Transport properties Wannier90/WanT + ABINIT

Tonatiuh Rangel Gordillo, Andrea Ferretti
and Gian-Marco Rignanese

Institute of Condensed Matter and Nanosciences (IMCN)
Université Catholique de Louvain, Belgium
European Theoretical Spectroscopy Facility

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Outline

- Wannier Functions basis
- Wannier functions in ABINIT
- Quantum Transport
- Wannier90 and WanT interfaces with ABINIT

Wannier Functions

Single band

$$|\omega_{\mathbf{R}}\rangle = \frac{V}{(2\pi)^3}\int_{BZ} d\mathbf{k}\, e^{-i\mathbf{k}\cdot\mathbf{R}} e^{i\phi_{\mathbf{k}}} |\psi_{\mathbf{k}}\rangle$$

G. H. Wannier, Phys Rev. 52, 191 (1937)

Wannier Functions

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Multiple bands

$$|\omega_{\mathbf{R},m}\rangle = \frac{V}{(2\pi)^3}\int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_n U^{\mathbf{k}}_{nm} |\psi_{\mathbf{k},n}\rangle$$

Properties

- Orthogonal
- Exactly span the starting Bloch subspace
- Strongly non-unique

G. H. Wannier, Phys Rev. 52, 191 (1937)

Maximally Localized Wannier Functions (MLWFs)

$$|\omega_{\mathbf{R},m}\rangle = \frac{V}{(2\pi)^3}\int_{BZ} d\mathbf{k}\, e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_n U^{\mathbf{k}}_{nm} |\psi_{\mathbf{k},n}\rangle$$

Exploit freedom of choice of $U^{\mathbf{k}}_{nm}$

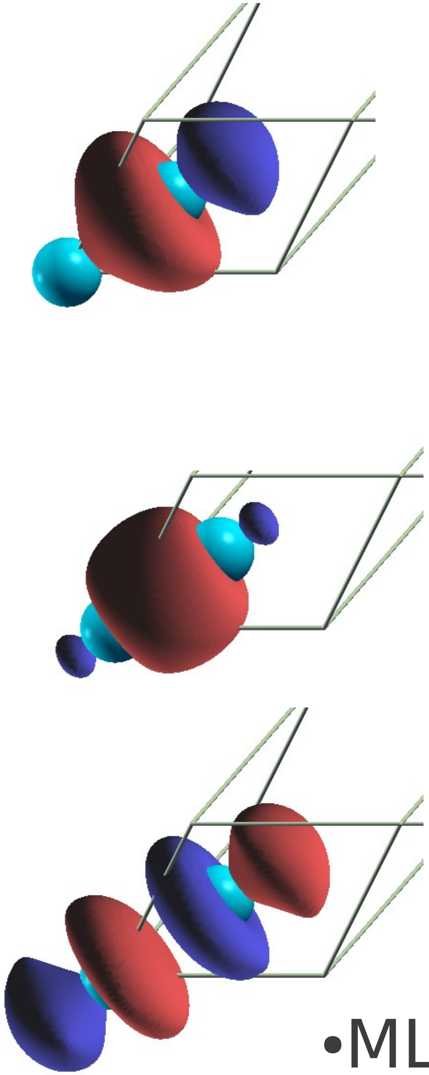
to minimize the spread

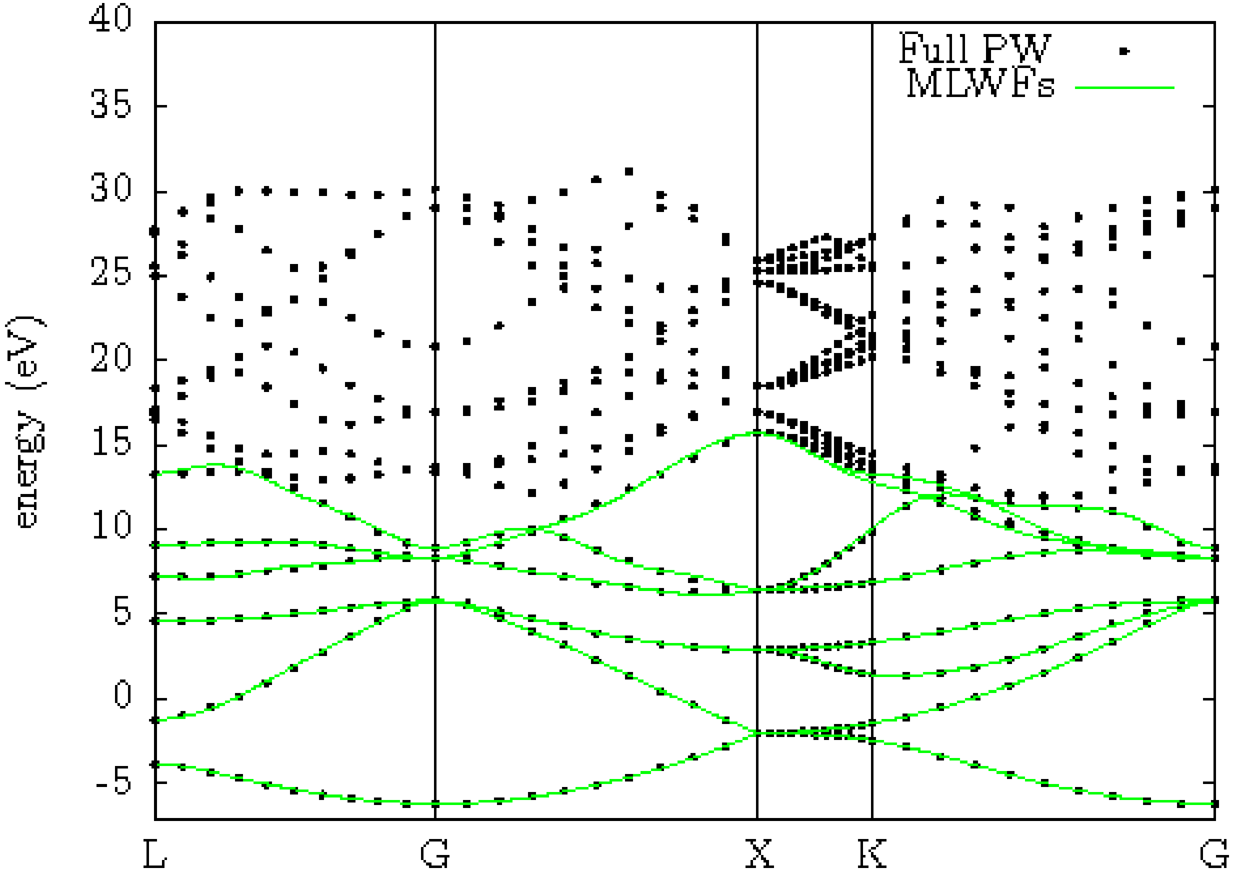
$$\Omega[U] = \sum_n \left[\langle \hat{r}^2 \rangle_n - \langle \hat{\mathbf{r}} \rangle_n^2 \right]$$

- MLWF's equivalent of the localized molecular orbitals.
- MLWFs provide a minimal basis set.

N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)

Example: MLWFs in silicon





- MLWF's atomic or chemical orbitals.
- MLWFs span the same space as initial Bloch functions.

MLWFs with Wannier90+ABINIT

Simply use: prtwant 2 or 3

Actual status
- PAW, NC
- *GW approaches*

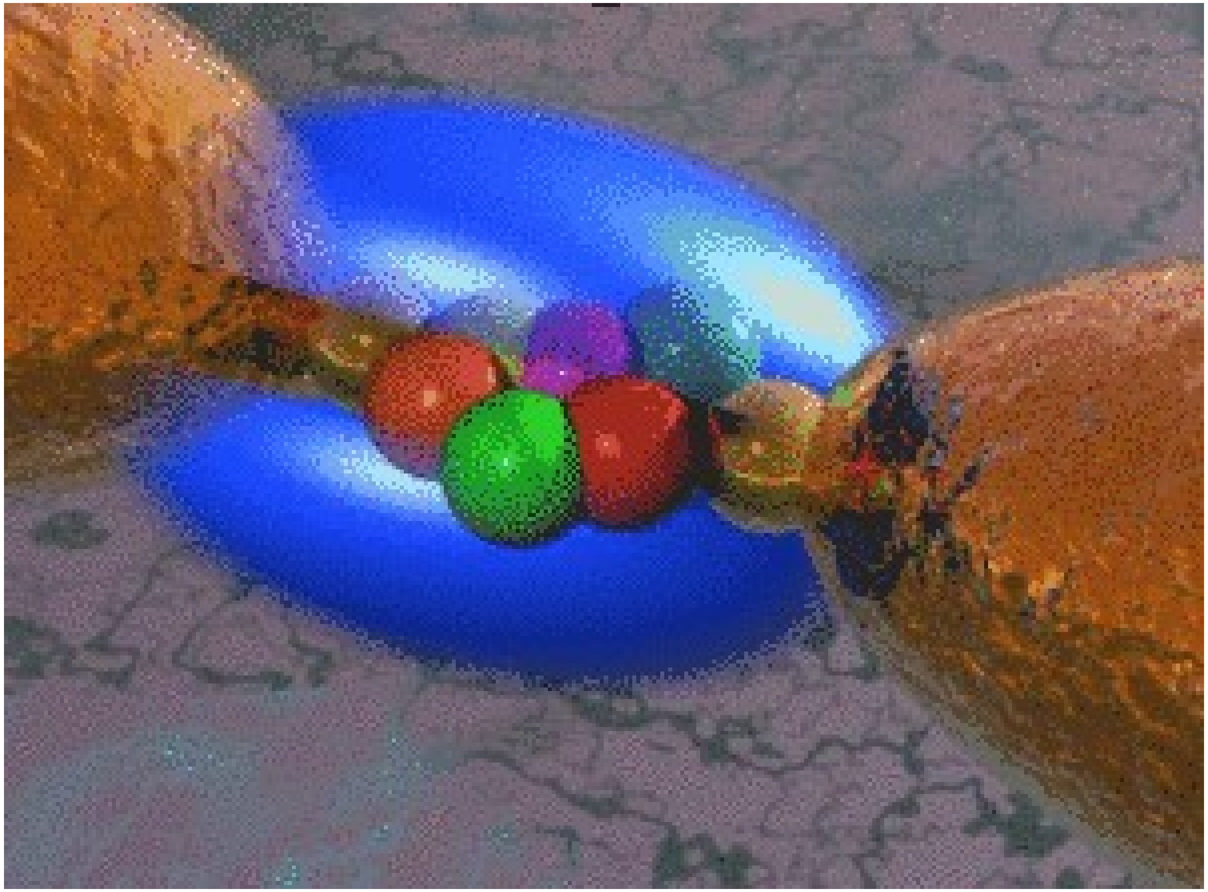
Tutorial + tests included

Testing
- Spin polarization, spinors

Post-processing:
- Van-der Waals forces (Camilo Espejo).
- De Haas-van Alphen (Simon Blackburn).
- DMFT (Bernard Amadon).

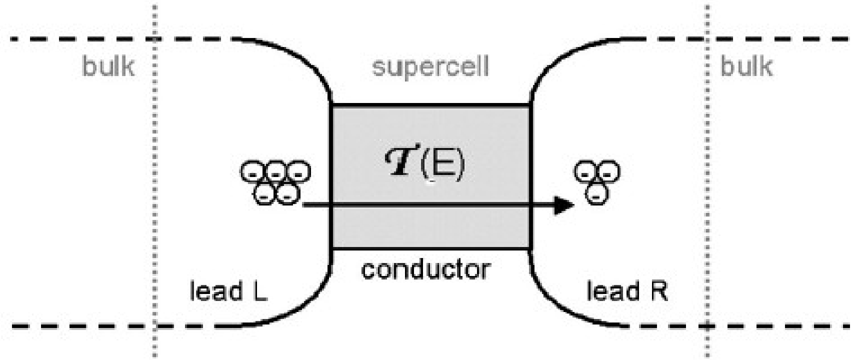
http://dieffi.deviantart.com/art/The-forces-Van-Der-Waals-128358132

Quantum transport



http://www.eng.yale.edu/reedlab/

Landauer Approach



A. Calzolari PRB 69, 035108 (2004)

- Conductance:

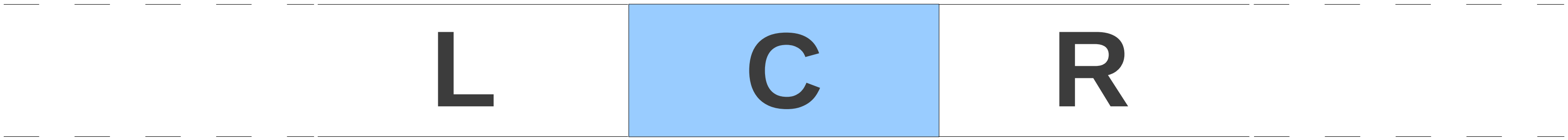
$$C(E) = \frac{2e^2}{h} T(E)$$

Hypotheses:

- Non-interacting system
- Local equilibrium in the leads
- Stationary problem

S. Datta “Electronic transport in mesoscopic systems”, 1995

Landauer Approach



- Green's functions of the system: $G=(\omega-H)^{-1}$

$$G_C(\omega)=(\omega-H_C-\Sigma_L(\omega)-\Sigma_R(\omega))$$

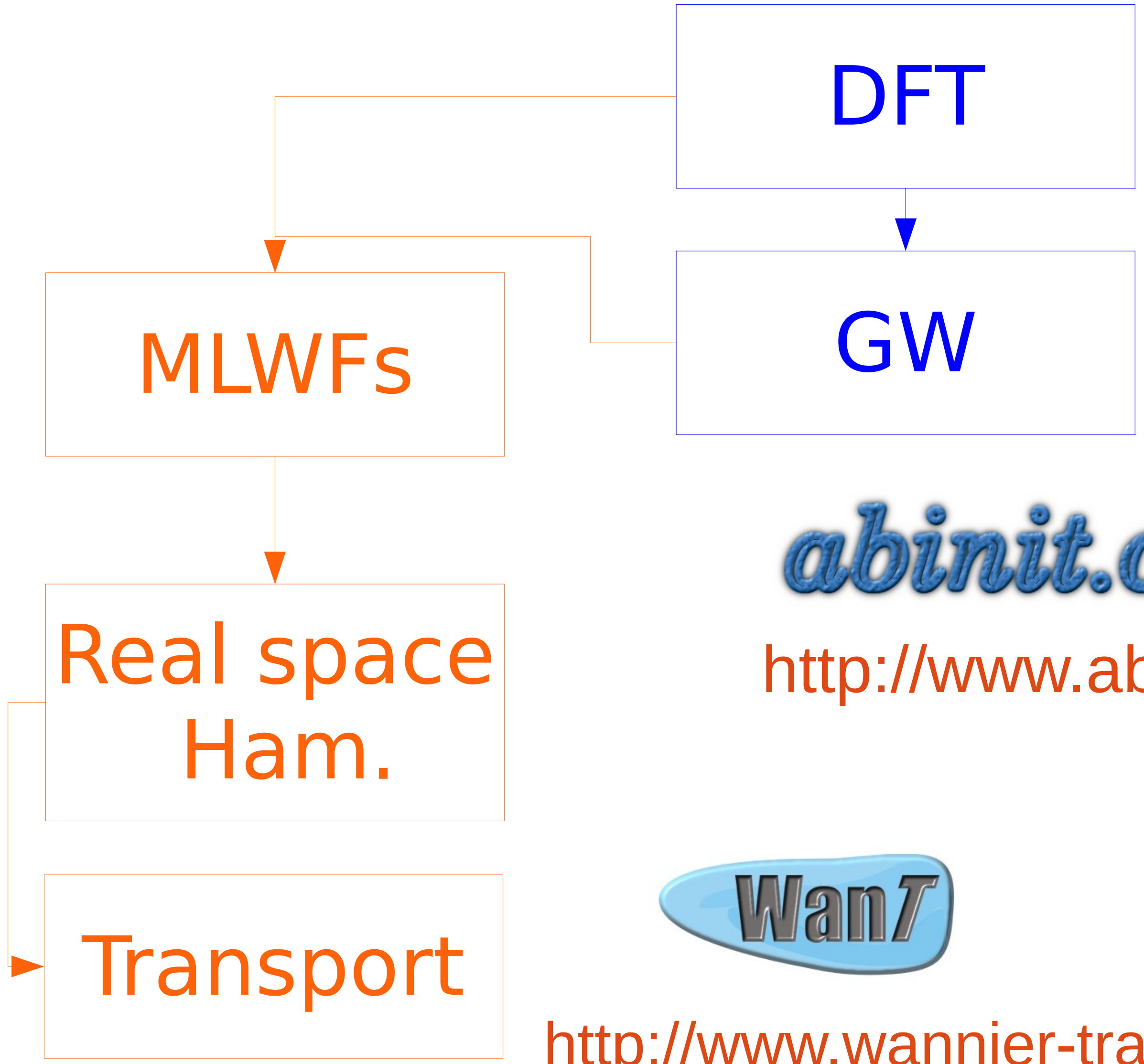
- All from:

$$H=\begin{pmatrix} H_{LL} & H_{LC} & 0 \\ H_{CL} & H_{CC} & 0 \\ 0 & H_{RC} & H_{RR} \end{pmatrix}$$

- Fisher and Lee:

$$T(\omega)=Tr[\Gamma_L G_C^r \Gamma_R G_C^a]$$

Flow diagram



http://www.abinit.org

http://www.wannier-transport.org

http://www.wannier.org

Transport with ABINIT+Wannier90

Wannier Functions:

Wannier90 call as library inside ABINIT.
Just use prtwant 2/3

Transport:

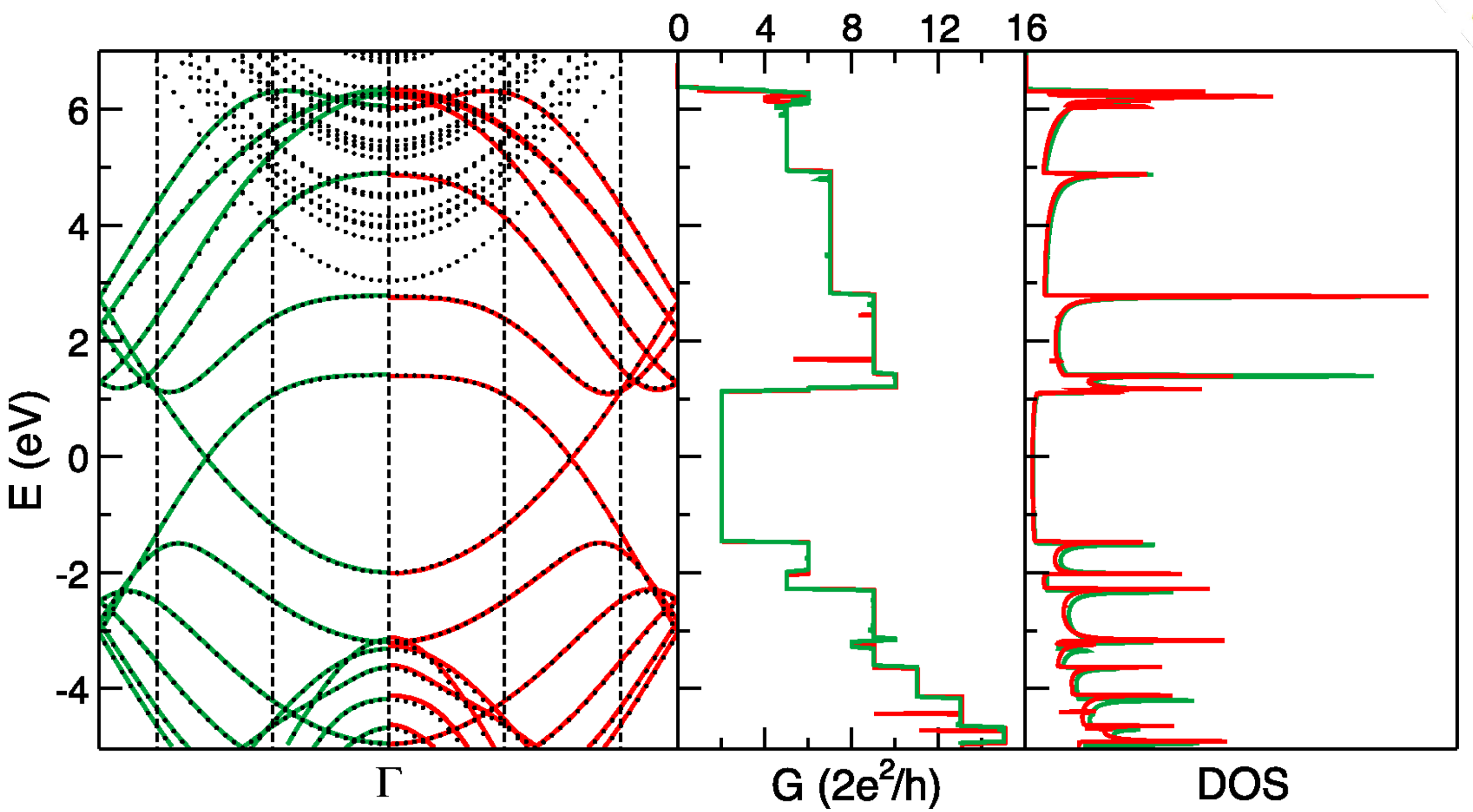
Post-processing tool of Wannier90
(See Wannier90 manual)

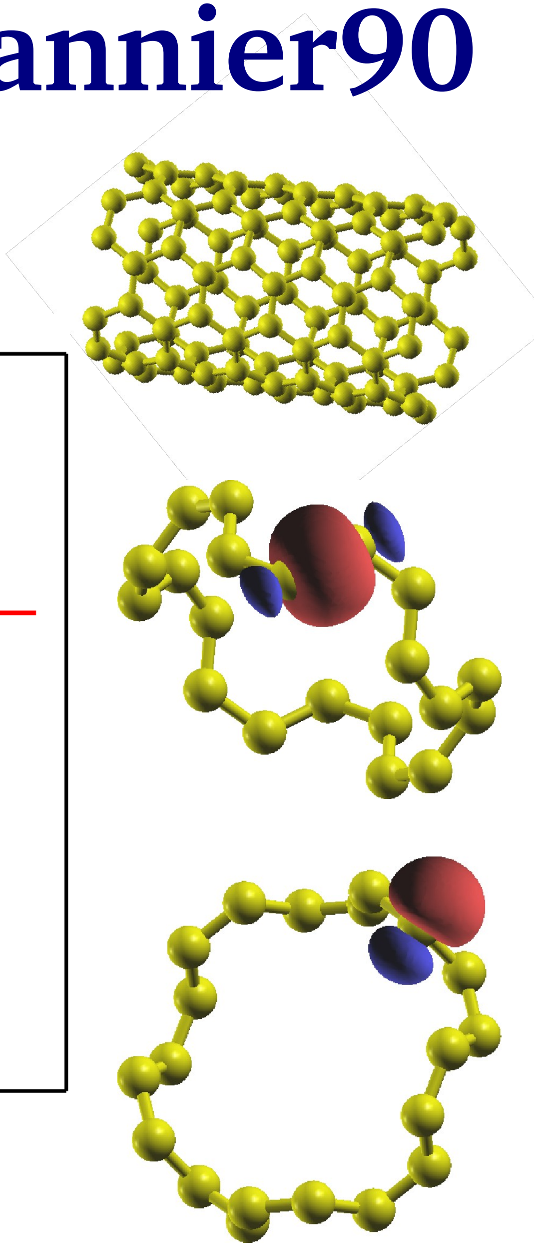
Restrictions:

Only 1D systems

Transport with ABINIT+Wannier90

Carbon nanotube (5 ,5)





Red: ABINIT + Wannier90

Green: Y-S Lee, M. B. Nardelli and N. Marzari. PRL 95, 076804 (2005)

Transport with WanT

Wannier Functions:
Interface with WanT through the ETSF format

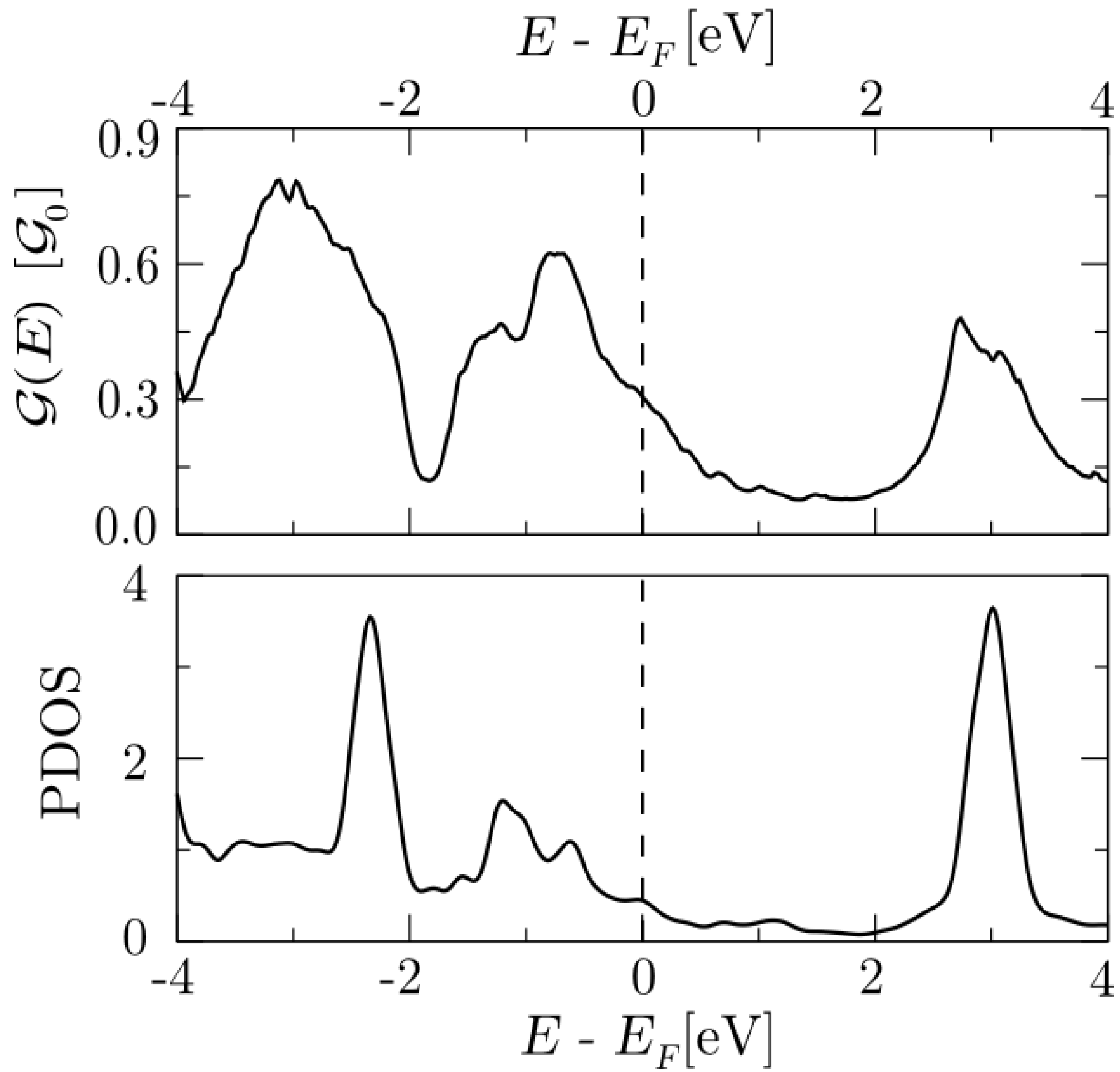
Transport:
1D-3D systems
Examples in the WanT test suite.

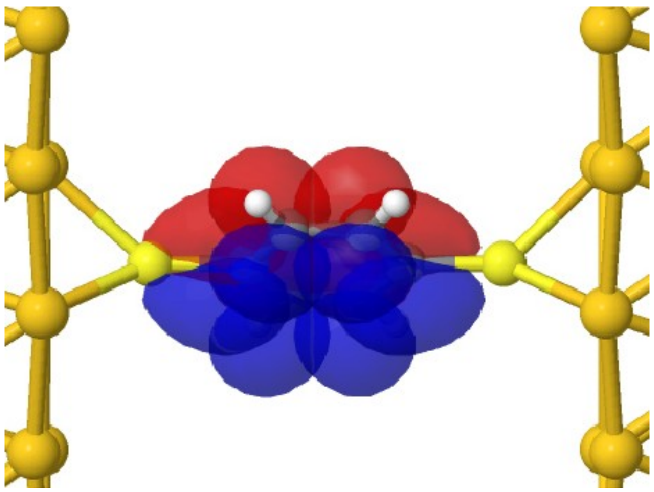
Restrictions:
1) ETSF format in ABINIT is not parallelized.
Solution: Use wfk2etsf.x distributed with WanT
2) Only for NC and DFT.
Solution: Wannier90-WanT interface.
Wannier functions with Wannier90 +Transport with WanT.

Future:
WanT as a pluging in ABINIT?

Transport with WanT

Benzene-dithiol attached to gold leads





Summary

Landauer transport can be calculated with:

ABINIT+Wannier90
1D systems
NC and PAW
GW

ABINIT+WanT
1D-3D systems
NC

ABINIT+Wannier90+WanT
For 3D systems (*GW* or DFT)
Wannier90-WanT interface.

Summary

Landauer transport can be calculated with:

1D-3D systems
NC and PAW
GW

Soon:
Spin transport

GW transport see: arXiv:1102.1880v1

ACknowledge

Thanks for your attention

Questions?