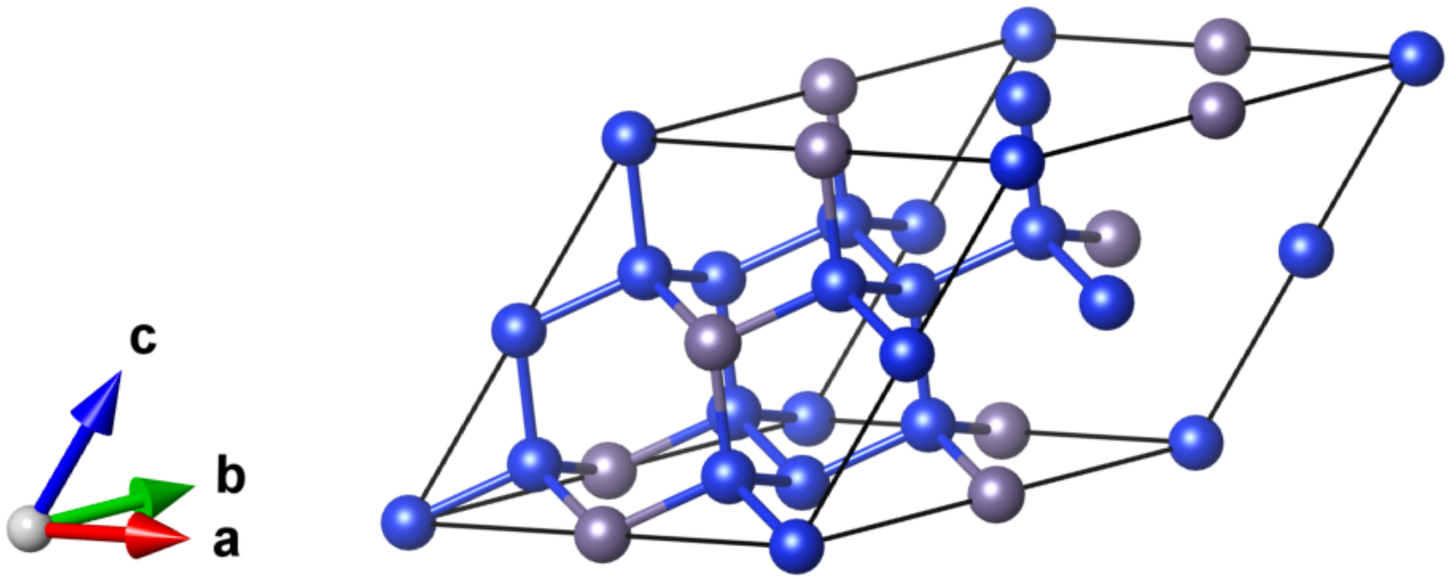
- Unfold band structure
  - `fold2Bloch [-c] case.vector "'2 0 0:0 1 0:0 0 1'"`



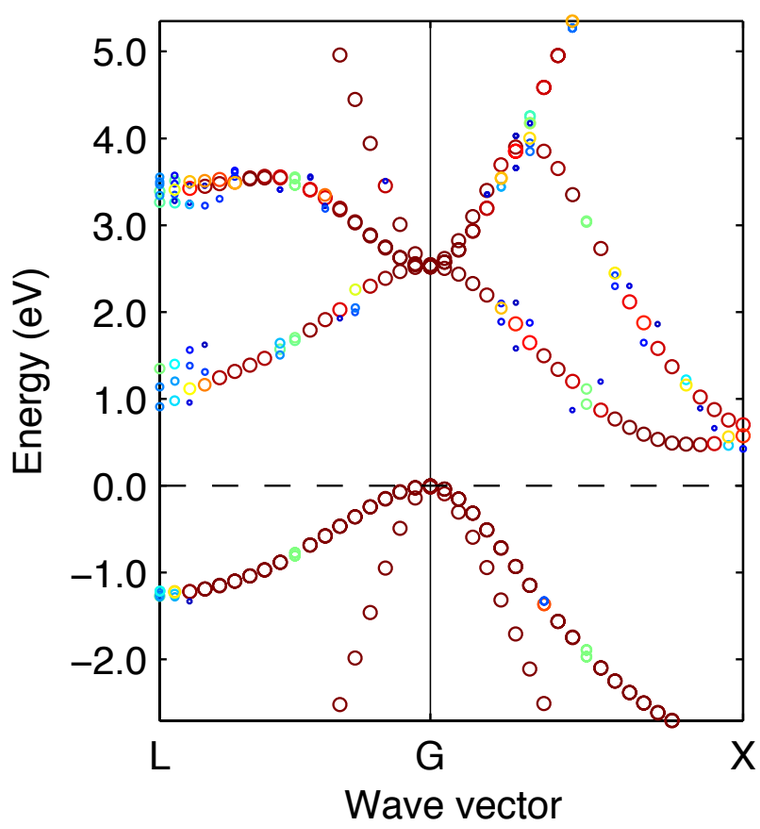
MATLAB

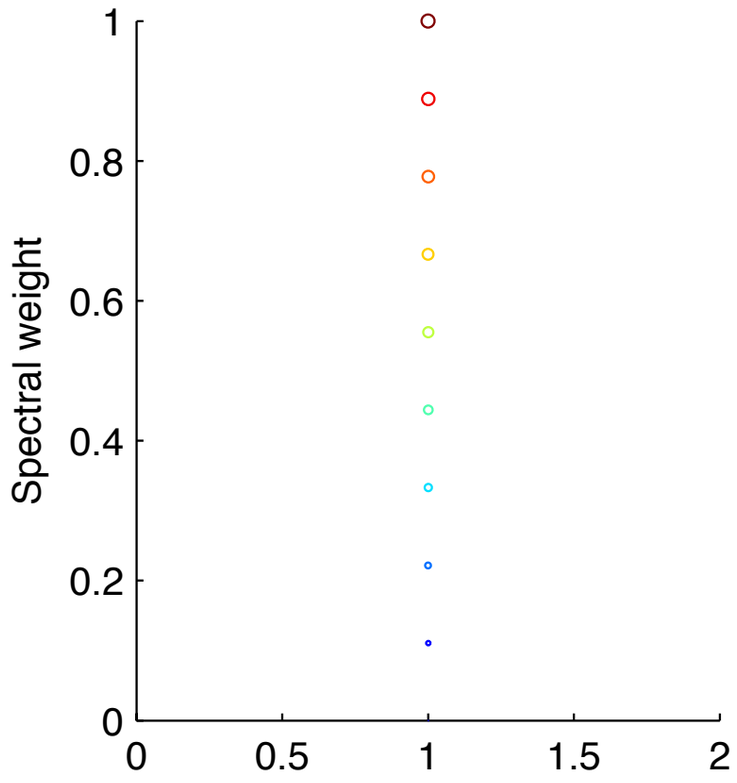
- Plot effective band structure (`ubs_dots*.m`)

Demonstration: Band structure of $Si_{1-x}Ge_x$ alloy (x ~ 0.2)

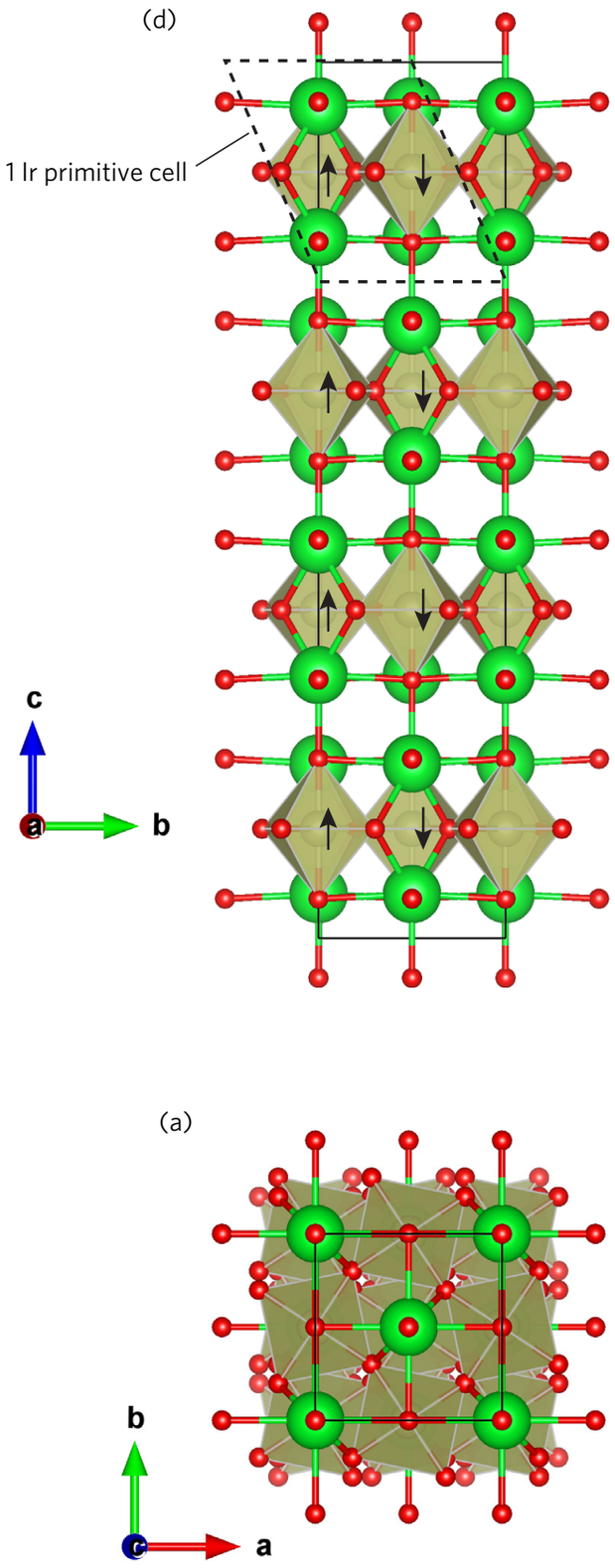


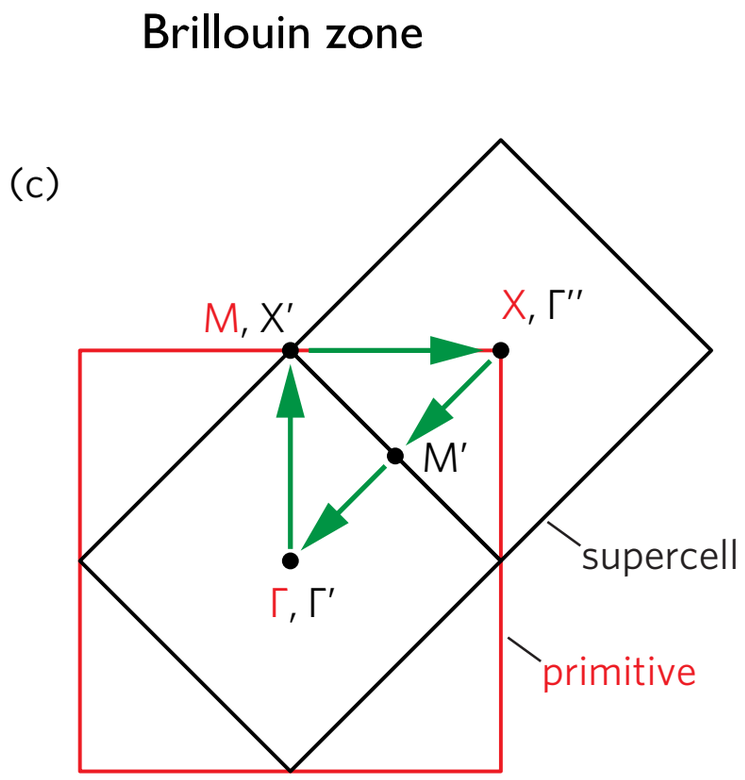
Tutorial

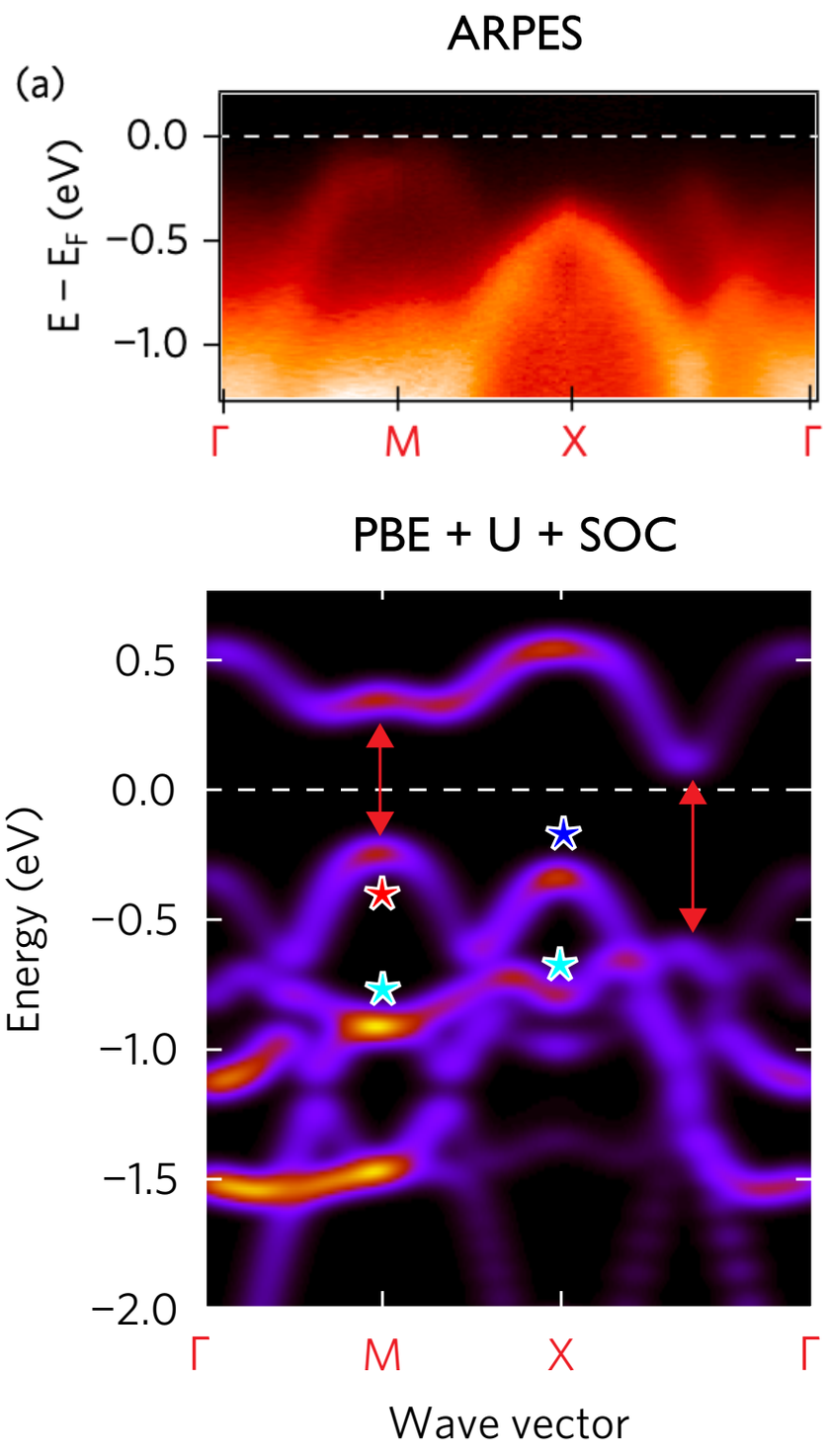




Strongly-correlated material: Sr_2IrO_4







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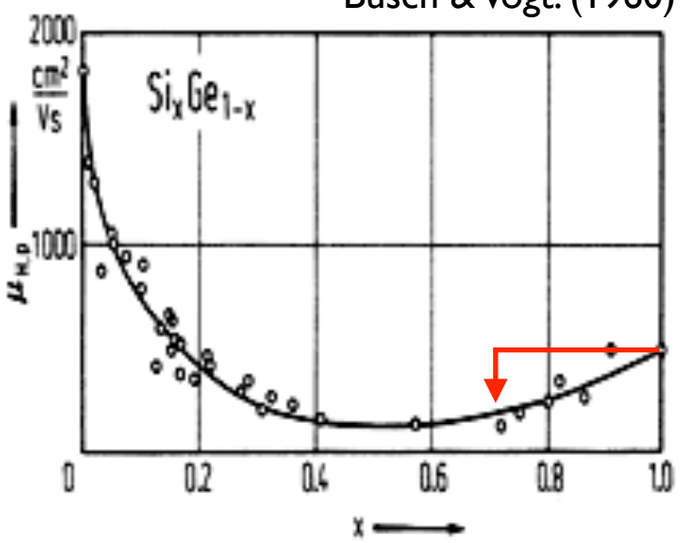
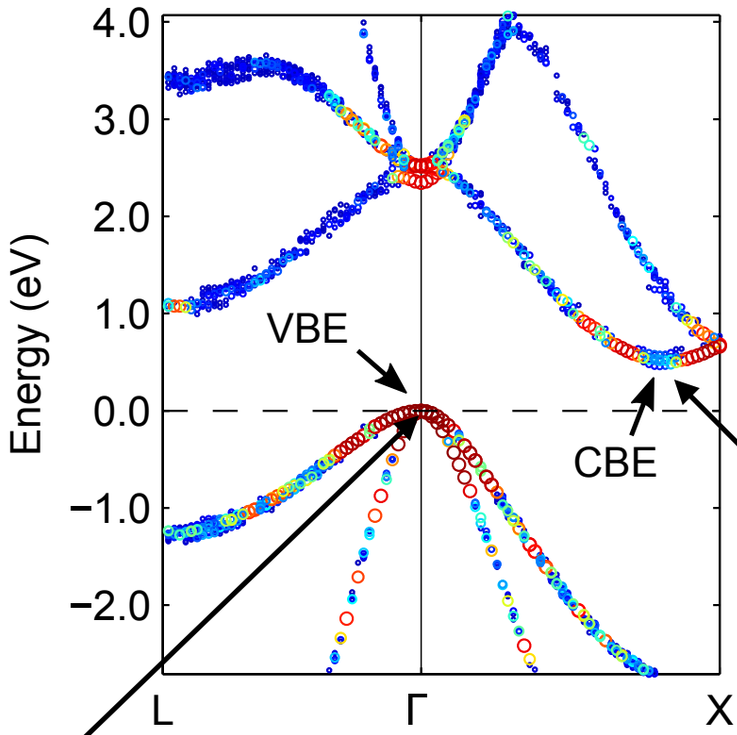
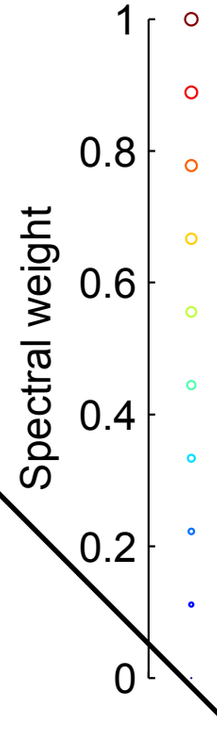
Thermoelectric material: $Si_{0.7}Ge_{0.3}$

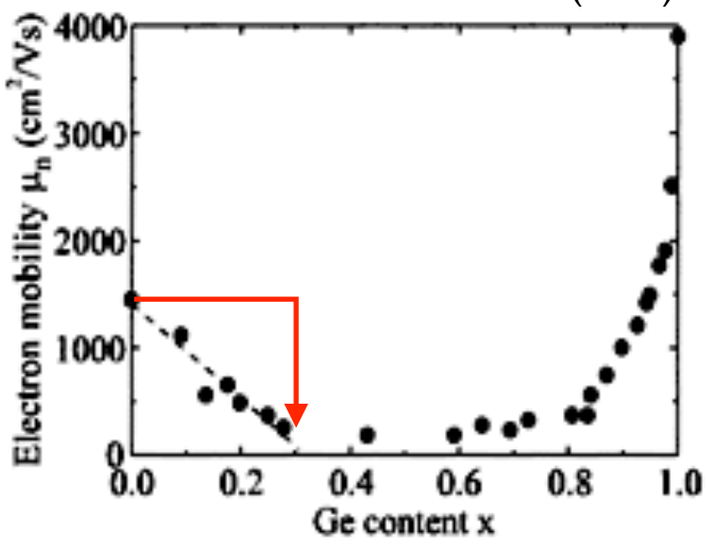
Busch & Vogt. (1960)







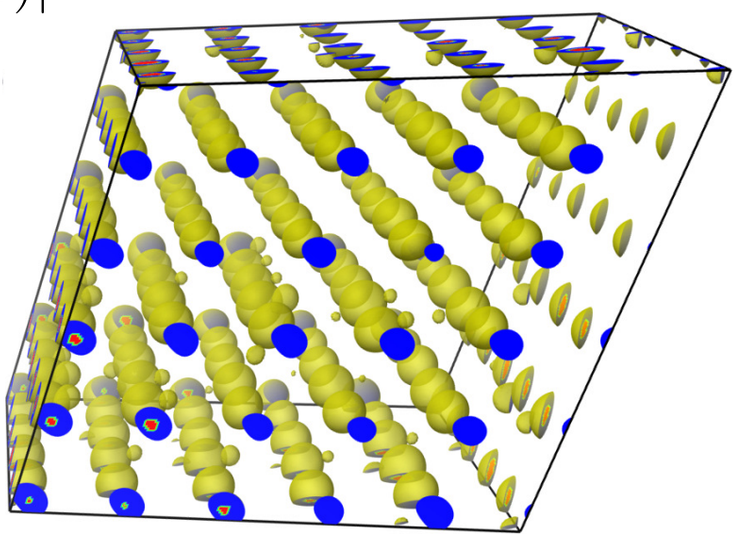
Landoldt-Bornstein (1982, 1987);
Sasaki et al. (1984).



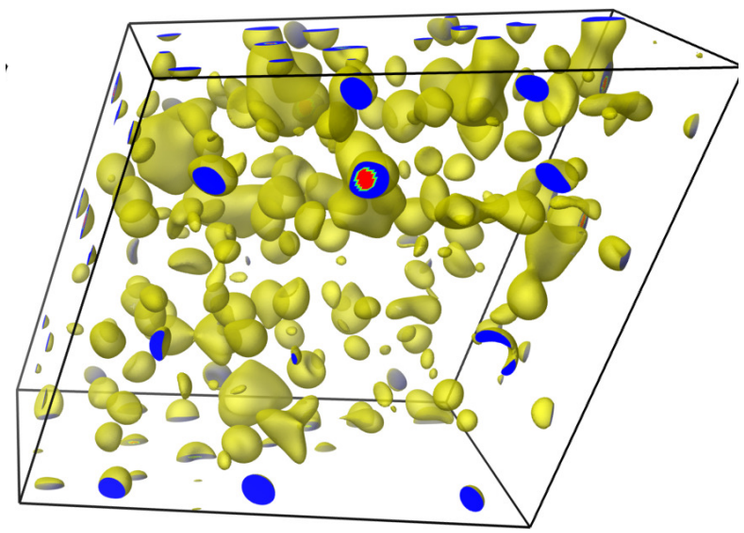
$\Delta r \Delta k \sim 1$

VBE

$|\psi(\mathbf{r})|^2$



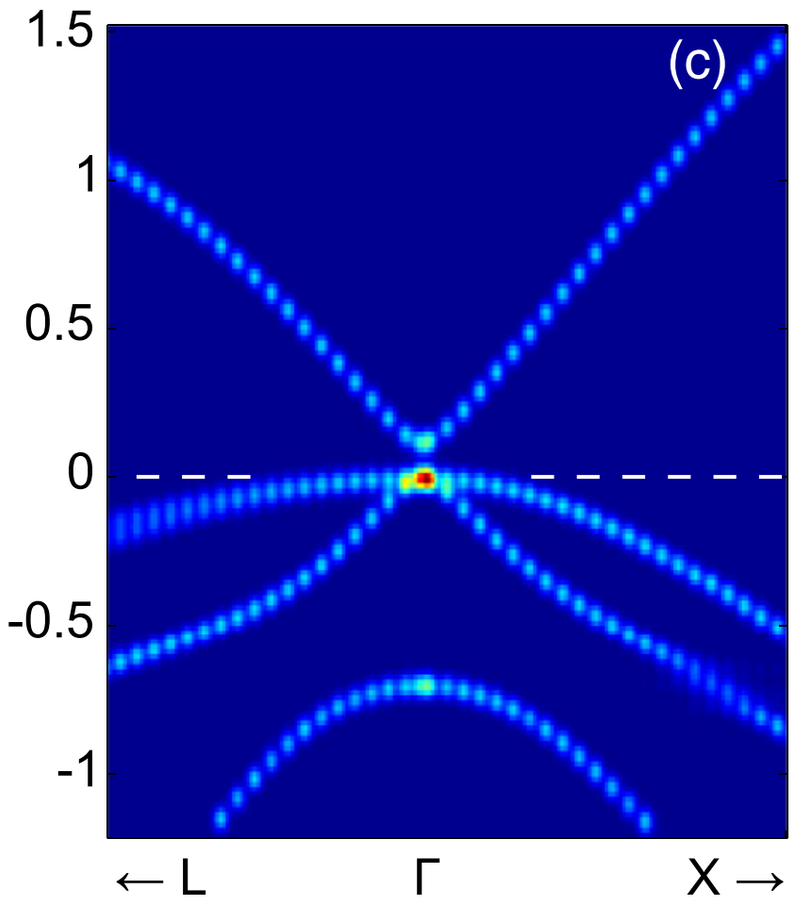
CBE



Comput. Phys. Commun. **205**, 106 (2016)

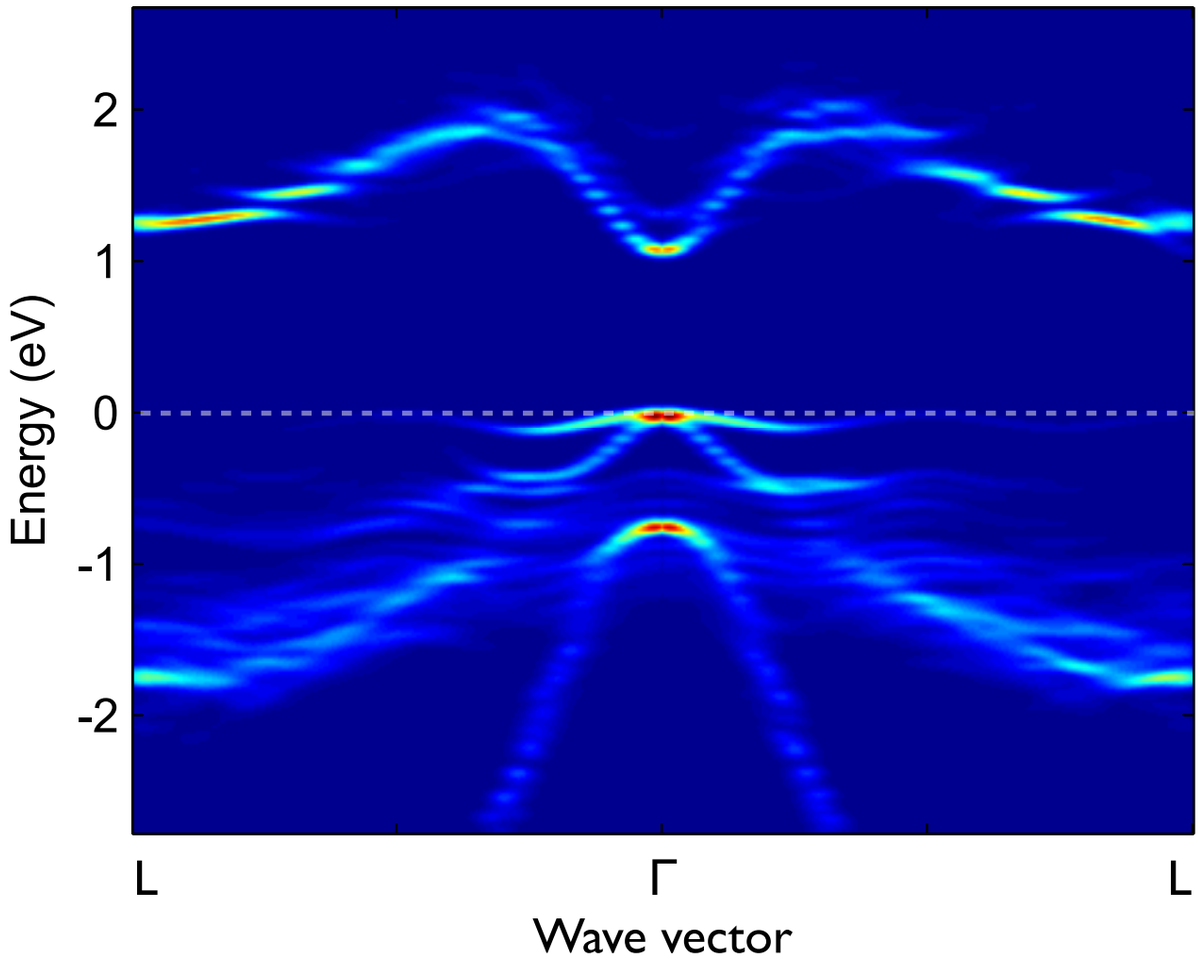
Impact of alloying disorder on charge transport

CdTe → (HgCd)Te



μ_e = 1,100 → 1,000,000 $cm^2V^{-1}s^{-1}$

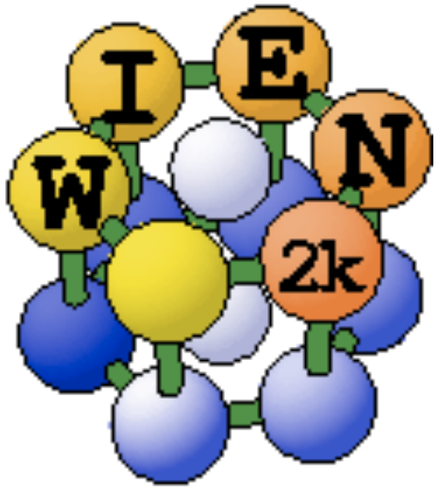
GaAs → Ga(AsBi)



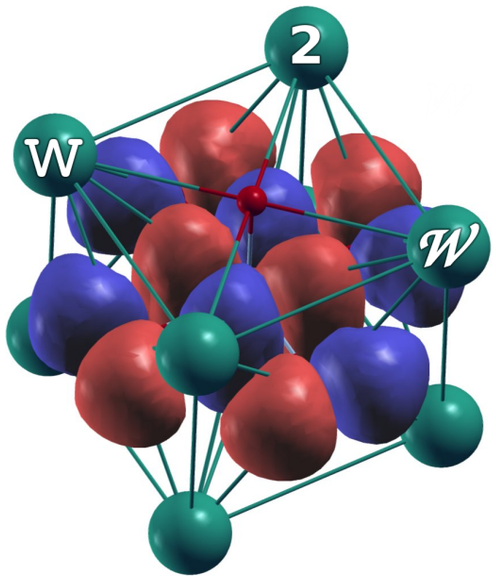
μ_h = 200 → 10 $cm^2V^{-1}s^{-1}$

μ_e = 4,000 → 2,500 $cm^2V^{-1}s^{-1}$

Wannier functions



+



+

WANNIER90

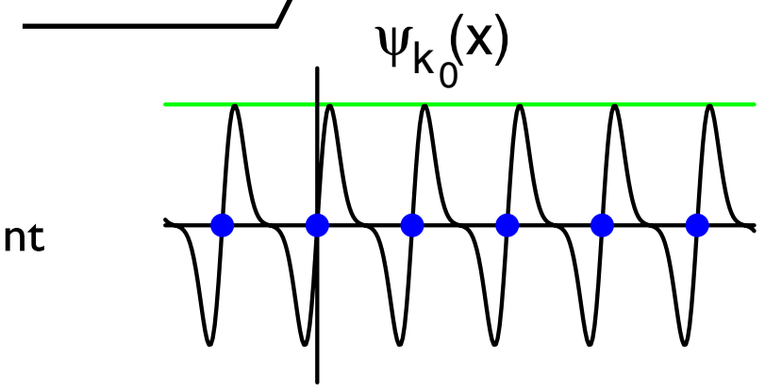
Bloch *vs* Wannier functions

Bloch functions

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

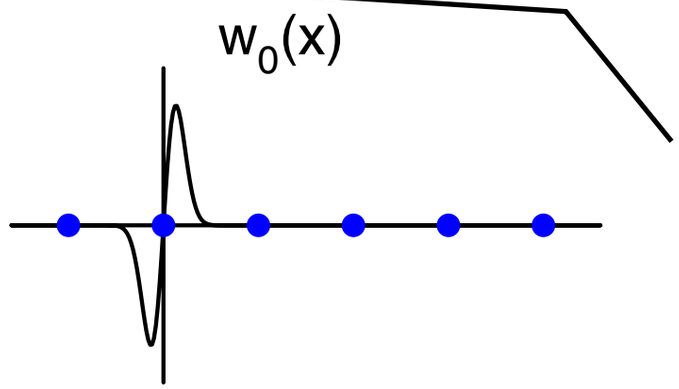
Indexed by band number (n) and wave vector (**k**)

Γ point

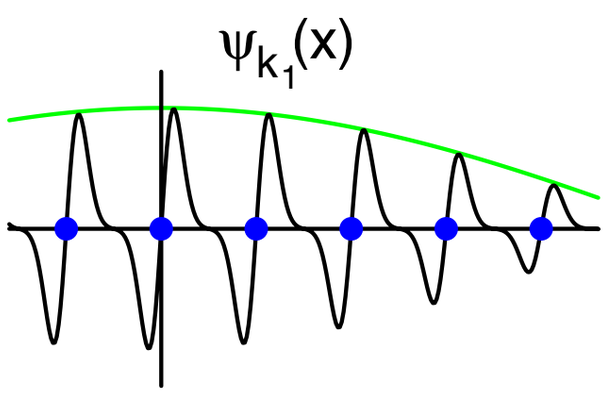


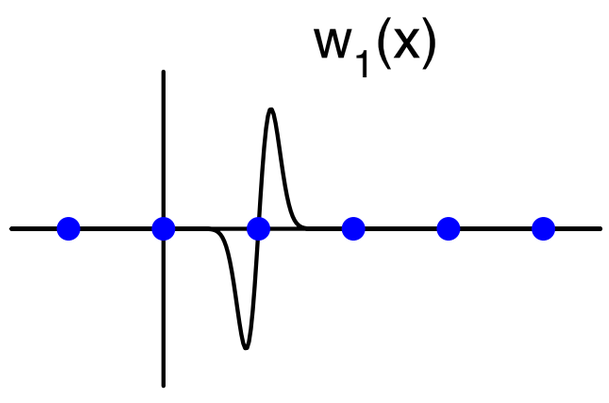
Wannier functions (localized orbitals)

$$|\mathbf{R}n\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\; e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{m=1}^{N} U_{mn}^{(\mathbf{k})}\,|\psi_{n\mathbf{k}}\rangle$$



Indexed by the lattice vector in real space





Number of WF = number of bands,
but band n does **not** correspond to WF n

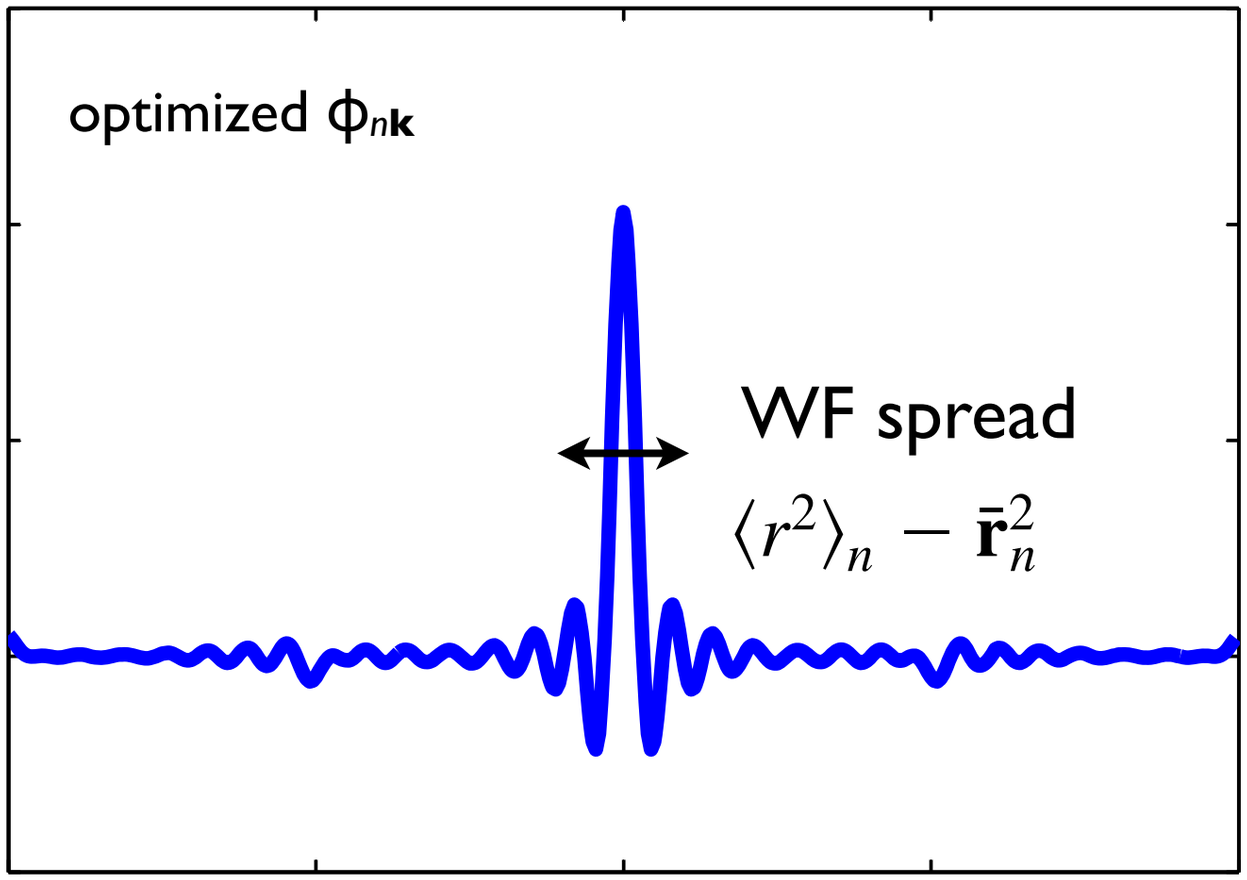
Wannier:
PRB **52**, 191 (1937)
Marzari et al.:
PRB **56**, 12847 (1997)
Rev. Mod. Phys. (2012)

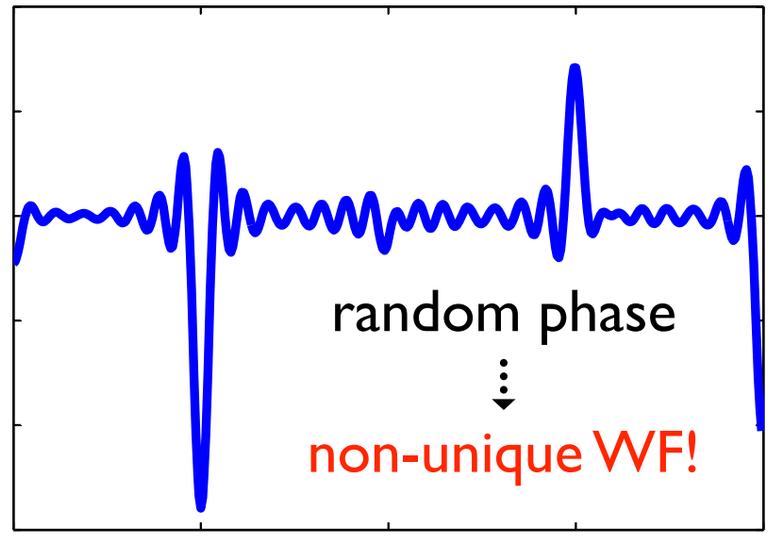
Max. localized Wannier functions (MLWF)

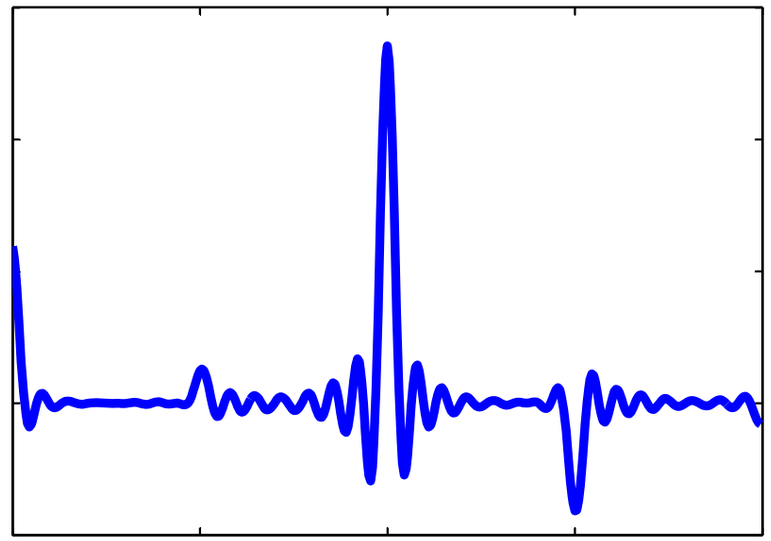
Bloch functions (more precisely):

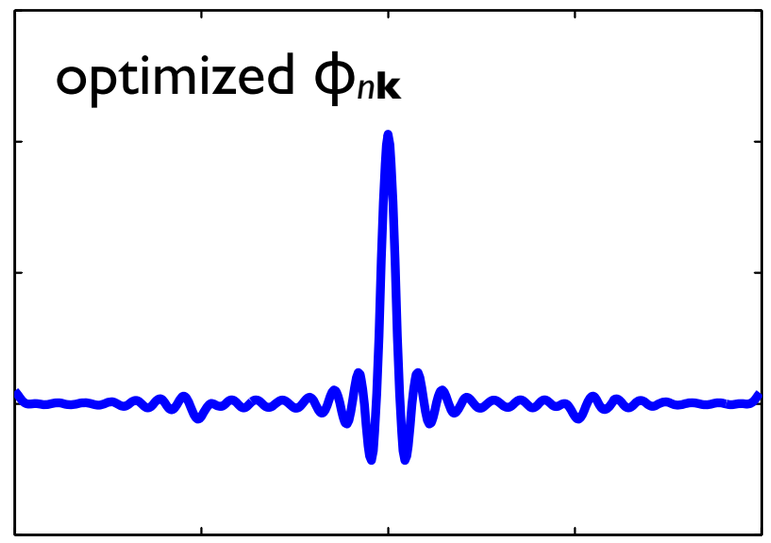
$$\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}}\, e^{i\phi_{n\mathbf{k}}}$$

gauge freedom → ambiguity



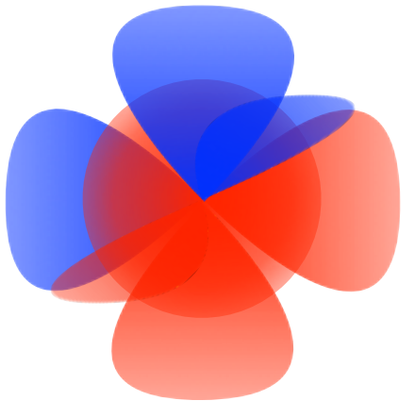






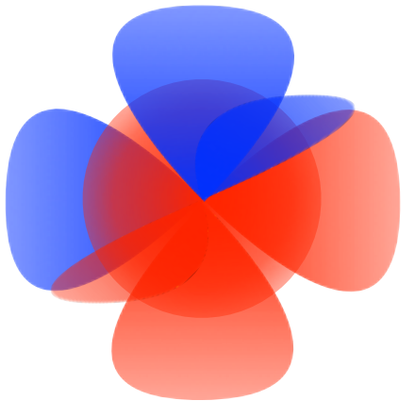
$$\Omega = \sum_n [\langle \mathbf{0}n|r^2|\mathbf{0}n\rangle - \langle \mathbf{0}n|\mathbf{r}|\mathbf{0}n\rangle^2] = \sum_n [\langle r^2\rangle_n - \bar{\mathbf{r}}_n^2]$$

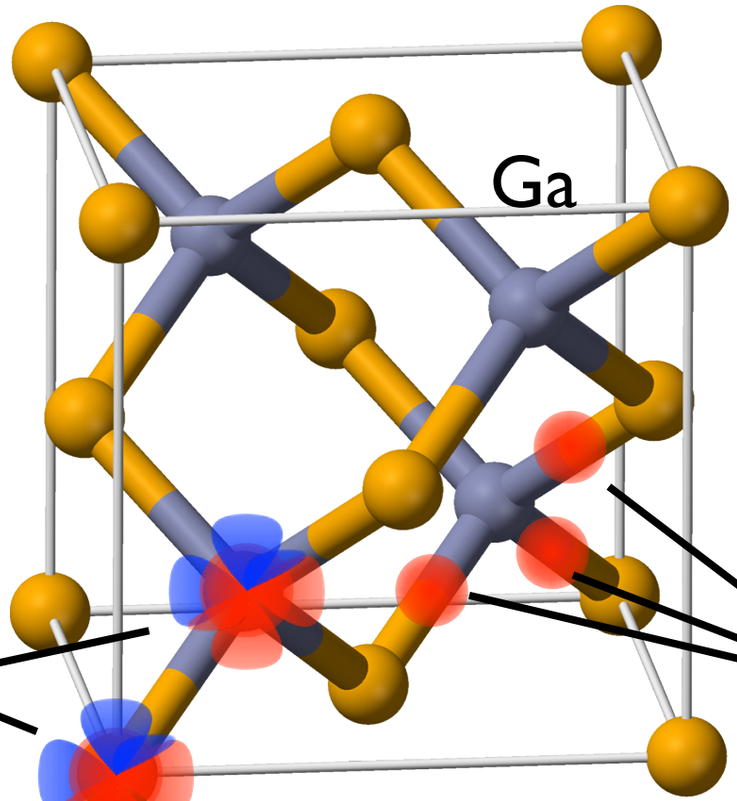
Two flavours of Wannier functions

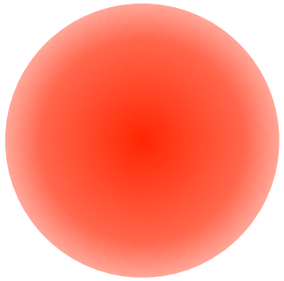


- includes *bonding* and *antibonding* states
- building effective hamiltonian

Two flavours of Wannier functions

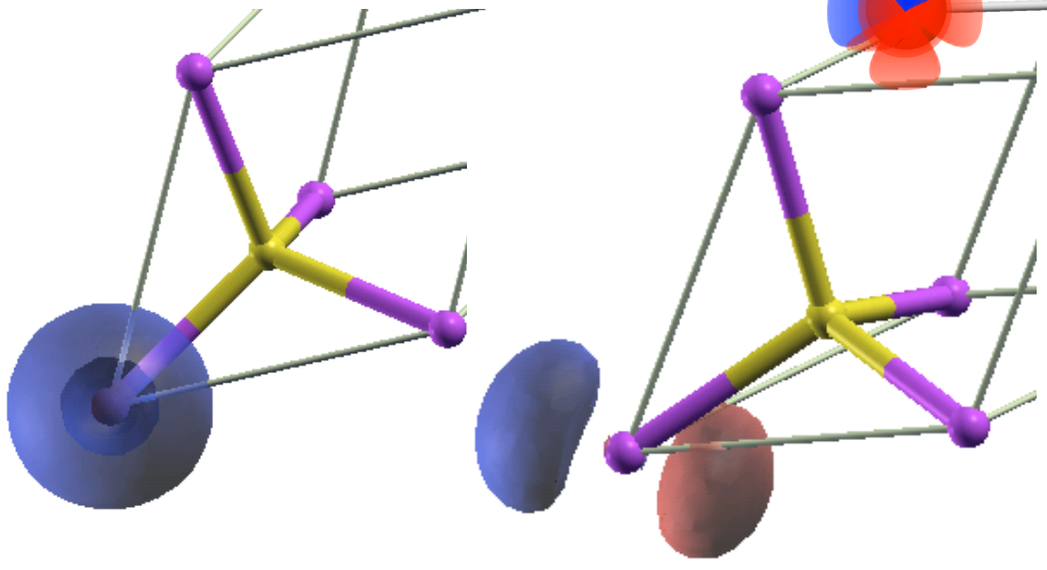


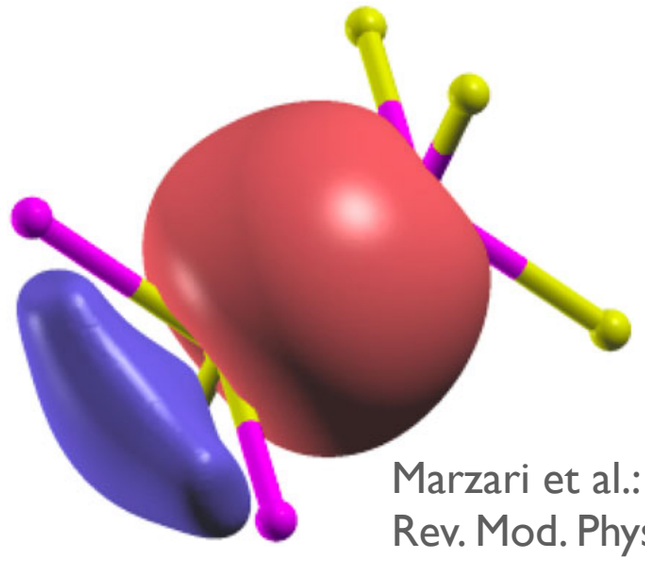




Atom centered sp^3-like

Bond centered s-like





Marzari et al.:
Rev. Mod. Phys. (2012)

- includes *bonding* and *antibonding* states
- building effective hamiltonian

- includes *valence* states
- charge transfer and polarization

Atom centered FWs as an LCAO basis (if you are lucky)

$ less GaAs-WANN_hr.dat

```
...
    0     0     0     1     1    -4.335108    0.000000
    0     0     0     2     1    -0.000001
    0     0     0     3     1     0.000000
    0     0     0     4     1    -0.000001
    0     0     0     5     1    -1.472358
    0     0     0     6     1    -1.157088
    0     0     0     7     1    -1.157088
    0     0     0     8     1    -1.157088
...
    0     0     1     1     1    -0.001219
...
```

Home

unit cell

⟨s1| |s1⟩

Matrix element (eV)
⟨s1|H|s1⟩ = Es1

0.000000 Im part = 0

⟨s2|

Matrix element (eV)
⟨s2|H|s1⟩ = Vssσ

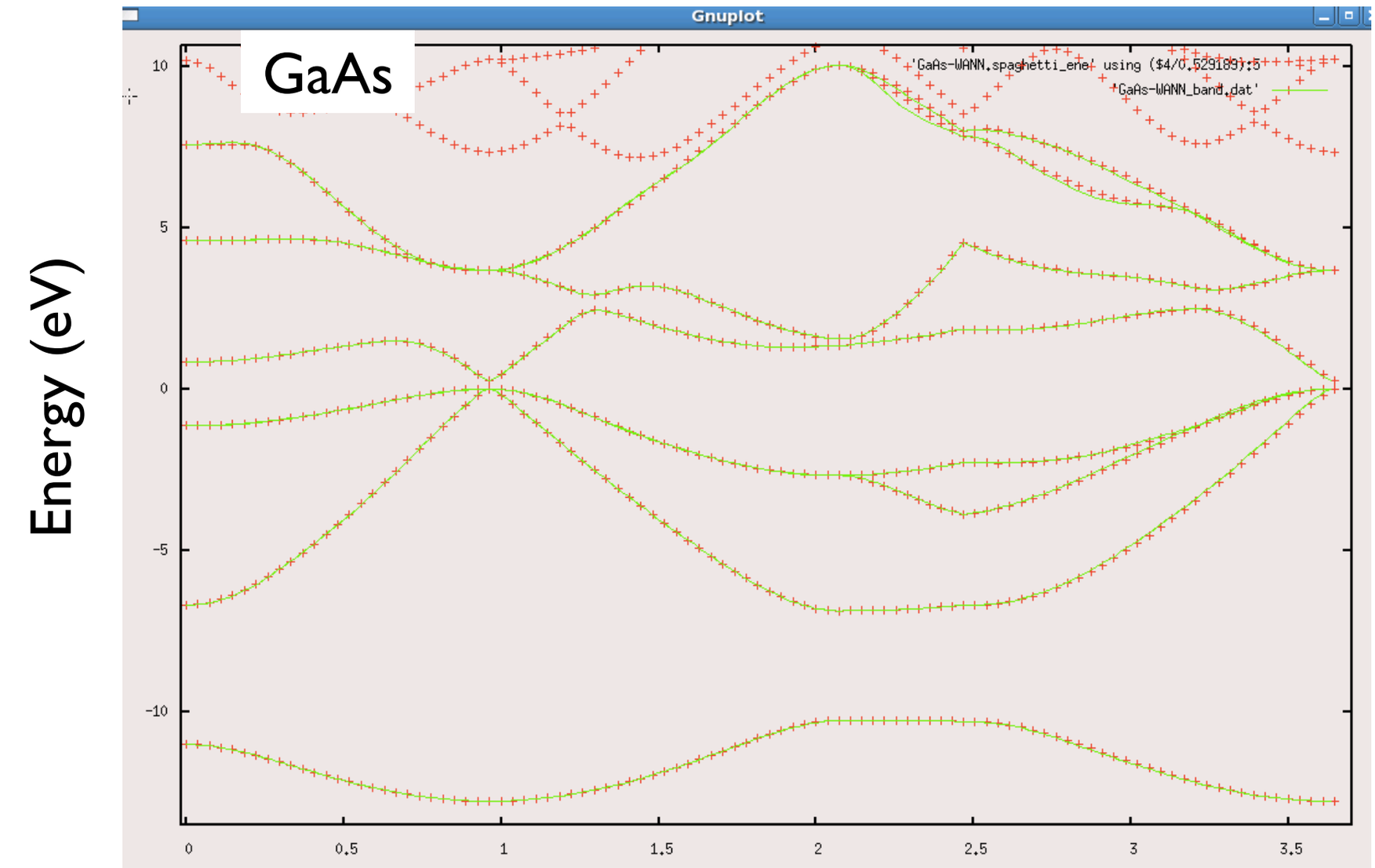
⟨p2|H|s1⟩ = Vsp

Neighbour unit cell

WF are well localized
⇒ nearest-neighbour suffice

Tutorial

Band structure interpolation

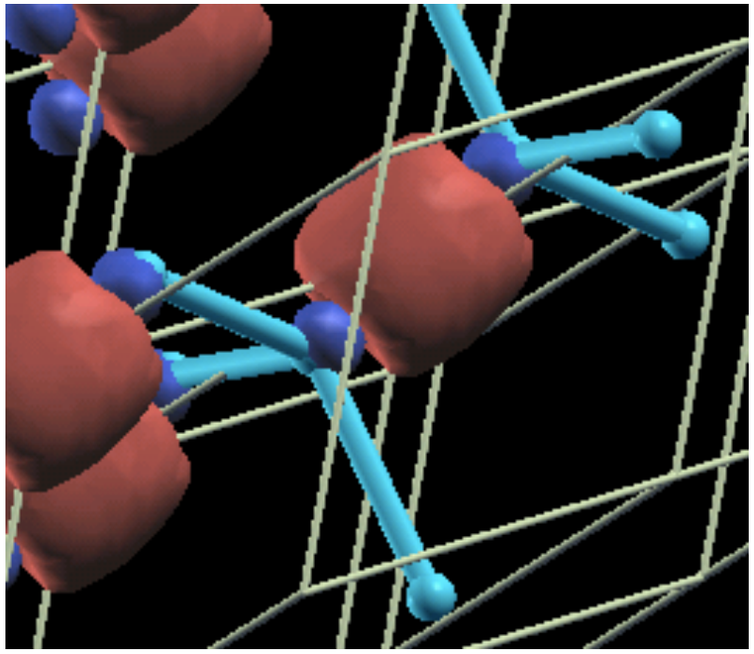


\+ original Wien2k band structure

– Band structure computed from Wannier hamiltonian

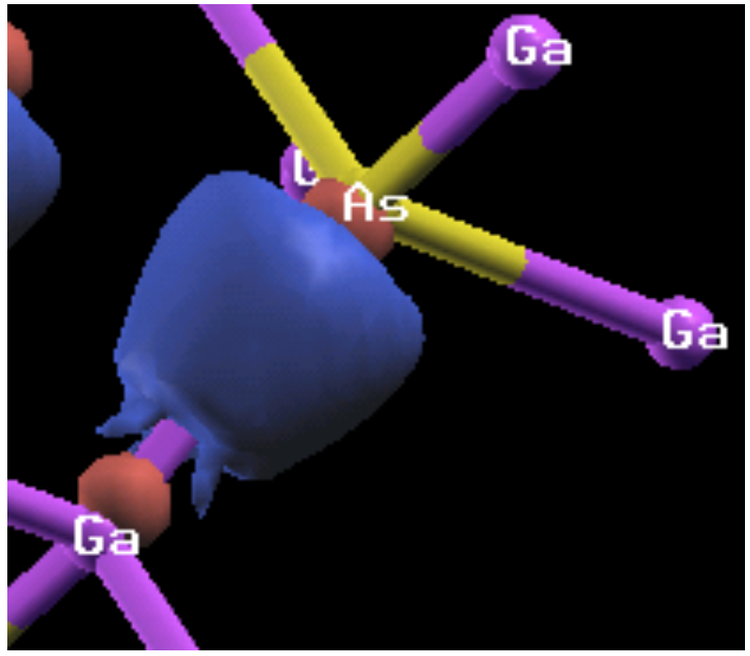
Relation to polarization (bond centered WF)

Si

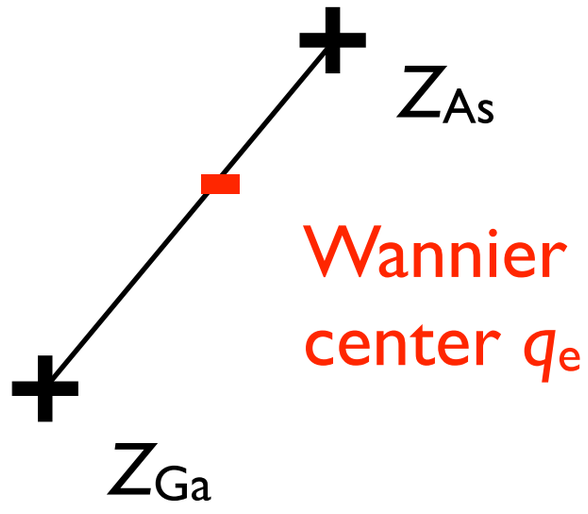


symmetric
(non-polar)

GaAs



non-symmetric
(polar)



$$\mathbf{P} = \frac{e}{V}\left(\sum_{\tau} Z_{\tau}\mathbf{r}_{\tau} - \sum_{n}\mathbf{r}_{n}\right)$$

Ionic part
(sum over all ions)

Electronic part
(sum over all WFs centres;
Wannierization to include
occupied bands only)

King-Smith & Vanderbilt,
Phys. Rev. B **47**, 1651 (1993)

Wannier90 "ecosystem"

Topological properties, surface states, band unfolding, and more

Z2Pack

Topological properties, $\mathbb{Z}_2$ invariants, Chern numbers, Weyl points

WANNIER BERRI

Topological properties, Berry curvature, related charge transport phenomena

WANNIER90

EPW®

Interpolation of e-ph interaction to a fine k-mesh

TRIQS

Correlated materials beyond DFT (dynamical mean-field theory)

Marrazzo *et al.*, arXiv:2312.10769 (2023), DOI: 10.48550/arXiv.2312.10769

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