Superconducting DFT in the SIESTA method and code

Riccardo Reho, Nils Wittemeier, **Arnold Kole**, Pablo Ordejón, Zeila Zanolli

Debye Institute for Nanomaterials Science, Utrecht University

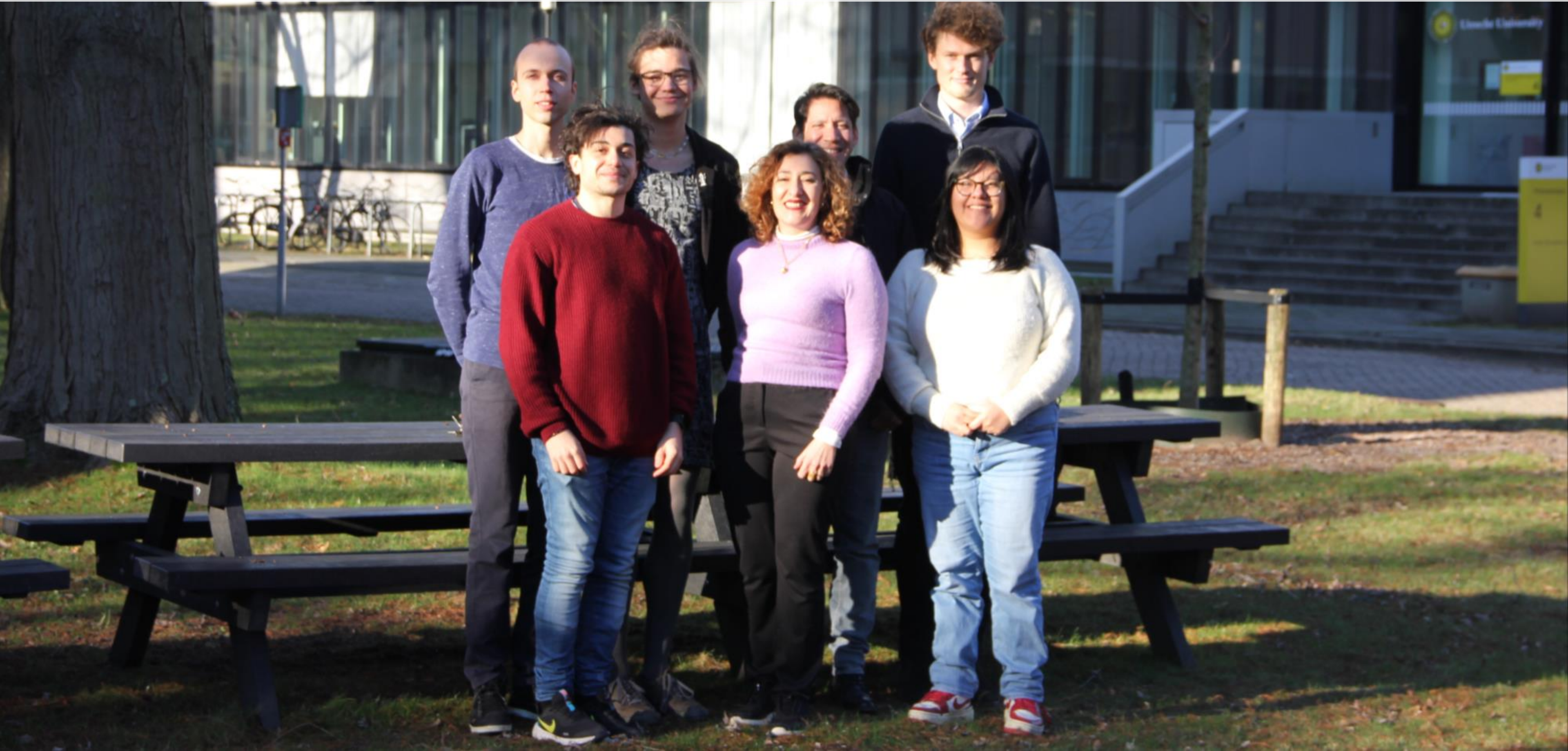
z.zanolli@uu.nl

Advanced SIESTA Workshop 2025

03/06/2025, Barcelona, Spain

Quantum Materials by Design

2025 Team



Overview

1. Motivation + Theoretical background

2. Guided Tour

3. Hands-on with sisl-bdg

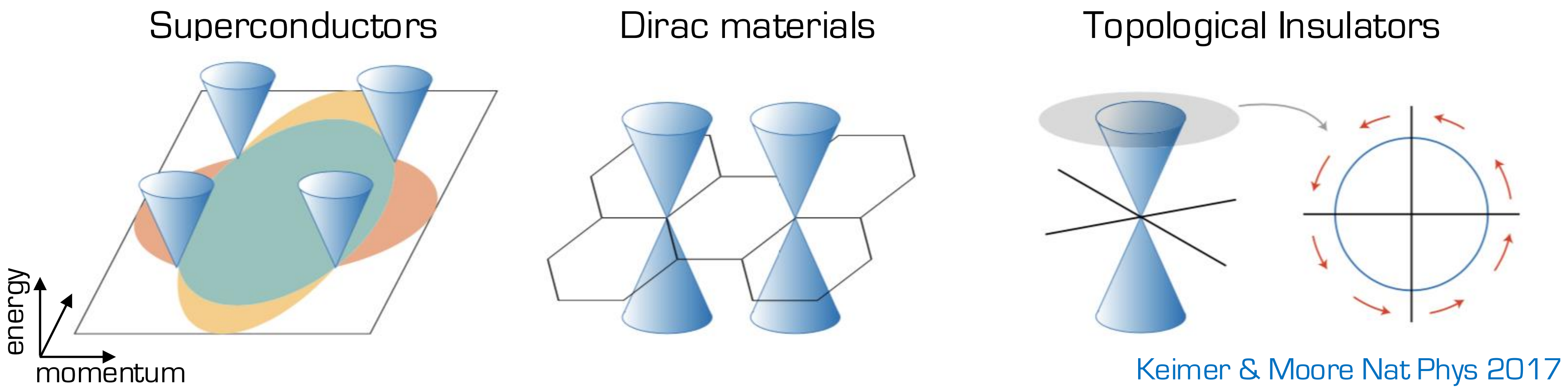
All materials are quantum

But some materials are more quantum than others.

[ZZ]

Quantum Materials

Quantum effects manifest over a wide range of energy and length scales



Keimer & Moore Nat Phys 2017

- Topological effects
- entanglement

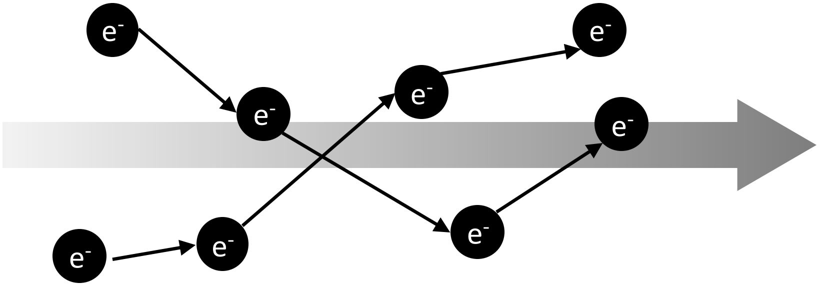
Quantum behaviour at macroscopic scales

Quantum technology:
Low-dissipation electronics
Photovoltaics
Quantum information

How do we do it?

Normal metals vs superconductors

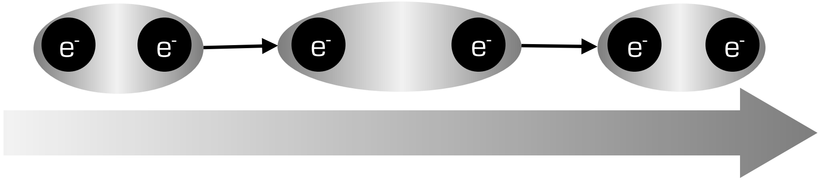
Normal metal



Electrons repel each other (Coulomb)

Electron-electron scattering
→ finite resistance

Conventional Superconductor



Attractive Electron-Electron interaction mediated by lattice vibrations (BCS theory)

→ Formation of Cooper pairs

→ collective motion without scattering

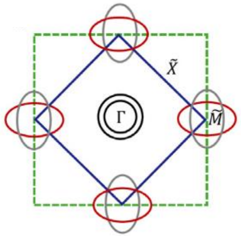
But… at very low T !

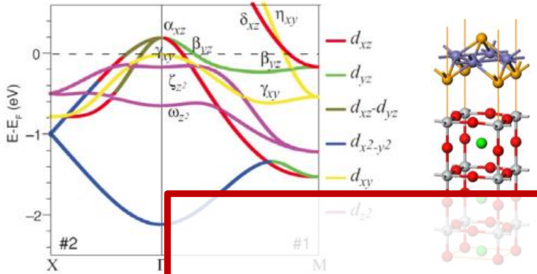
z.zanolli@uu.nl

Unconventional superconductivity

Fermiology of electronic states

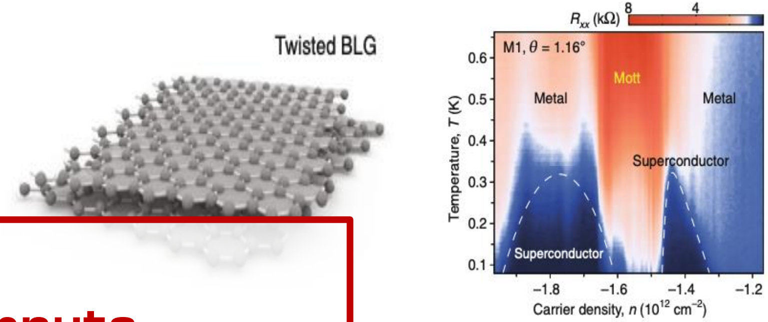
FeSe ML





Liu *et al* JPCM 2015

Electron-electron correlations



Cao, Nature 2018

How can we compute (un)conventional superconductivity?

Interplay between disorder and dimensionality

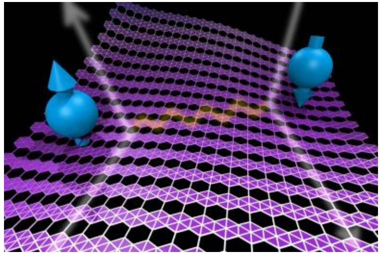
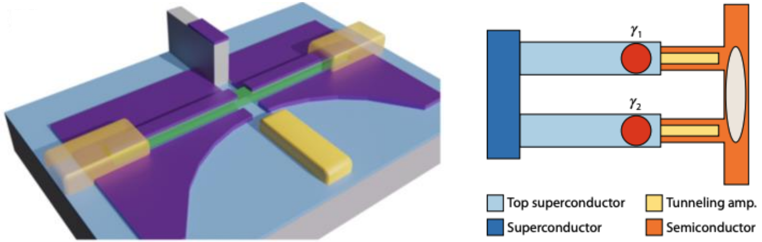


Image: E Penev, Rice U

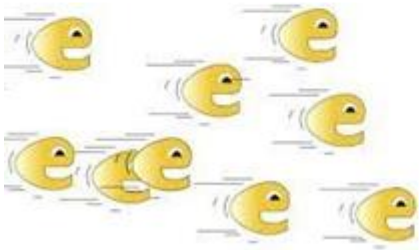
Balents *et al* Nature 2020

Topological superconductivity

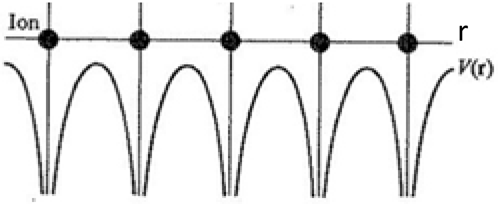


Zhang *et al* *Phys. Rev. Mat.* 2023

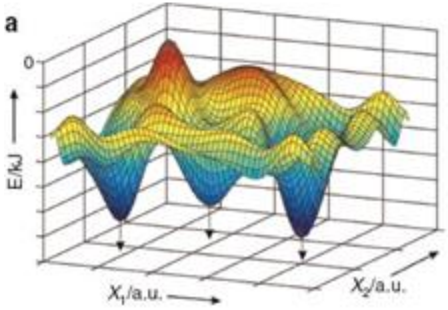
First-principles Quantum Modelling



Kinetic energy of electrons



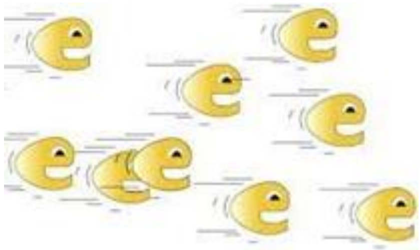
Electron-nuclei interaction

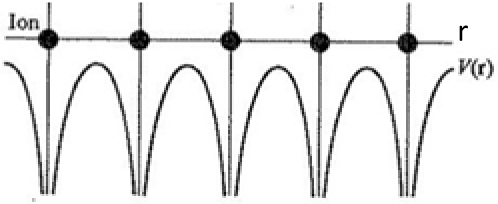


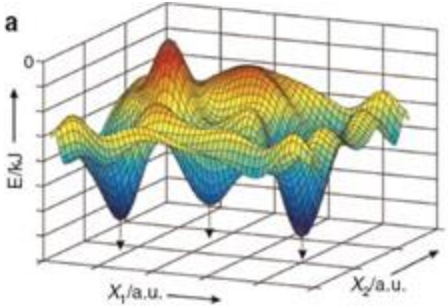
Electron-electron interaction

z.zanolli@uu.nl

First-principles Superconductivity

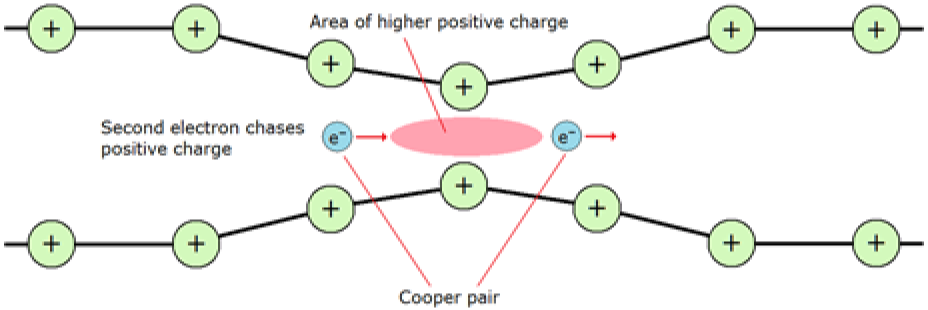






Kinetic energy of electrons + Electron-nuclei interaction + Electron-electron interaction

+



Superconducting (anomalous) charge

Modelling (exotic) superconductivity

- Fully capture the quantum nature of atomistic interactions
- Predict:
  - Structure
  - Electronic band structure
  - Magnetism, SOC
  - Topology
  - Dimensionality effects
  - Heterostructures
  - Electron transport

DFT

Electronic Wavefunction

$$\begin{pmatrix} \psi_\uparrow(\boldsymbol{r}) \\ \psi_\downarrow(\boldsymbol{r}) \end{pmatrix}$$

Electronic Hamiltonian

$$H_{\sigma\sigma'}(\boldsymbol{r})$$

- A unified treatment of normal and superconducting electronic properties
- Model unconventional pairing, beyond BCS theory

BdG

Nambu spinor

$$\begin{pmatrix} u_\uparrow(\boldsymbol{r}) \\ u_\downarrow(\boldsymbol{r}) \\ v_\uparrow(\boldsymbol{r}) \\ v_\downarrow(\boldsymbol{r}) \end{pmatrix}$$

Bogoliubov Hamiltonian

$$\begin{pmatrix} H_{\sigma\sigma'}(\boldsymbol{r}) & \Delta_{\sigma\sigma'}(\boldsymbol{r}) \\ -\Delta^*_{\sigma\sigma'}(\boldsymbol{r}) & -H^*_{\sigma\sigma'}(\boldsymbol{r}) \end{pmatrix}$$

From DFT to SuperConducting DFT

Kohn-Sham DFT

$$H\,\varphi = \left(T - E_F + V_{eff}\right)\varphi = E\varphi$$

Kohn-Sham Bogoliubov-de-Gennes equations (Oliveira PRL 1988)

$$(T - E_F + V_{eff})\,u_n(\boldsymbol{r}) + \int d^3\boldsymbol{r}'\Delta^{eff}(\boldsymbol{r},\boldsymbol{r}')v_n(\boldsymbol{r}') = \epsilon_n\,u_n(\boldsymbol{r})$$

$$(-T - E_F + V_{eff})\,v_n(\boldsymbol{r}) - \int d^3\boldsymbol{r}'\Delta^{eff*}(\boldsymbol{r},\boldsymbol{r}')u_n(\boldsymbol{r}') = -\epsilon_n\,v_n(\boldsymbol{r})$$

Effective single-particle potentials

$$V_{eff}(\boldsymbol{r}) = V_{ext}(\boldsymbol{r}) + \int \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{x}' + \frac{\delta E_{xc}[\rho]}{\delta\rho(\boldsymbol{x})}$$

$$V_{eff}(\boldsymbol{r}) = V_{ext}(\boldsymbol{r}) + \int \frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{x}' + \frac{\delta E_{xc}[\rho,\chi]}{\delta\rho(\boldsymbol{r})}$$

χ = anomalous charge density

$$\Delta_{eff}(\boldsymbol{r},\boldsymbol{r}')[\rho,\chi] = D_{ext}(\boldsymbol{r},\boldsymbol{r}') - \frac{\delta E_{xc}[\rho,\chi]}{\delta\chi^*(\boldsymbol{r},\boldsymbol{r}')}$$

Exchange correlation energy

$E^0_{xc}[\rho]$ (LDA, GGA, Hybrids, ...)

$$E^0_{xc}[\rho] - \int d^3[\boldsymbol{r}\,\boldsymbol{r}'\boldsymbol{r}''\boldsymbol{r}''']\chi^*(\boldsymbol{r},\boldsymbol{r}')\Lambda[\rho,\chi](\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\boldsymbol{r}''')\chi(\boldsymbol{r}'',\boldsymbol{r}''')$$

Local approximation: $\Delta_{eff}(\boldsymbol{r}) = \Lambda\chi(\boldsymbol{r})$ (Suvasini PRB 1993)

Λ = superconducting kernel from:

- el.-ph. (fully ab-initio DFT)
- Model (e.g. strong correlation)
- Experiment (fitting parameter)

SIESTA-BdG

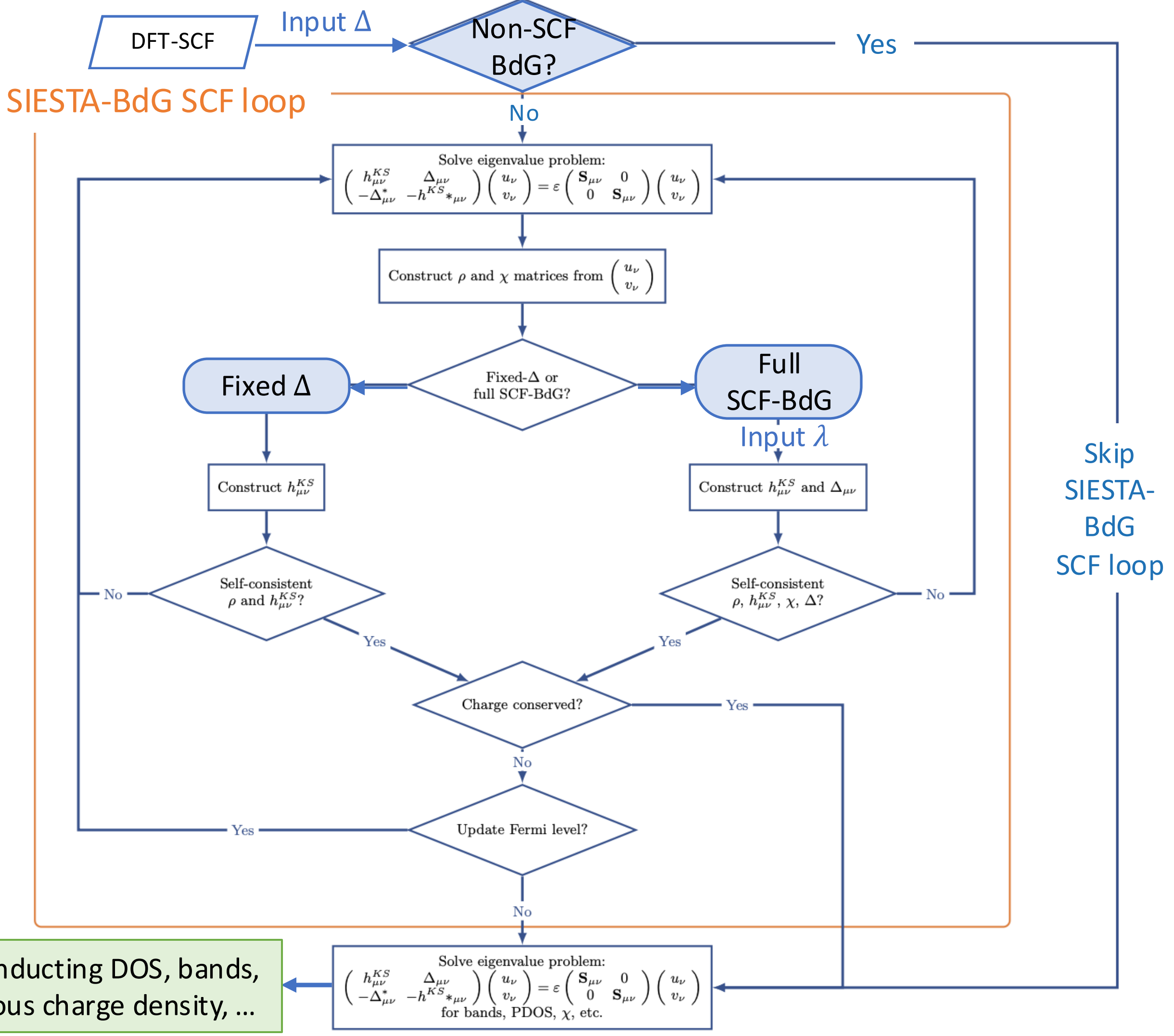
- Simultaneous treatment of normal and superconducting electronic properties

- SIESTA-BdG self-consistency can be performed at different level of accuracy:
  - Non-SCF BdG
  - Fixed Δ
  - Full SCF BdG

- General form of superconducting pairing potential Δ specified as
  - Interaction between orbitals
  - Real-space function

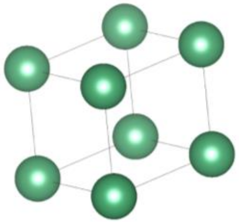
=> (un)conventional superconductivity

Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code
Reho, Wittemeier, Kole, Ordejón, Zanolli
Physical Review B, 110(13), 134505

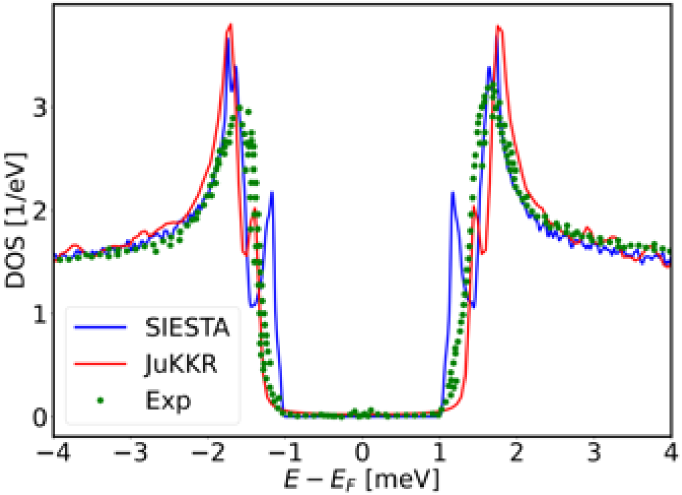


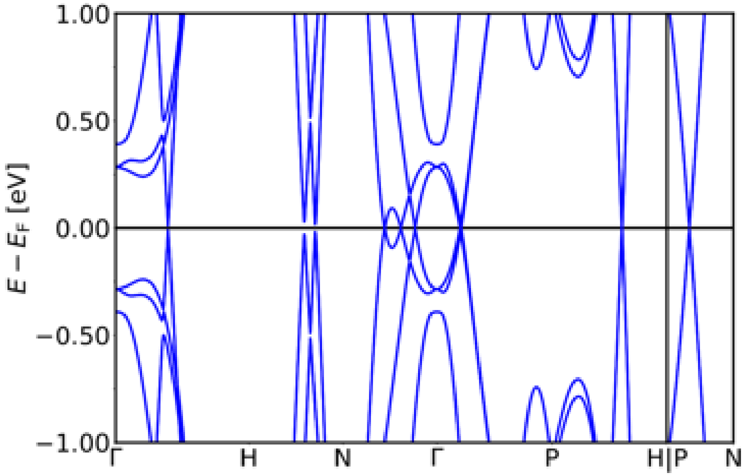
Computing Conventional Superconductivity

Bulk Nb



Finnemore
PhysRev 1966





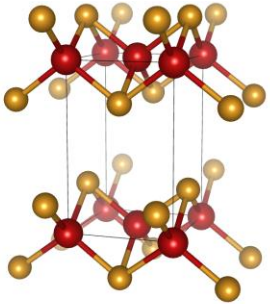
A. Kole

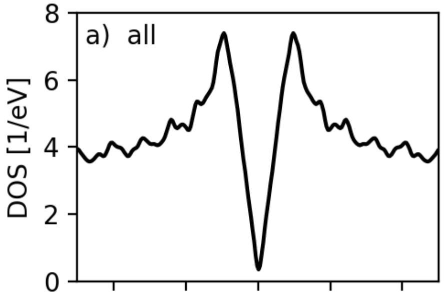
- ✓ U shaped DOS => SIESTA-BdG correctly predicts conventional superconductivity
- ✓ Agreement with Jülich-KKR (Rußmann PRB. **105,** 125143, 2022)
- ✓ Agreement with experiment (Schneider, PhD thesis 2021)
- ✓ Electron-hole symmetry visible in band structure

siesta

Computing Unconventional Superconductivity

bulk FeSe





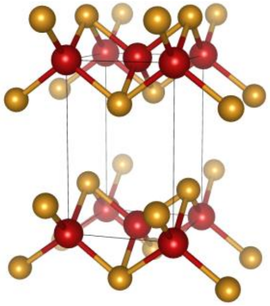
N. Wittemeier

siesta

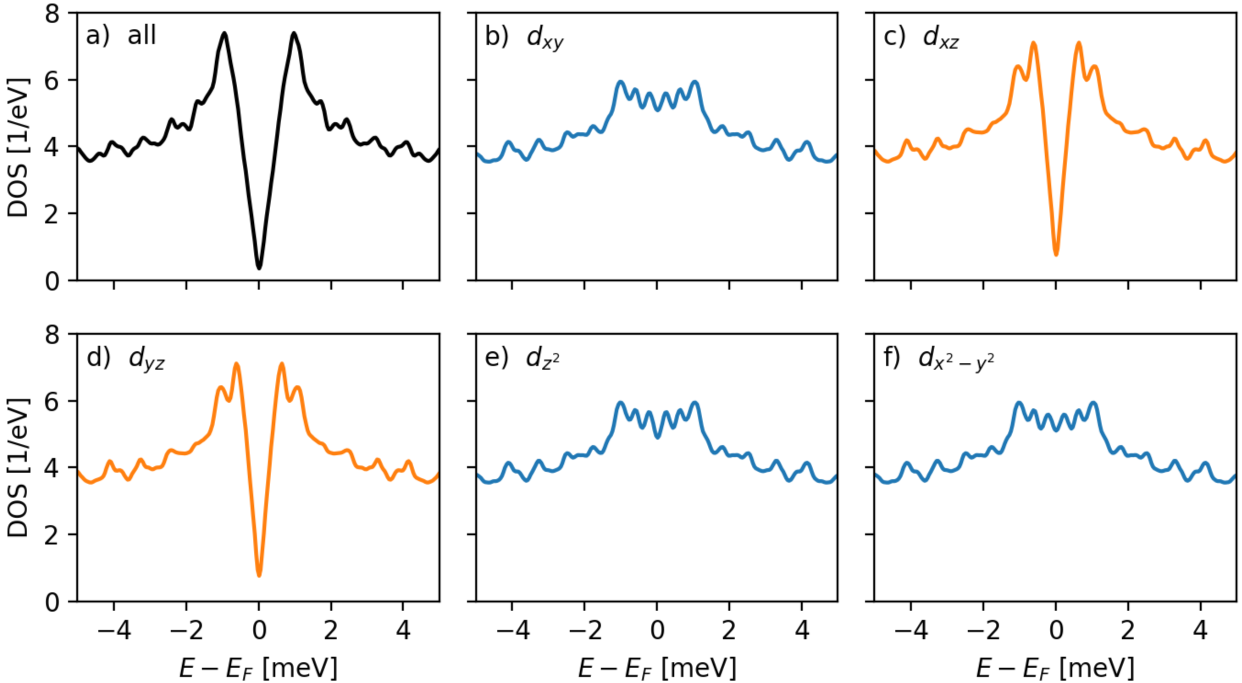
✓ V-shaped DOS: agreement with experiment (Kasahara PNAS **11** 46 16309, 2014)

Computing **Unconventional** Superconductivity

bulk FeSe



N. Wittemeier



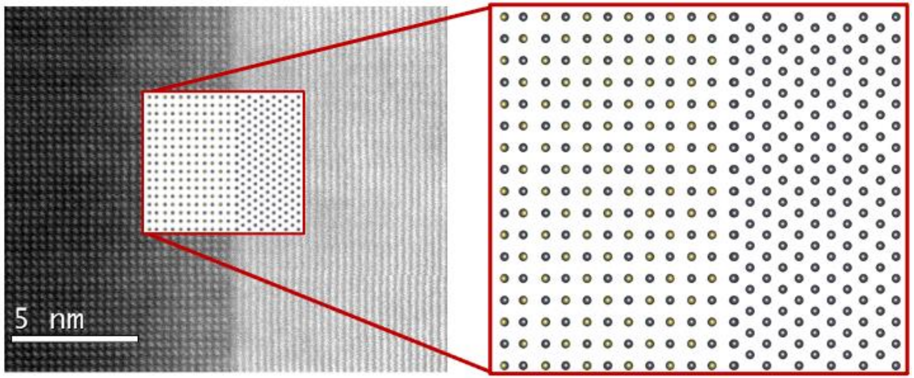
siesta

- ✓ V-shaped DOS: agreement with experiment (Kasahara PNAS **11** 46 16309, 2014)
- ✓ Superconductivity due to Fe d_{xz} and d_{yz} orbitals (Zhang PRB **91** 214503, 2015)
- ✓ No superconducting gap if pairing interaction restricted to other Fe(3d) orbitals

Proximity Induced Superconductivity

Emerging properties depend on the **atomic/electronic interaction** at the **interface**

- Lattice mismatch, strain, crystal symmetry
- Disorder, scattering by non-magnetic impurities
- Electronic band structure
- Band offset, Schottky barrier
- SOC
- formation & stability of the topological phase



HRTEM Verheijen, TU/e

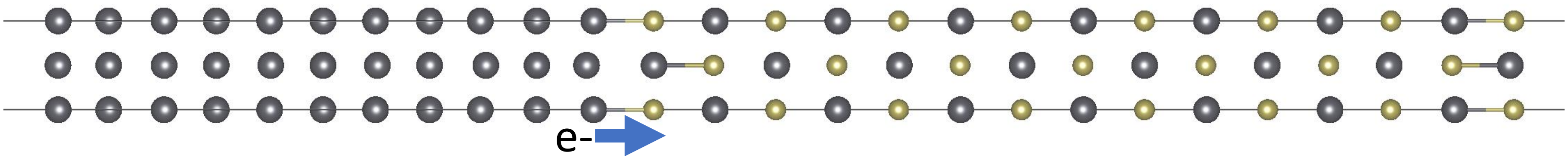
Models: either too simple or too complex.
Interface features hard to access experimentally

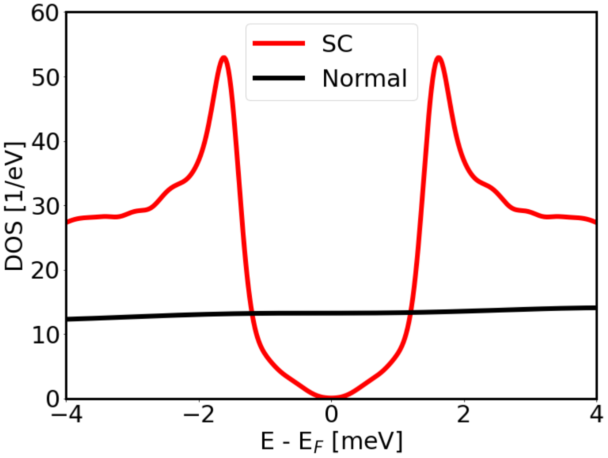
Need:

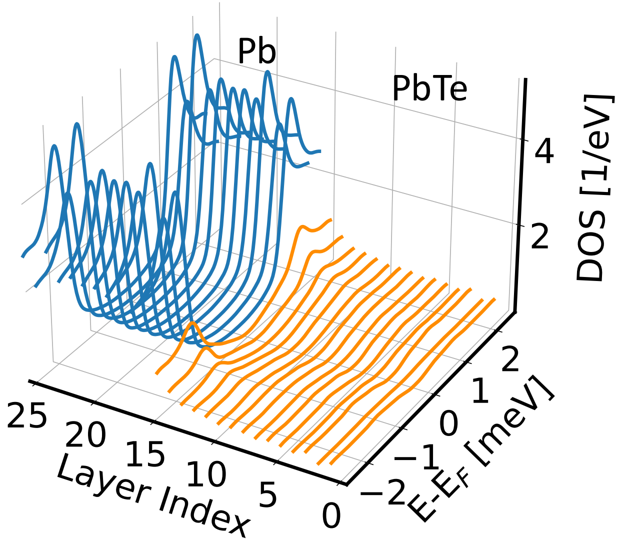
- Actual material parameters at the interface: **first-principles simulations**
- **Simultaneous treatment of normal and superconducting electrons**

z.zanolli@uu.nl

Proximity Induced Superconductivity: PbTe/Pb







<u>PbTe/Pb Interface effects:</u>

- Structural relaxation
- Induced metallicity in PbTe
- **Induced superconductivity in PbTe**
- Charge transfer to Pb

R. Reho

Quantum Transport

Scattering theory for superconductors

Reflection and transmission probabilities:

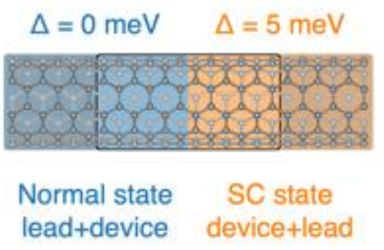
$$R_{\mathfrak{e}} \rightarrow \begin{pmatrix} R_{\mathfrak{e}}^{pp} & R_{\mathfrak{e}}^{hp} \\ R_{\mathfrak{e}}^{ph} & R_{\mathfrak{e}}^{hh} \end{pmatrix} \qquad T_{\mathfrak{e}\mathfrak{e}'} \rightarrow \begin{pmatrix} T_{\mathfrak{e}\mathfrak{e}'}^{pp} & T_{\mathfrak{e}\mathfrak{e}'}^{hp} \\ T_{\mathfrak{e}\mathfrak{e}'}^{ph} & T_{\mathfrak{e}\mathfrak{e}'}^{hh} \end{pmatrix}$$

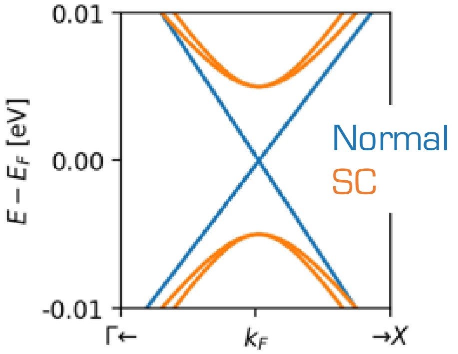
normal

$$I_{\mathfrak{e}} \approx \frac{2e}{h} \int_{\mathrm{BZ}} d\mathbf{k} \sum_{\mathfrak{e}' \neq \mathfrak{e}} T_{\mathfrak{e}\mathfrak{e}'}^{pp}(\mu)[\mu_{\mathfrak{e}'} - \mu_{\mathfrak{e}}]$$

$$+ \sum_{\mathfrak{e}' \neq \mathfrak{e}} T_{\mathfrak{e}\mathfrak{e}'}^{ph}(\mu)[2\mu - \mu_{\mathfrak{e}'} - \mu_{\mathfrak{e}}] + 2R_{\mathfrak{e}}^{hp}(\mu)[\mu - \mu_{\mathfrak{e}}]$$

anomalous Andreev



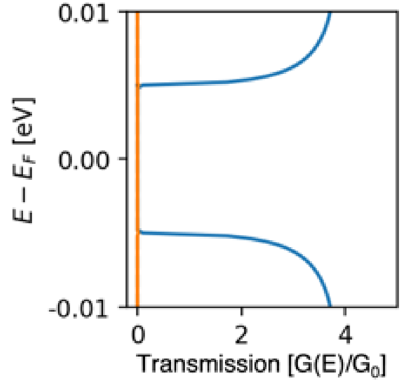


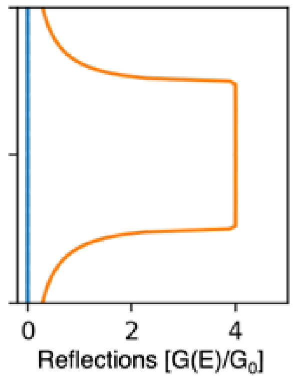
T^{pp} = normal transmission

T^{ph} = anomalous transmission

R^{pp} = normal reflection

R^{ph} = Andreev reflection





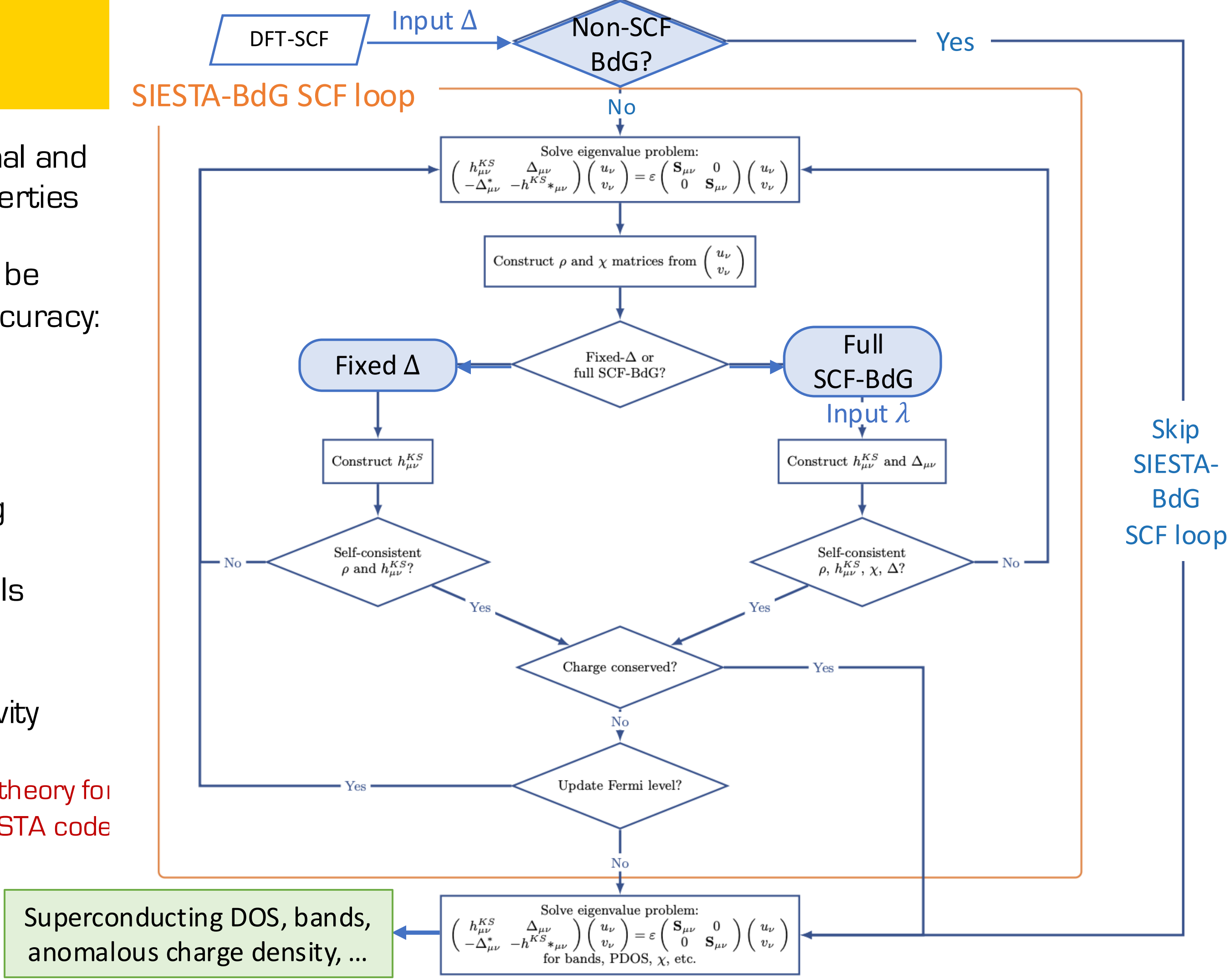
Guided Tour

SIESTA-BdG

- Simultaneous treatment of normal and superconducting electronic properties
- SIESTA-BdG self-consistency can be performed at different level of accuracy:
  - Non-SCF BdG
  - Fixed Δ
  - Full SCF BdG
- General form of superconducting pairing potential Δ specified as
  - Interaction between orbitals
  - Real-space function

=> (un)conventional superconductivity

Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code
Reho, Wittemeier, Kole, Ordejón, Zanolli
Physical Review B, 110(13), 134505

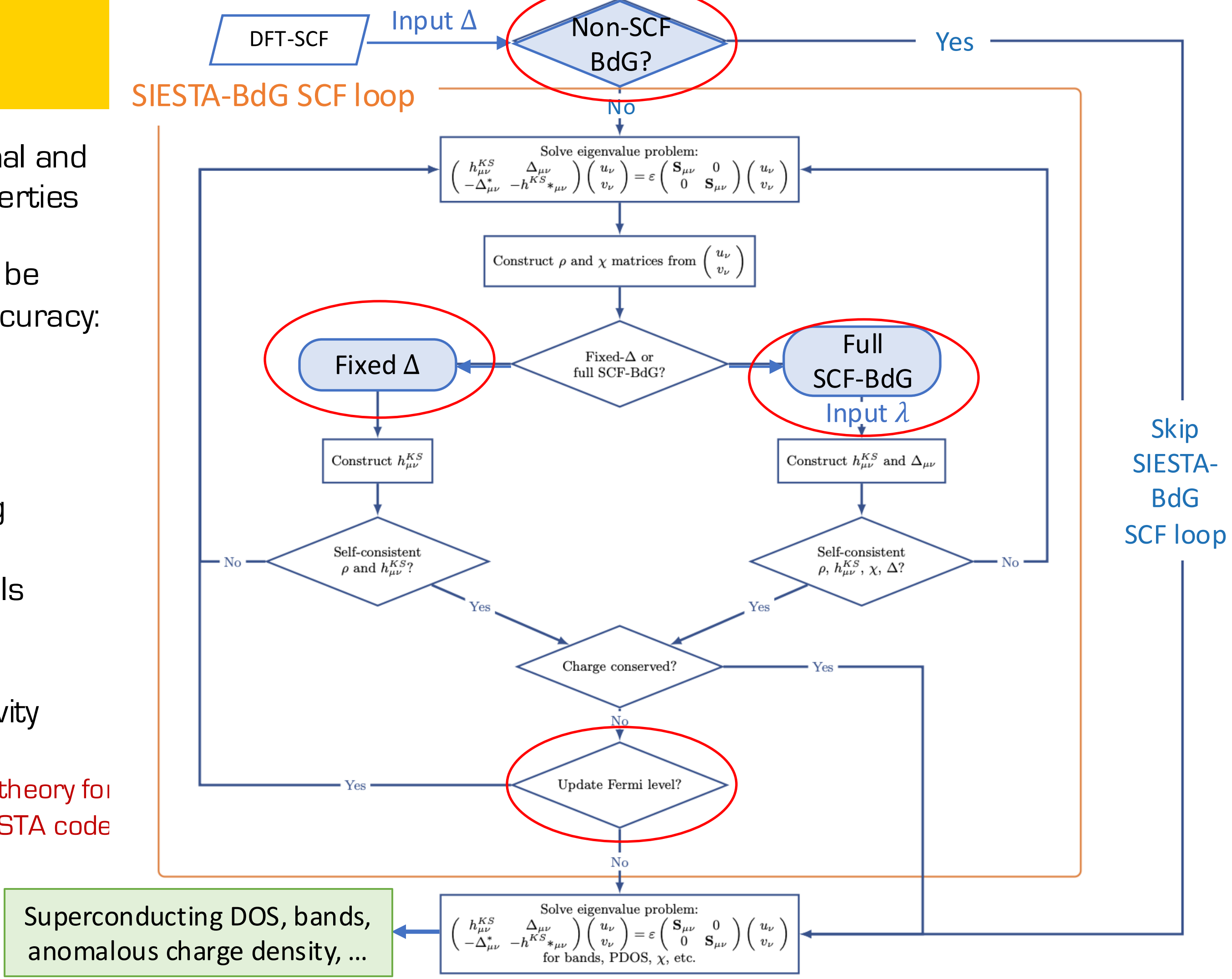


SIESTA-BdG

- Simultaneous treatment of normal and superconducting electronic properties
- SIESTA-BdG self-consistency can be performed at different level of accuracy:
  - Non-SCF BdG
  - Fixed Δ
  - Full SCF BdG
- General form of superconducting pairing potential Δ specified as
  - Interaction between orbitals
  - Real-space function

=> (un)conventional superconductivity

Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code
Reho, Wittemeier, Kole, Ordejón, Zanolli
Physical Review B, 110(13), 134505



Inputs – Top level control flags

At the top level you can specify:

- Which level of self-consistency
- Enable charge conservation during BdG
- Control of charge conservation loop

```
BdG.Method OneShot | FixedDelta | FixedLambda
```

```
BdG.SCF.dQ.Converge true | false
BdG.SCF.dQ.Tolerance [float]
BdG.dQ.Fermi.Max [float] [energy unit]
BdG.dQ.Fermi.Scale [float]
```

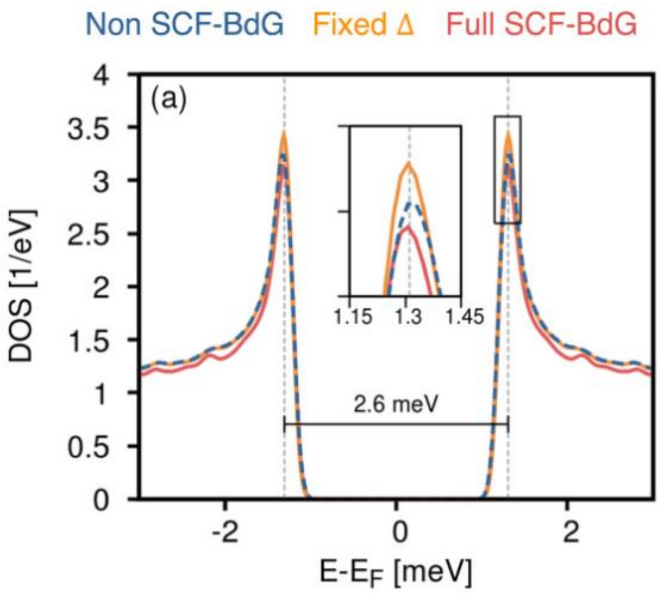
It is possible to restart SIESTA-BdG calculations. For this you need:

- "normal" DM (diagonal part)
- "anomalous" ADM (off-diagonal part)
- The Fermi energy
  - Can be read from SystemLabel.EIG
  - Or set manually via 'Nambu.ChemPot'

Inputs – Different levels of self-consistency

Comparison of BdG-DOS for bulk Pb with different levels of self-consistency

- Bulk Pb is conventional BCS superconductor
- Only minor differences in the DOS



N. Wittemeier

Inputs – Tuning SIESTA-BdG SCF loop

For full SCF-BdG the anomalous quantities (χ, Δ) are being mixed

- The quantity being mixed is derived from the 'SCF.Mix' flag
  - χ if mixing DM
  - Δ if mixing H
- All regular mixing options also work for the anomalous quantities
- Additional options to delay updating the anomalous quantities

```
SCF.BdG.Mixer.[flag] [value]
(i.e. Method, Weight, History)
```

```
SCF.BdG.Mixer.DelayedUpdate true | false
SCF.BdG.Mixer.Update.Scale [float]
SCF.BdG.Mixer.Reset true | false
SCF.BdG.Mixer.Reset.Scale [float]
```

```
%block SCF.BdG.Mixer.<>
  H.tolerance [float] [energy unit]
  H.converge true | false
  DM.tolerance [float]
  DM.converge true | false
%endblock
```

Inputs – Charge conservation

Charge conservation during "normal" SCF

- Set Fermi energy to get correct Qtot
- No re-computation of the eigenvalues needed

$$Q_{\mathrm{tot}} = \sum_{\mathbf{k},i} \frac{1}{\exp\left[\left(\epsilon_i(\mathbf{k}) - E_F\right) / \left(k_B T\right)\right] + 1} w_{\mathbf{k}}$$

Charge conservation during BdG-SCF

- Fermi energy enters directly into the KS-BdG equations
  - Updating Fermi energy requires re-computation of eigenvalues
- Only update in loop outside of SCF possible

$$(T - E_F + V_{eff})\, u_n(\boldsymbol{r}) + \int d^3\boldsymbol{r}' \Delta^{eff}(\boldsymbol{r},\boldsymbol{r}') v_n(\boldsymbol{r}') = \epsilon_n\, u_n(\boldsymbol{r})$$

$$(-T - E_F + V_{eff})\, v_n(\boldsymbol{r}) - \int d^3\boldsymbol{r}' \Delta^{eff*}(\boldsymbol{r},\boldsymbol{r}') u_n(\boldsymbol{r}') = -\epsilon_n\, v_n(\boldsymbol{r})$$

SIESTA-BdG

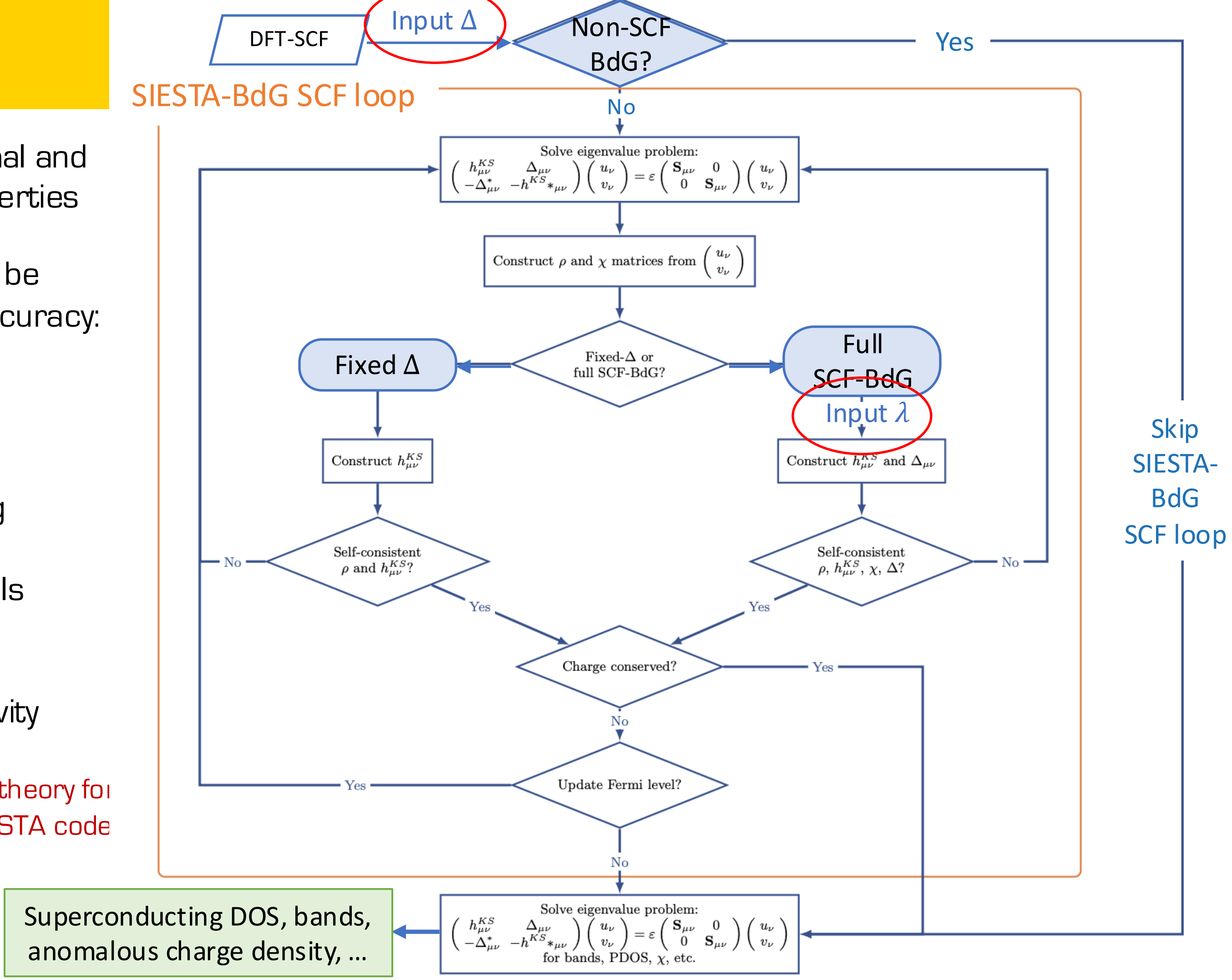
- Simultaneous treatment of normal and superconducting electronic properties

- SIESTA-BdG self-consistency can be performed at different level of accuracy:
    - Non-SCF BdG
    - Fixed Δ
    - Full SCF BdG

- General form of superconducting pairing potential Δ specified as
    - Interaction between orbitals
    - Real-space function

=> (un)conventional superconductivity

Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code
Reho, Wittemeier, Kole, Ordejón, Zanolli
Physical Review B, 110(13), 134505



Inputs – Different options for initializing Delta/Lambda

Initialize Delta:

- Matrix elements in orbital space
- On a grid in real-space

```
BdG.Delta.Init   orbital | real-space
BdG.Lambda.Init            real-space
```

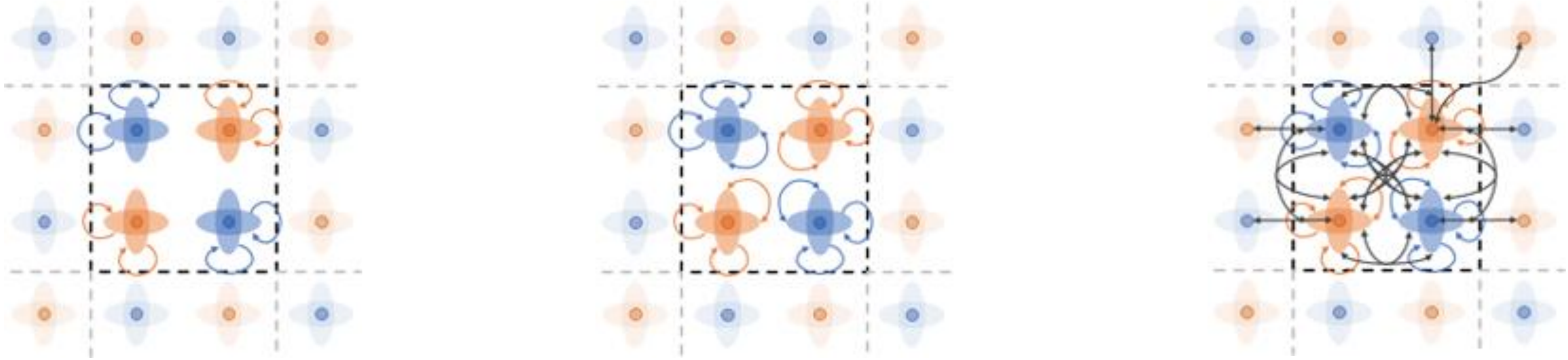
Initialize Lambda:

- On a grid in real-space

$$\Delta_{eff}(\boldsymbol{r}) = \Lambda\chi(\boldsymbol{r})$$

‘Orbital’ Initialization of the superconducting coupling

Intra orbital coupling	Onsite inter orbital coupling	Full inter orbital coupling



Same atom Same orbital	Same atom Different orbitals	All atoms All orbitals

- Fe
- Se

- Localized atomic orbitals $\varphi_\mu(\boldsymbol{r})$ with $\mu = (I, n, l, m)$, I = atom index; n, l, m = quantum numbers
- Coupling between one electron in orbital φ_μ and one hole in orbital φ_ν : $\Delta_{\mu\upsilon} = \int \varphi_\mu \Delta \varphi_\upsilon$

z.zanolli@uu.nl

‘Orbital’ Initialization of the superconducting coupling

- Directly set coupling between different orbitals
- Sparsity pattern inherited from H
  - Coupling between orbitals with zero overlap ignored

```
%block BdG.Delta.SelectiveCouplings

# Spin channel indices (possible values: 1,2,3,4)

          #    - 1  => S          (singlet)
          #    - 2  => T_up,up    (triplet)
          #    - 3  => T_down,down (triplet)
          #    - 4  => T_0        (triplet)

# channel jo_s io_u    abs(Delta) phase(Delta) energy_unit
  1       1    2       3.0        0.           meV
%endblock

%block BdG.Delta.FullOverlap
# channel jo_s io_u    abs(Delta) phase(Delta) energy_unit
  4       12   35      3.0        0.           meV
%endblock
```

Real-space initialization of the superconducting coupling

We currently support four types of real-space pairing:

- Hardwell
- Softwell
- Gaussian
- PlaneWave

$$\Delta(\mathbf{r}) = \bar{\Delta} g(\mathbf{r})$$

$$g(\mathbf{r};\mathbf{x},\sigma) = e^{-|\mathbf{r}-\mathbf{x}|^2/(2\sigma^2)}$$

$$g(\mathbf{r};\mathbf{x},\sigma) = \theta\left(|\mathbf{r}-\mathbf{x}|;\sigma;\eta\right)$$

$$g(\mathbf{r};\mathbf{k},\phi) = \cos\left(\mathbf{k}\cdot\mathbf{r}+\phi\right)$$

```
%block BdG.[Delta|Lambda].RealSpacePairings
  Label1 Hardwell  # Sphere with constant value
  Label2 Softwell  # Sphere with finite broadening
  Label3 Gaussian  # Gaussian shaped pairing
  Label4 PlaneWave
%endblock
```

Real-space initialization of the superconducting coupling

Input block for Hardwell

```
Label1 Hardwell  # Sphere with constant value
```

```
%block BdG.[Delta|Lambda].Pairing.Label1
  channel  1          # Super conducting channel
                      #   1 = Singlet
                      #   2,3,4 = Triplet (T_up,T_down,T_0)
  radius   2. Ang     # Radius of the sphere where pairing applies
  strength 5. meV     # Strength of the pairing
  cphase   0.         # Complex phase of the pairing
  # centers
    species Pb        # Placed on all atoms of species Pb
%endblock
```

Real-space initialization of the superconducting coupling

Input block for Softwell

```
    Label2 Softwell  # Sphere with finite broadening
```

```
%block BdG.[Delta|Lambda].Pairing.Label2
  channel  1
  radius   2. Ang
  strength 5. meV
  cphase   0.
  sigma    0.125 Ang  # Smearing width at the edge of the sphere
  # centers
    atom   [1-3,5]    # Placed on atoms 1, 2, 3 and 5
%endblock
```

Real-space initialization of the superconducting coupling

Input block for Gaussian

```
    Label3 Gaussian  # Gaussian shaped pairing
```

```
%block BdG.[Delta|Lambda].Pairing.Label3
  channel    1
  strength   5. meV
  cphase     0.
  sigma      2. Ang      # Broadening of the Gaussian
  # centers              # Multiple centers are possible
    xyz      0. 0.2 0.3 #   at (0. 0.2 0.3) uses AtomicCoorinatesFormat
    atom     [1]         #   Allows different types of center definitions
    species Pb           #   Species 2
%endblock
```

Real-space initialization of the superconducting coupling

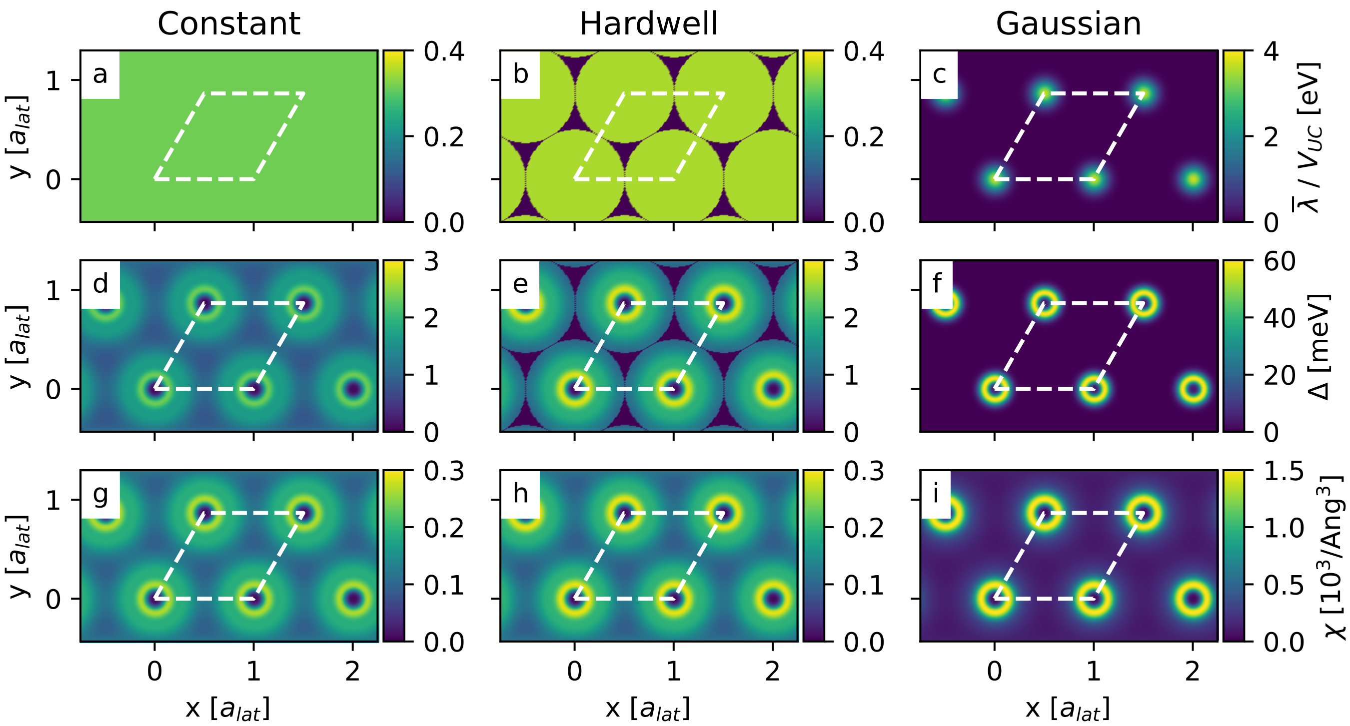
Input block for PlaneWave

```
Label4 PlaneWave
```

```
%block BdG.[Delta|Lambda].Pairing.Label4
  channel  1
  strength 1. eV
  cphase   0.
  nk       1
  # Using k = 0 is equivalent to setting Delta constant in real-space everywhere in simulation cell
  k        0. 0. 0.
%endblock
```

Real-space initialization of the superconducting coupling

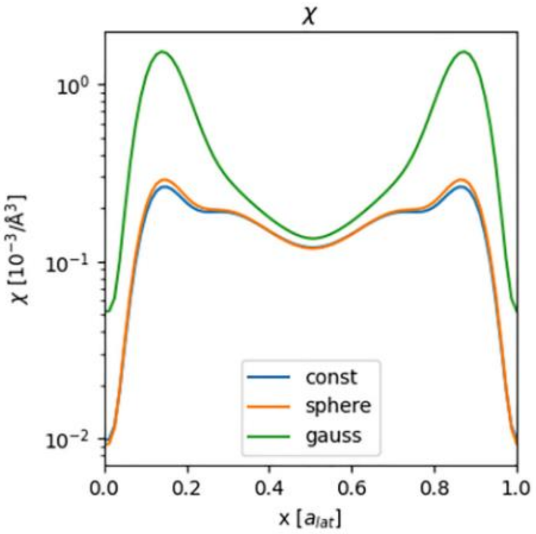
Example of using the different real-space initializations for Lambda for a full-SCF BdG calculation for bulk Pb

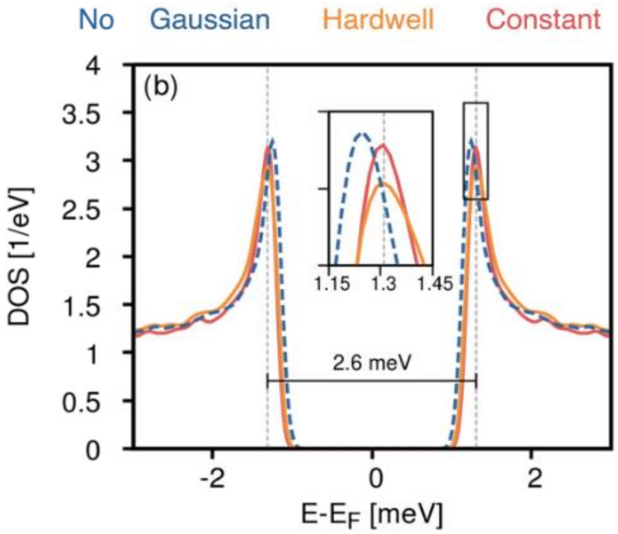


N. Wittemeier

Real-space initialization of the superconducting coupling

N. Wittemeier





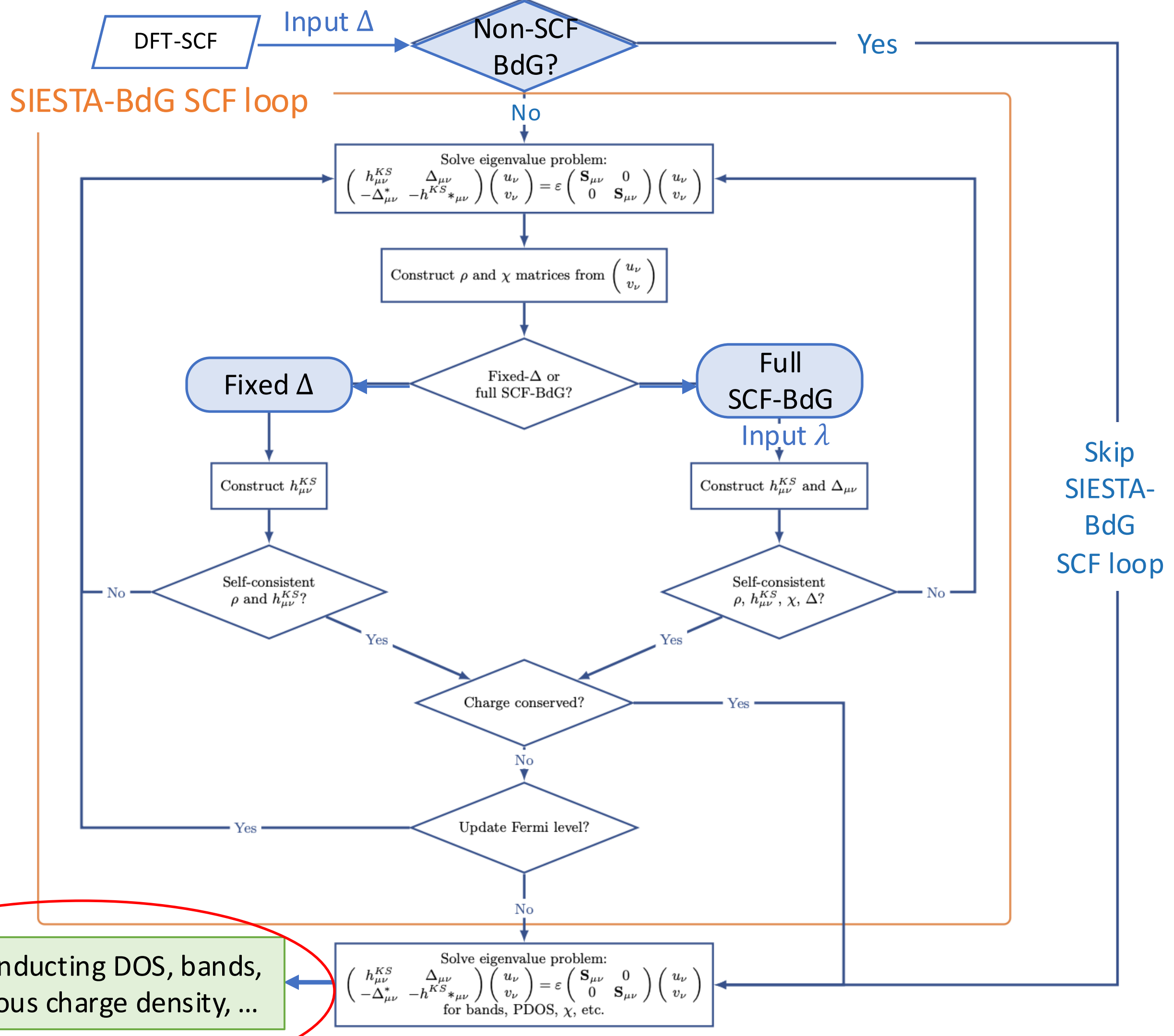
- PDOS shape changes little upon changing real-space initialization
  - Note that strength was tuned to give the same gap size
- Anomalous charge in-between atoms also changes little upon changing initialization

SIESTA-BdG

- Simultaneous treatment of normal and superconducting electronic properties
- SIESTA-BdG self-consistency can be performed at different level of accuracy:
  - Non-SCF BdG
  - Fixed Δ
  - Full SCF BdG
- General form of superconducting pairing potential Δ specified as
  - Interaction between orbitals
  - Real-space function

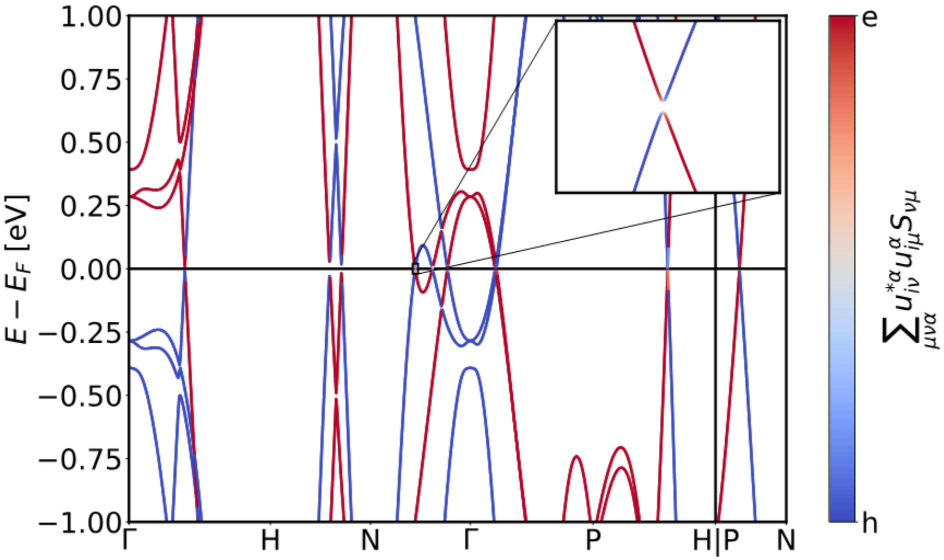
=> (un)conventional superconductivity

Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code
Reho, Wittemeier, Kole, Ordejón, Zanolli
Physical Review B, 110(13), 134505



Outputs - Bands

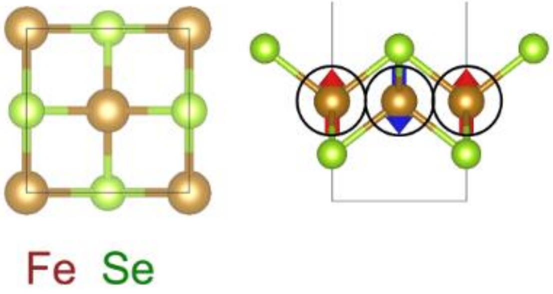
- Bands block for BdG is the same as for "normal" SIESTA
- Output is stored in SystemLabel.bands
  - Twice as many bands per k-point as for SOC (i.e. four times the number of orbitals)
- Note the particle-hole symmetry
- Fatbands can be done with latest version of sisl



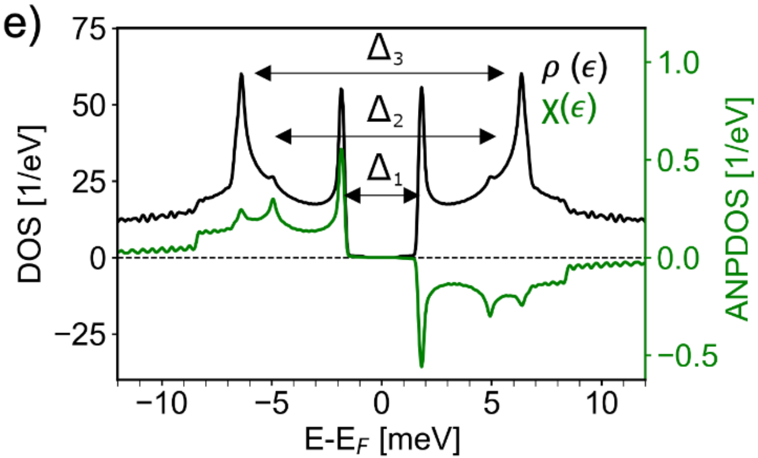
Outputs – PDOS + ANPDOS

PDOS
- Combine u+u or v+v
- 8 spin components
  - 4 soc electron
  - 4 soc hole
- Stored in SystemLabel.PDOS.xml

$$\begin{pmatrix} u_{\uparrow}(\boldsymbol{r}) \\ u_{\downarrow}(\boldsymbol{r}) \\ v_{\uparrow}(\boldsymbol{r}) \\ v_{\downarrow}(\boldsymbol{r}) \end{pmatrix}$$

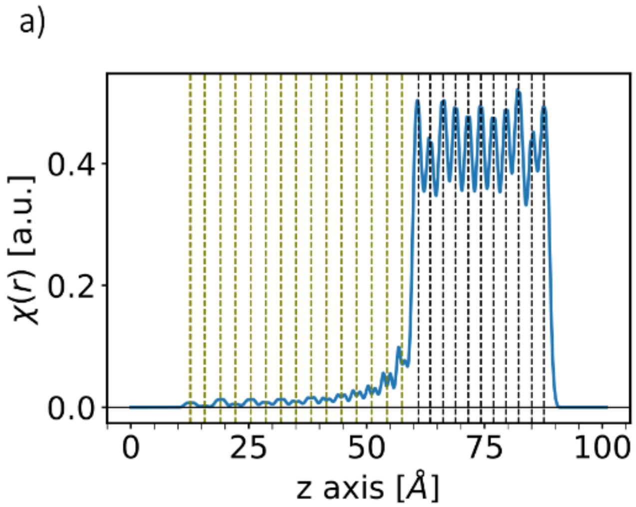


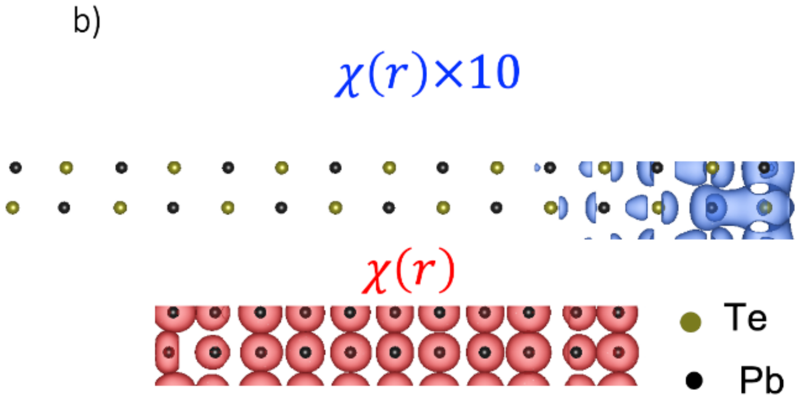
ANPDOS
- Combine u+v or v+u
- 8 spin components
  - 4 electron-hole
  - 4 hole-electron
  - S, T_z, T_x, T_y
- Stored in SystemLabel.ANPDOS.xml



Outputs – Anomalous Charge Density

R. Reho





- Projection onto real-space grid using ADM (off-diagonal part of BdG density matrix)
- Stored in SystemLabel.CHI

```
SaveChi true | false
```

Outputs – Other SIESTA quantities

Other SIESTA output quantities are currently being tested. For example,

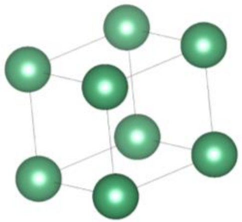
- Energies
- Atomic moments (i.e. Mulliken, Hirshfeld)
- Many more

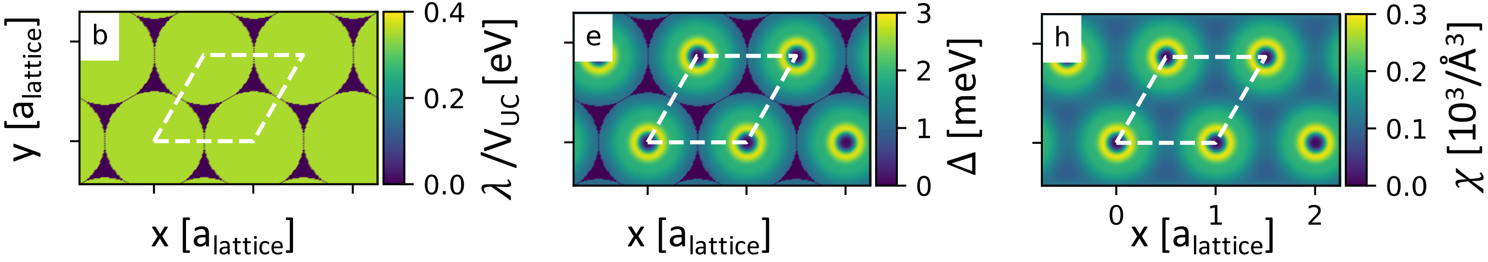
Notable exception:

- Contributions of BdG to forces and stresses are **not** computed
    - Relaxation cannot be done simultaneously with superconductivity
    - Effects should be small for small superconducting pairing

Energy scales and parameter convergence

Nb

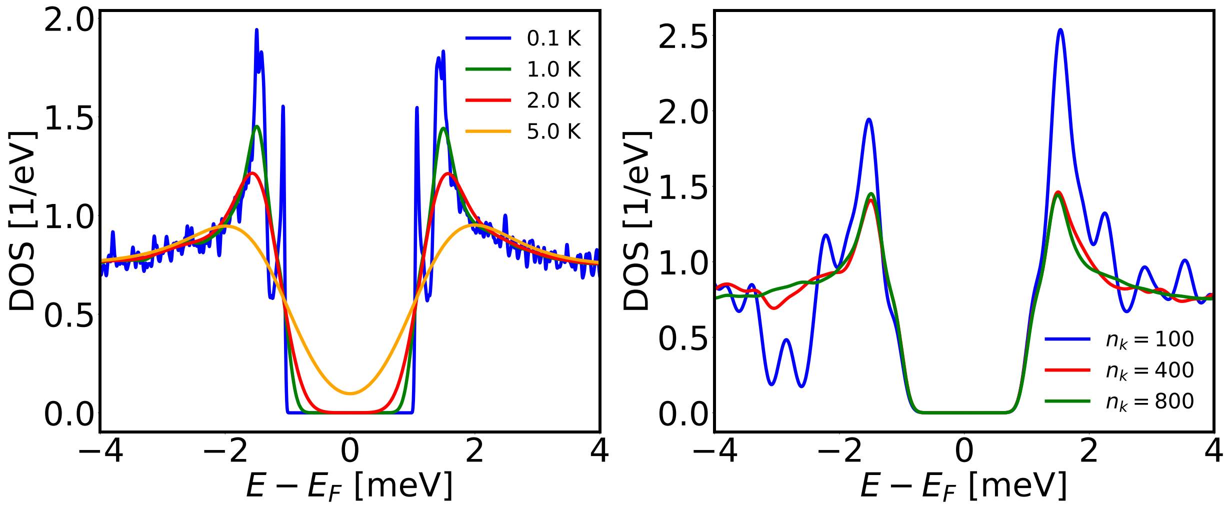




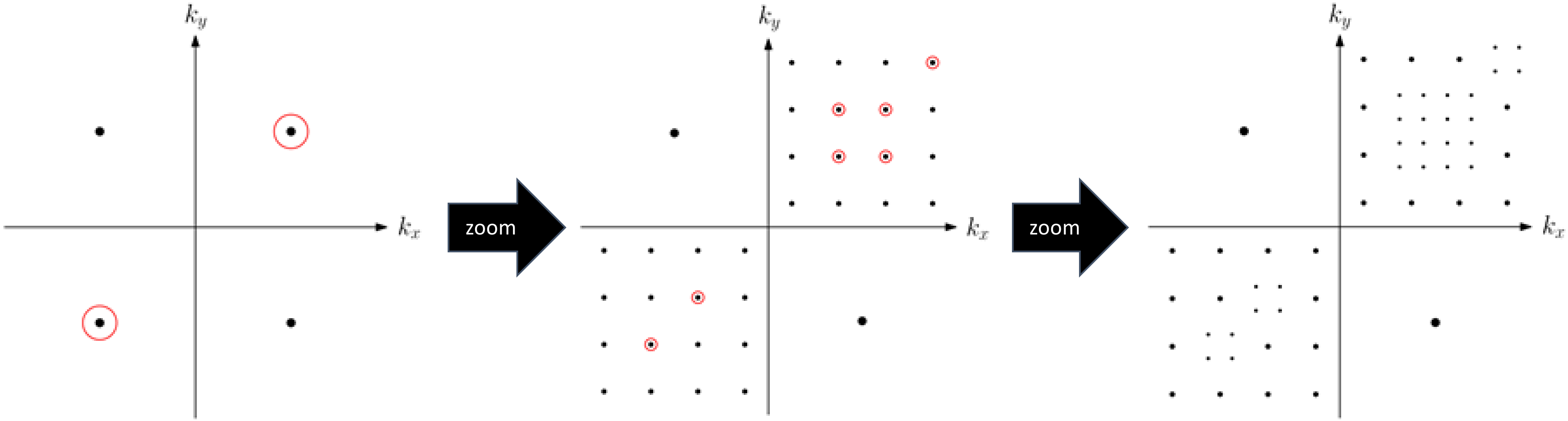
- SOC fully included
- Real-space initialization of superconducting coupling parameter λ
- full SCF-BdG
- Converged for

  T_{el} = 0.1 K

  800x800x800 k points



Adaptive Brillouin Zone Sampling



Original | Original + 1 zoom | Original + 2 zoom

K-points circled in **red** have eigenvalues lying in a specified energy range

Adaptive Brillouin Zone Sampling

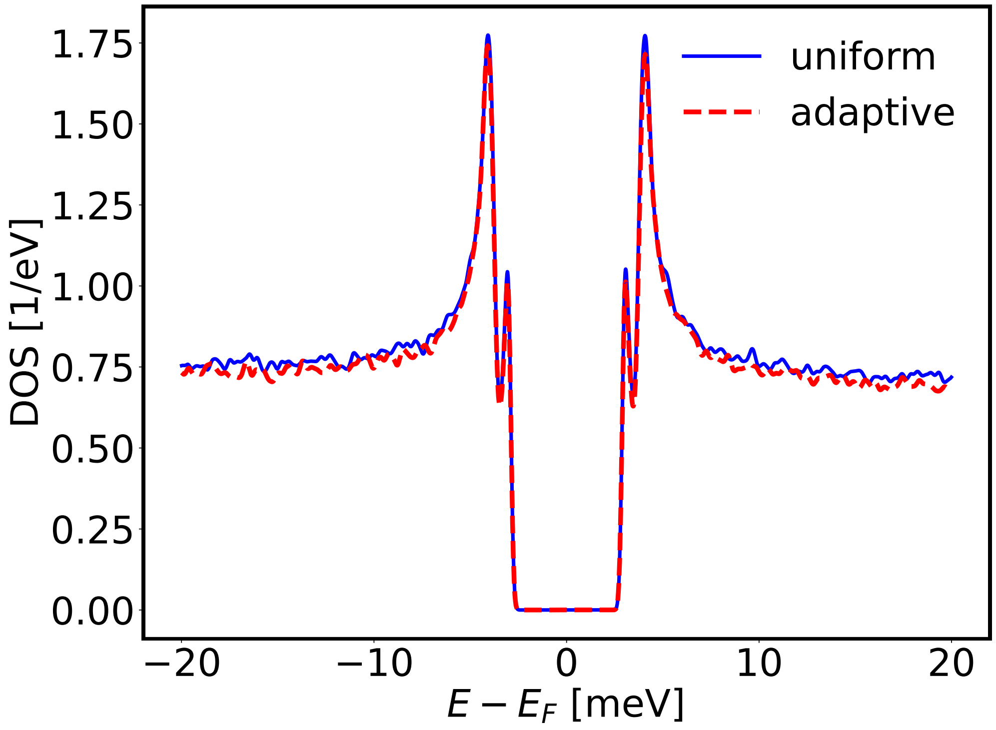
```
PDOS.Adaptive.kgrid.Steps [int]

%block PDOS.Adaptive.kgrid.EnergyWindow
  EF -50.0 50.0 meV
%endblock

%block PDOS.Adaptive.kgrid.MonkhorstPack
  3 0 0  0.
  0 2 0 -0.5
  0 0 3  0.
%endblock
```

For even number of points in sub-grid we recommend using a shift of –0.5 to ensure the subgrid is centered on the replaced point

Adaptive Brillouin Zone Sampling

DOS of bulk Niobium computed with
a uniform 800 × 800 × 800 k-grid and
an adaptive grid generated starting from a
100 × 100 × 100 uniform grid and using,
for three iterations, a 2 × 2 × 2 sub-grid.

Δ = 5 meV



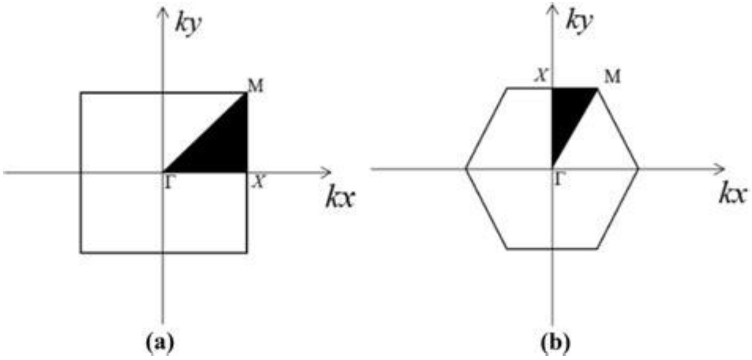
Symmetries in SIESTA

Further reduction in number of k-points using symmetries

Implementation of symmetries in SIESTA

- Currently supports
  - Determination of space group
  - Symmetrization of atomic positions and cell
  - Symmetrization of forces and stresses
    - Conserve space group during relaxation
- Uses external library 'spglib'

```
Symmetry.Impose true | false
Symmetry.Tolerance [float] [length unit]
```



MR

z.zanolli@uu.nl

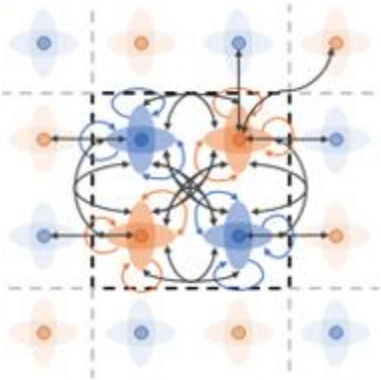
Symmetries in SIESTA

Extension to symmetries for the k-grid adds significant complexity

- Requires applying symmetry operations to wave functions or the DM
- In particular, this involves rotations of the basis-set
  - Requires implementation of Wigner D-matrices in SIESTA for spherical harmonics
- Care must be taken that symmetries of SOC and BdG are respected

$$Y_\ell^m(\mathbf{r}') = \sum_{m'=-\ell}^{\ell} [D^{(\ell)}_{mm'}(\mathcal{R})]^* Y_\ell^{m'}(\mathbf{r})$$

SIESTA + BdG: take home messages



- ✓ Theory & Implementation of DFT+BdG in SIESTA
- ✓ conventional & (un)conventional superconductors
- ✓ proximity induced superconductivity
- ✓ Extension to quantum transport in superconductors: DFT+BdG+NEGF

Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code

R. Reho, N. Wittemeier, A. H. Kole, P. Ordejón, Z. Zanolli
Physical Review B, 110(13), 134505

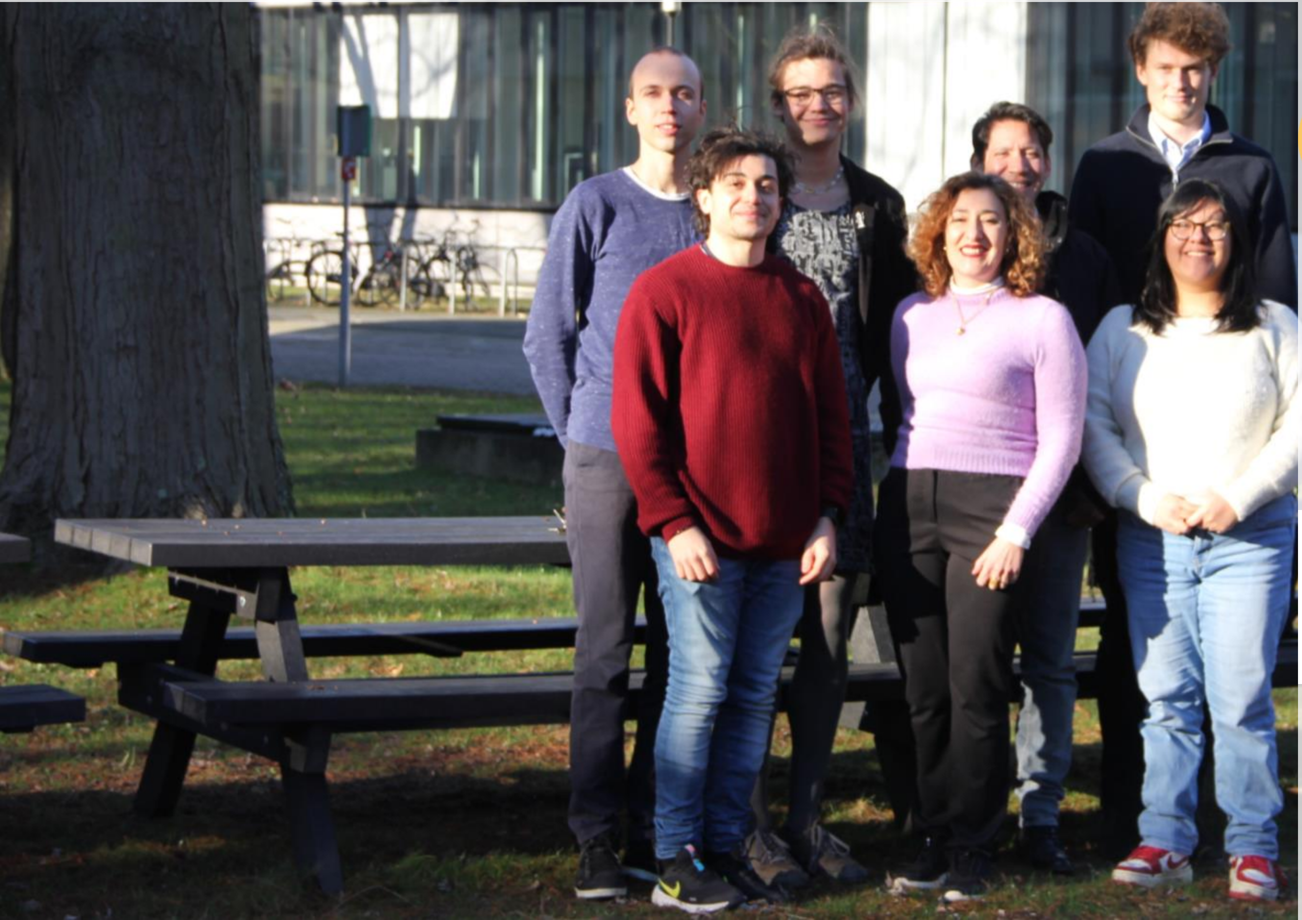
P Ordejón N Wittemeier A Kole R. Reho

ICN2 Utrecht University

Quantum Materials by Design
2025 Team

ETSF

Utrecht University



siesta

Yambo

QuMat
Materials for the Quantum Age

NWO

QUONDENSATE

European Innovation Council

SURF SARA

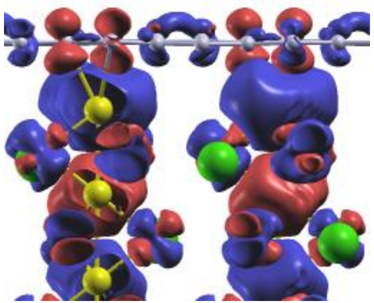
PRACE

Thank you!

Hands-on with sisl-bdg

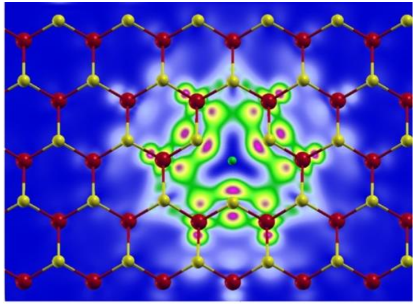
https://edu.nl/e7j9b

Research Lines



Topological Matter

Moes NL ‘24
Zanolli SciRep ‘16
Zanolli PRB ’18
Wittemeier JPhysMat ‘22
Garcia PRB 22

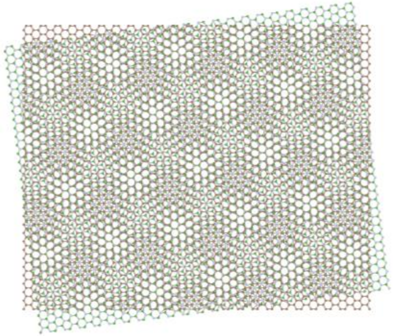


Exciton physics

Sohier 2D Mater ‘23
Libbi PRL ’22
Melo QUTE ‘21
Ersfeld NL ‘18

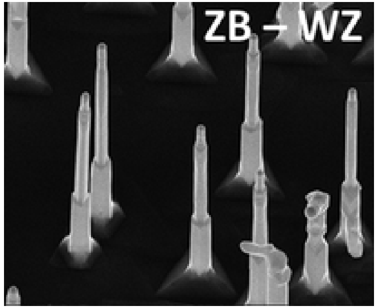
Quantum Materials

Twistronics
vdWaals heterostructures

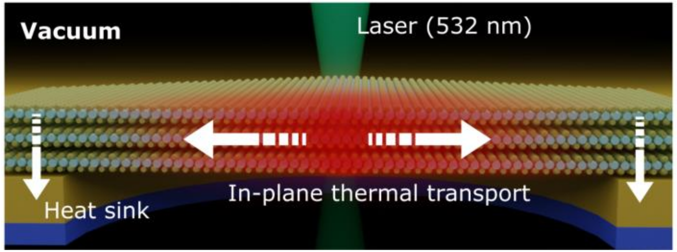


Wittemeier Carbon 22
Pezo 2D Mater 22

First-principles Superconductivity



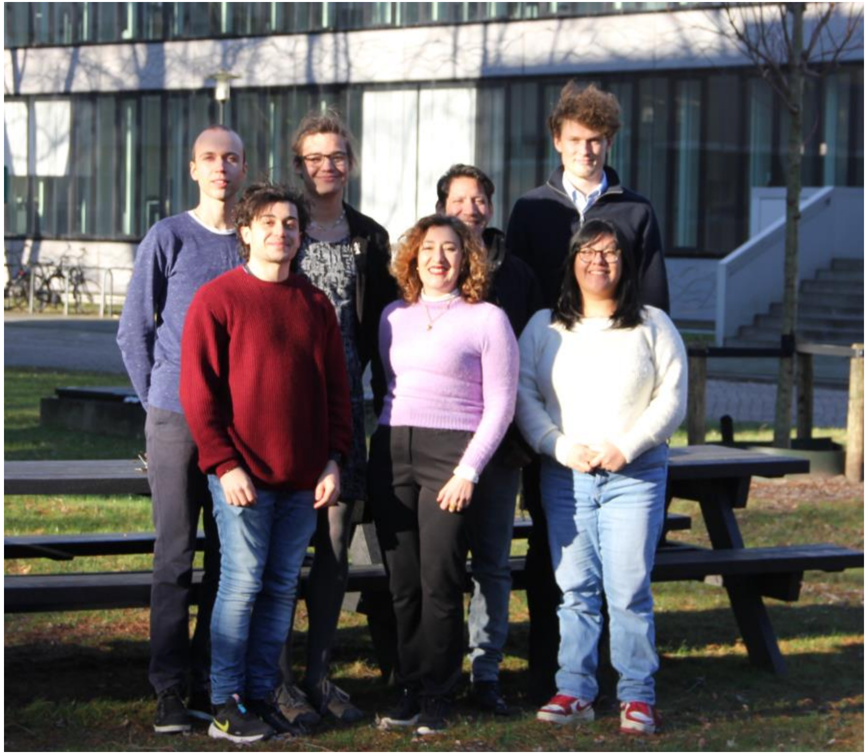
Quantum Electron & Thermal Transport



Saleta Adv Mater 22

ETSF

2023-24 Team



Developing: siesta Yambo

Funding:

QuMat Materials for the Quantum Age

NWO

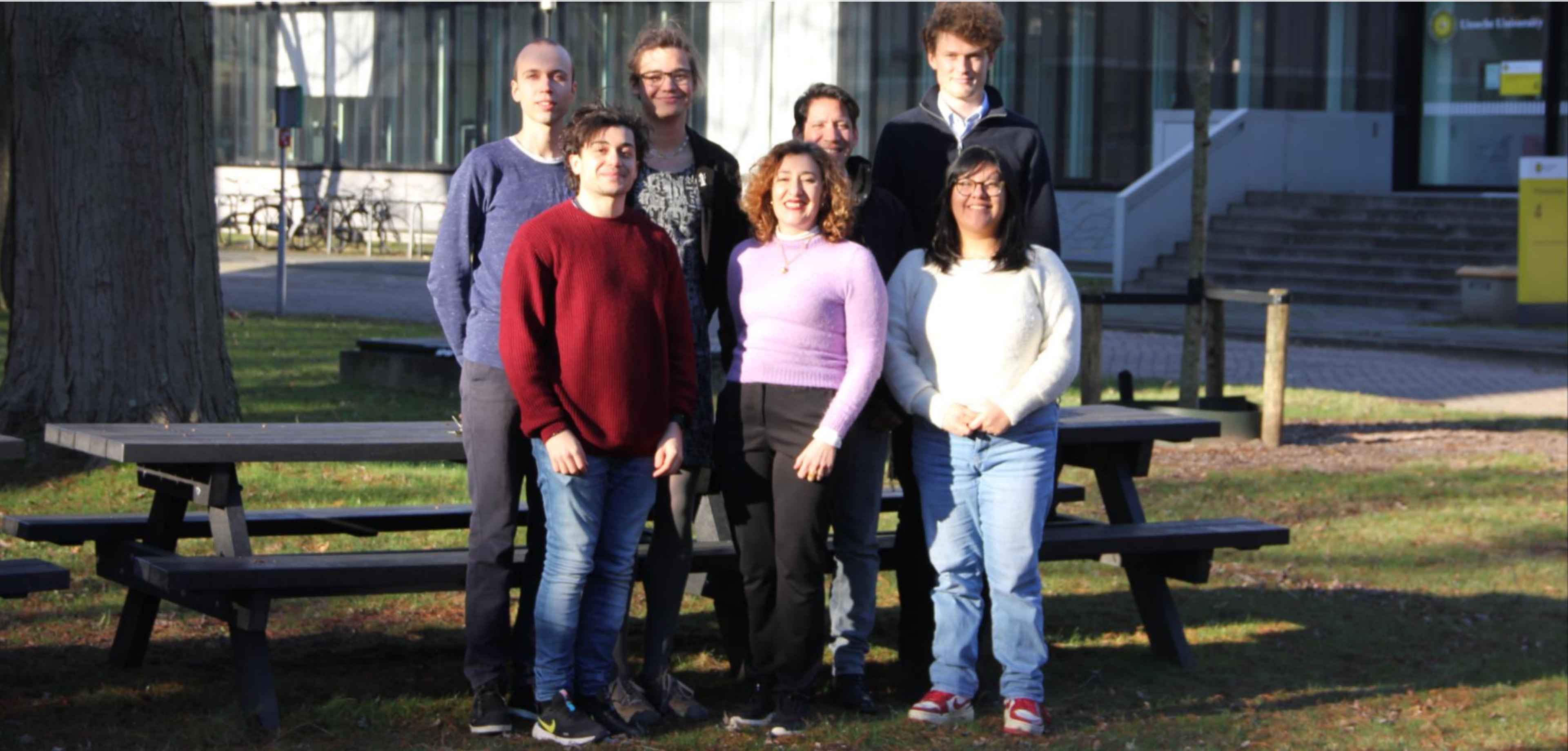
QUONDENSATE

European Innovation Council

Computing: SURF SARA PRACE

Quantum Materials by Design
2024 Team

Utrecht University



High-throughput & FAIR data

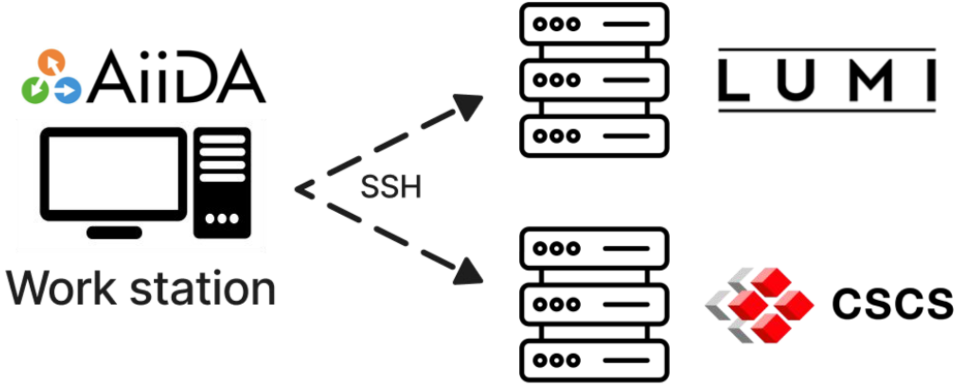
AiiDA Automated Interactive Infrastructure and Database for Computational Science

Open-source Python infrastructure to **automate, manage, share and reproduce** complex computational workflows & data

- ✓ Support for HPC
- ✓ Scalable workflows
- ✓ Multiple material science codes
- ✓ Full data provenance

=> FAIR Data MATERIALS CLOUD

Built-in support for HPC



Support for common schedulers

- Slurm
- PBS/Torque
- SGE
- ...

What if connection fails?

- Try again for 5 times with EBM
- Pause process

But won't that lead to too many connections?

- Tasks that require SSH are grouped
- "safe interval" is configurable

Advantages

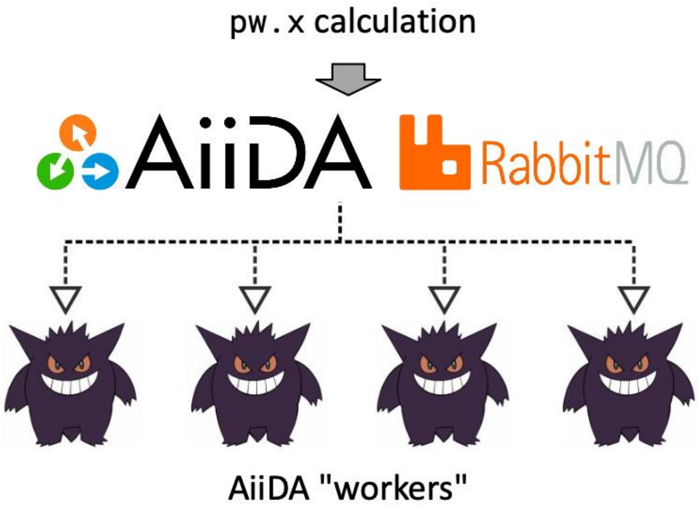
- Easy to understand and set up
- Nothing installed on cluster
- Easy to run on multiple systems

Disadvantages

- You have to set it up yourself
- Multi-factor authentication

Courtesy M Bercx, 2024

Scalable workflow engine

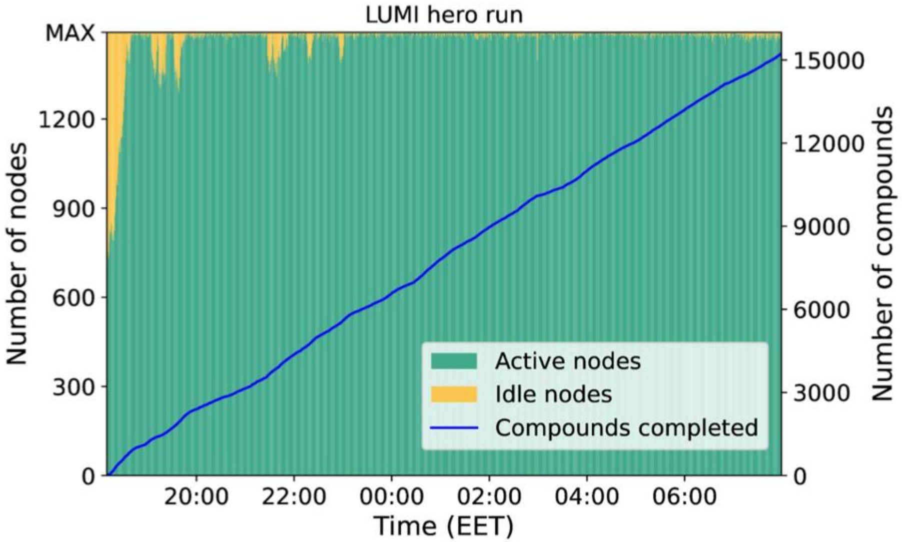


AiiDA workers take care of everything

1. Upload inputs
2. Submit to scheduler
3. Monitor queue
4. Retrieve outputs
5. Parse to nodes

LUMI

- Ran 55704 Quantum ESPRESSO calculations in 12 hours
- Handled 7887 errors on the fly
- Fully optimized 15324 geometries



However

- You need the RabbitMQ service
- Workers run in their own Python instance

Courtesy M Bercx, 2024

PAUL SCHERRER INSTITUT PSI

Flexible plugin system

AiiDA PLUGIN REGISTRY

[View on GitHub/register your package]

Registered plugin packages: 92

Calculations	139 plugins in 56 packages
Parsers	117 plugins in 57 packages
Data	105 plugins in 32 packages
Workflows	160 plugins in 42 packages
Console scripts	26 plugins in 15 packages
Other	100 plugins in 27 packages

https://aiidateam.github.io/aiida-registry/

Support for many materials science codes

QUANTUM ESPRESSO, Yambo, VASP, CP2K, WIEN2k, NWCHEM, WANNIER90, Fleur (www.flapw.de), EPW, Abinit

...

Courtesy M Bercx, 2024

PAUL SCHERRER INSTITUT PSI

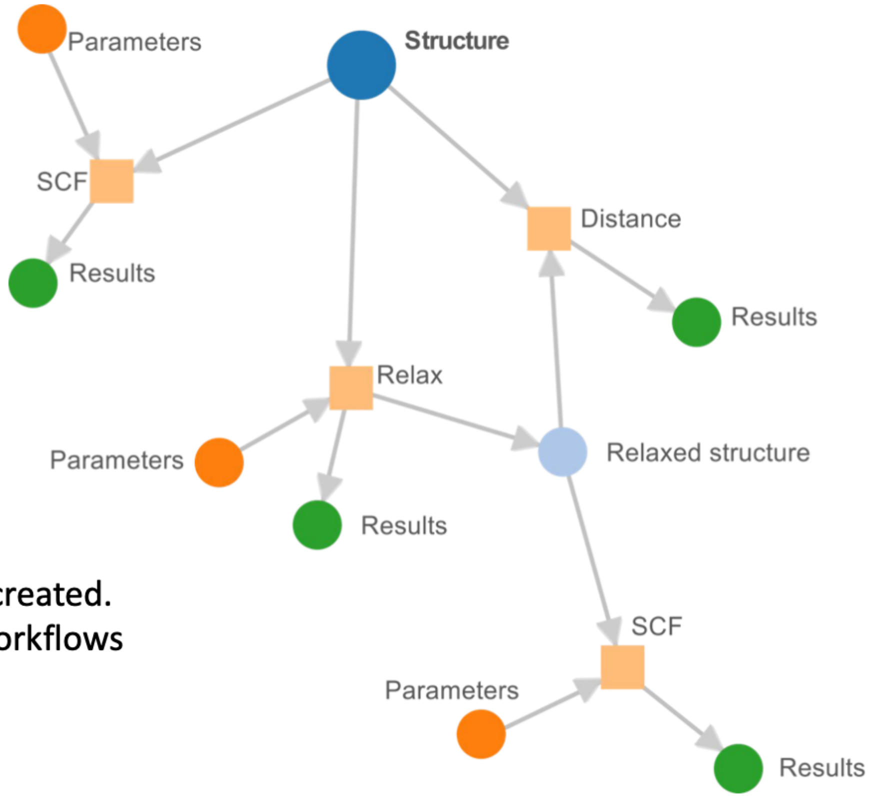
Data Provenance

Simple recipe

- Store data transformations or **"calculations"**.
- Store its **inputs** and **outputs**.
- Most crucially: store the inter-connections or **"links"**.

Provenance graphs

- When data is reused, a directed acyclic graph is created.
- Quickly grows in complexity even for "simple" workflows



Courtesy M Bercx, 2024

Sharing data

PAUL SCHERRER INSTITUT

Default records

Engineering frustrated lewis pair active sites in porous organic scaffolds for catalytic CO_2 hydrogenation

DOI 10.24435/materialscloud:31-wz

AiiDA-generated records

A Standard Solid State Pseudopotentials (SSSP) library optimized for precision and efficiency

DOI 4435/materialscloud:f3-ym

CalcJobNode

JOB ID 2570313

SCHEDULER STATE DONE

REMOTE WORKING DIRECTORY /scratch/snx3000/marrazzo/aiida_run/14/42/ba1a-88bc-494d-8d97-cfa5c295ca66

INPUT FILES
- aiida.in
- _aiidasubmit.sh
- .aiida/calcinfo.json
- .aiida/job_tmpl.json

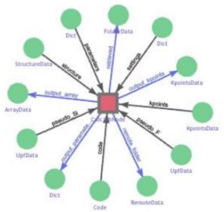
OUTPUT FILES
- aiida.out
- _scheduler-stderr.txt
- _scheduler-stdout.txt
- data-file.xml

Node metadata

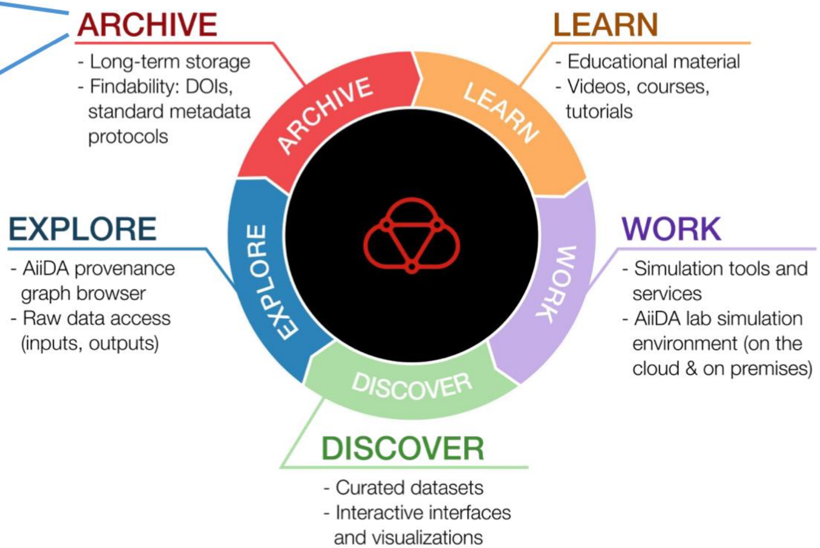
CUSTOM_SCHEDULER_COMMANDS #SBATCH --constraint=gpu #SBATCH --account=pr09

AiiDA Provenance Browser

Click on node to browse, drag to animate



MATERIALSCLOUD



GO FAIR

- **Findable**
- **Accessible**
- **Interoperable**
- **Reusable**

Courtesy M Bercx, 2024

Thank you!