# Spin-polarized transmission through correlated heterostructures

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# Goals, References

- Study correlation effects on transport properties of heterostructures
- ... by combining density functional and many-body dynamical mean field theory
- ... within the non-equilibrium Green's function approach
- ... as implemented, e.g., within the SMEAGOL package

  "Spin and Molecular Electronics on Atomically Generated Orbital Landscape"


— L. Chioncel et al., Transmission through correlated Cu-Co-Cu heterostructures, Phys. Rev. B 92, 054431 (2015)

— C. Morari et al., Spin-polarized ballistic conduction through correlated Au-NiMnSb-Au heterostructures, Phys. Rev. B 96, 205137 (2017)

— W. H. Appelt, PhD thesis, April 2016
A. Prinz-Zwick, PhD thesis, December 2017
A. Weh, MSc thesis, January 2018

# Outline

## Basic concepts

- Scattering / NEGF approach to transport
- Towards a more realistic description
- Electronic correlations: DMFT

## Test case

- Cu-Co-Cu heterostructure

## The half-Heusler compound NiMnSb

- Correlations in a model half-metal
- Correlations in bulk NiMnSb
- Transport through Au-NiMnSb-Au

# Scattering / NEGF approach to transport

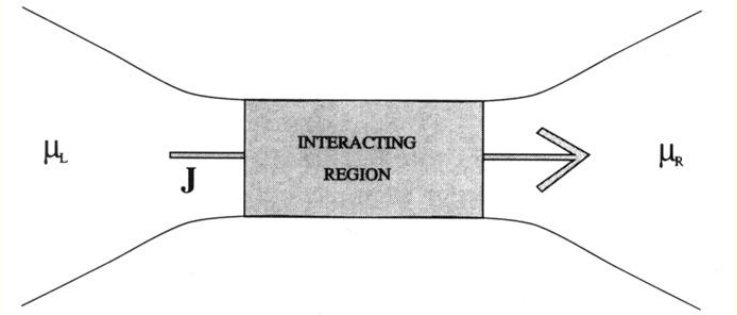



FIG. 1. Schematic diagram of the experimental configuration for which an *interacting* Landauer formula for the current is derived. Two leads, characterized by chemical potentials $\mu_L$ and $\mu_R$, are connected to a mesoscopic region where electrons may interact. If $\mu_L > \mu_R$, an electron current $J$ will flow from left to right.

- developed by Landauer & Büttiker, Meir & Wingreen, ...
- initial conditions $\rightarrow$ stationary currents
- $t \rightarrow -\infty$: $\Delta V \neq 0$, $\Delta T \neq 0$
- lead – "molecule" – lead: non-interacting leads, simple coupling
- express currents $I_n$, $I_\epsilon$ through the leads' (equ.) distribution functions and local properties of the "molecules"

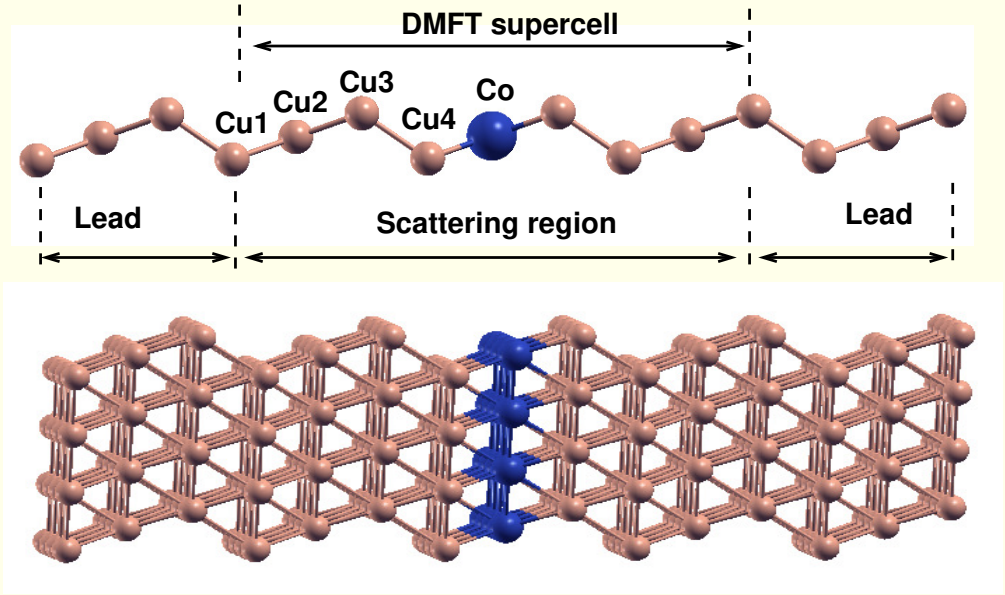
# Scattering / NEGF approach to transport

- consider total currents
- coupling: $\sim (V_{LC} c_L^+ d_C + \text{h.c.})$, $\sim (V_{RC} c_R^+ d_C + \text{h.c.})$
  L = left, C = center, R = right
- first step: $I_n \sim \text{tr}\left(V_{LC} G^<_{LC}\right) \sim \text{tr}\left(V_{CR} G^<_{CR}\right)$
- general result:
  $I_n = \frac{i}{2h} \int d\epsilon \, \text{tr}\left([f_L \Gamma^L - f_R \Gamma^R](G^R - G^A) + [\Gamma^L - \Gamma^R] G^<\right)$

- special case: non-interacting *or* $\Gamma^L = \Gamma^R$; then:
  $I_n = \frac{1}{h} \int d\epsilon \, [f_L(\epsilon) - f_R(\epsilon)] \mathcal{T}(\epsilon, ...)$
- $\mathcal{T}(\epsilon, ...)$ = transmission probability = function of energy, ...
- energy current: $I_\epsilon = \frac{1}{h} \int d\epsilon \, \epsilon \, [f_L(\epsilon) - f_R(\epsilon)] \mathcal{T}(\epsilon, ...)$
- including correlations via $G^R$, $G^A$

# Towards a more realistic description

- combining DFT (GGA) studies (SMEAGOL) with DMFT
- model system / test case: Cu(111) | Co | Cu(111)
- include correlations within the Co plane
- determine spin-resolved transmission




L. Chioncel et al., 2015

# Electronic correlations: DMFT

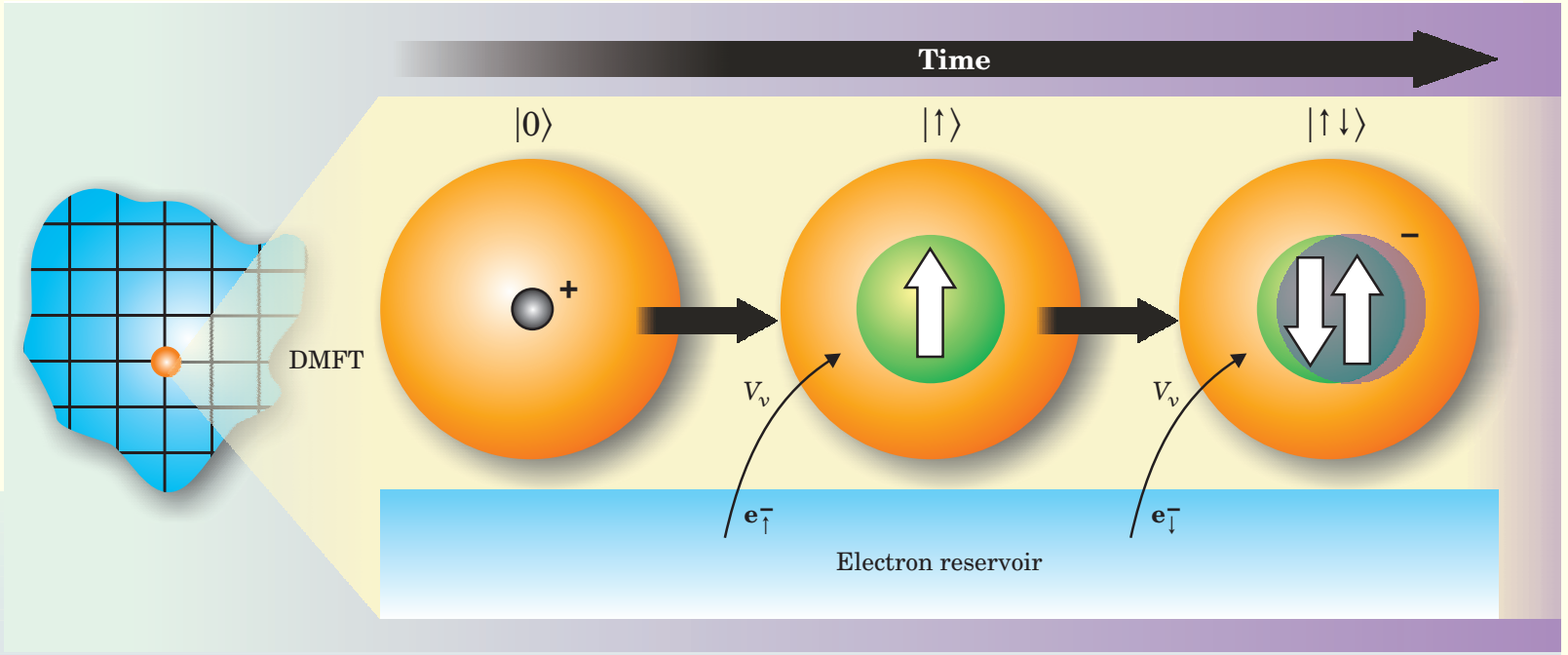
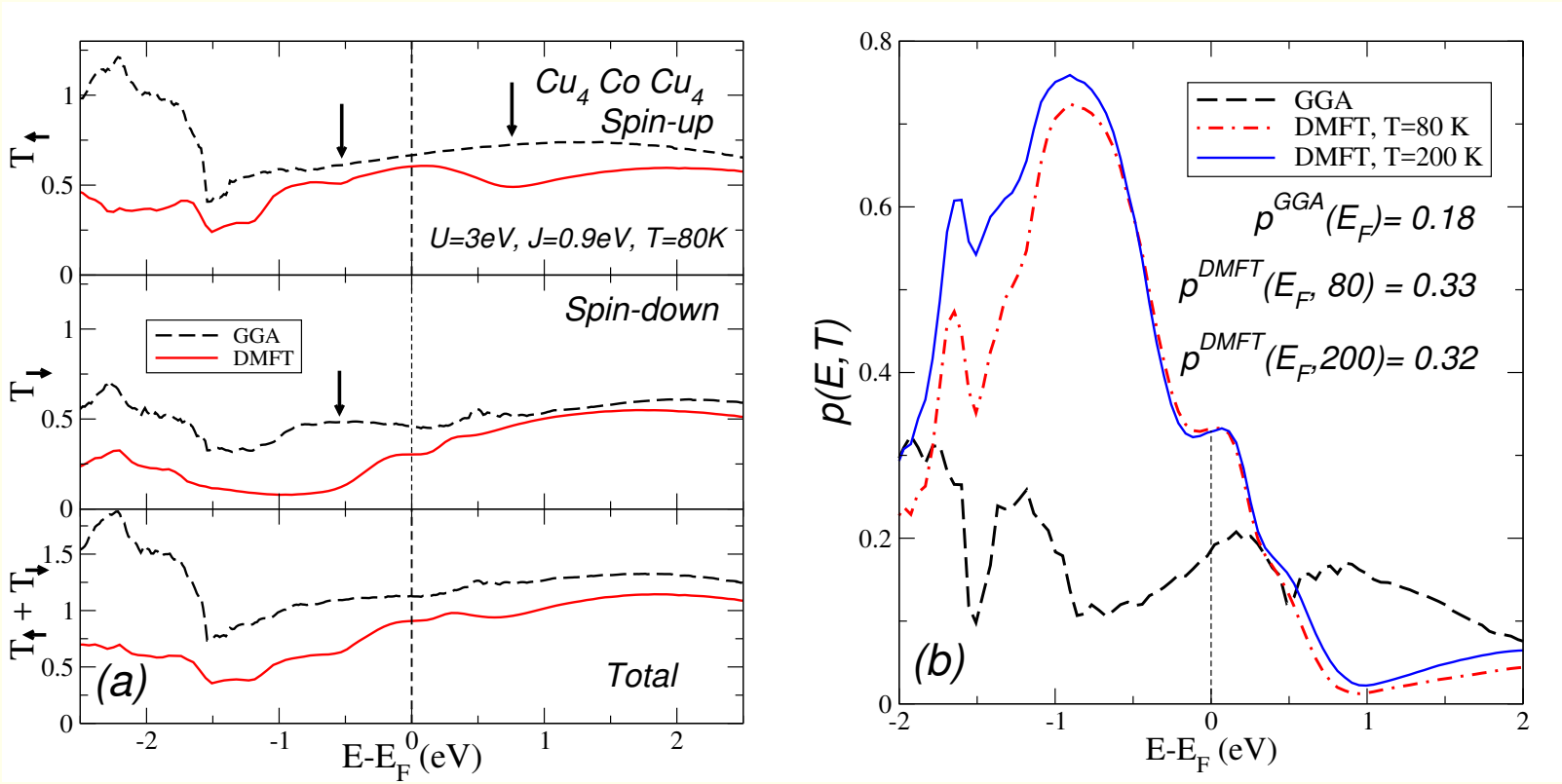



**Figure 1. Dynamical mean-field theory** (DMFT) of correlated-electron solids replaces the full lattice of atoms and electrons with a single impurity atom imagined to exist in a bath of electrons. The approximation captures the dynamics of electrons on a central atom (in orange) as it fluctuates among different atomic configurations, shown here as snapshots in time. In the simplest case of an *s* orbital occupying an atom, fluctuations could vary among $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, or $|\uparrow\downarrow\rangle$, which refer to an unoccupied state, a state with a single electron of spin-up, one with spin-down, and a doubly occupied state with opposite spins. In this illustration of one possible sequence involving two transitions, an atom in an empty state absorbs an electron from the surrounding reservoir in each transition. The hybridization $V_v$ is the quantum mechanical amplitude that specifies how likely a state flips between two different configurations.

G. Kotliar & D. Vollhardt, Physics Today 57(3), 53 (2004)

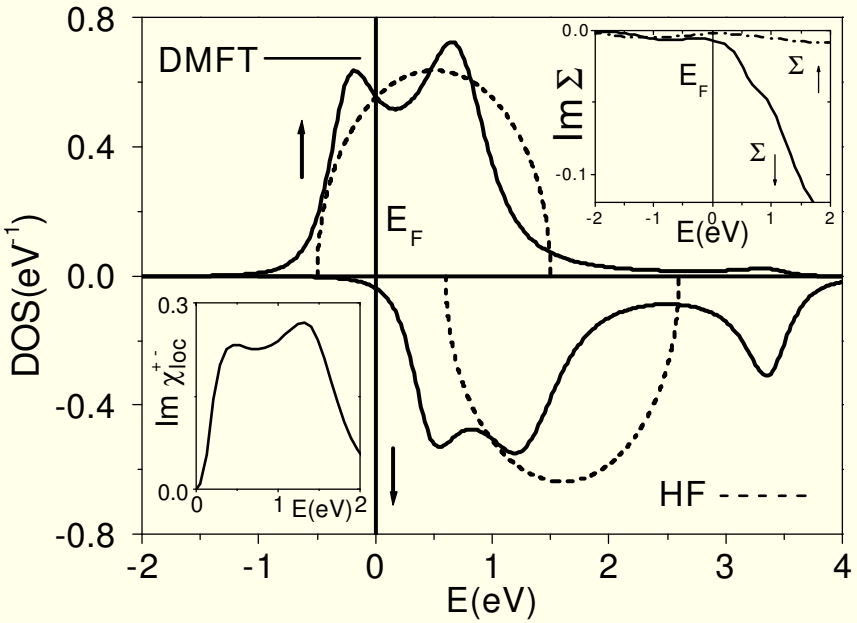
# Cu-Co-Cu heterostructure




Left: Spin-resolved transmission: majority spins (upper panel), minority spins (middle panel), and total (lower panel). Black dashed/red solid lines: GGA/GGA+DMFT results. Right: Transmission spin polarization obtained within the GGA (black dashed) and at $T = 80$ K (red dot dashed), $T = 200$ K (blue solid). Coulomb and exchange parameters: $U = 3$ eV, $J = 0.9$ eV. — Further results: transmission vs. $U$ and $J$ at fixed $T$

L. Chioncel et al., 2015

# Correlations in a model half-metal




Bethe lattice $\rightarrow$ semi-circular DOS

$$H = -t \sum_{<ij>} \sum_{\sigma} \left( c_{i\sigma} c^{\dagger}_{j\sigma} + c_{j\sigma} c^{\dagger}_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$U = 2$ eV, $W = 2$ eV
$\Delta = 0.5$ eV, $T = 0.25$ eV

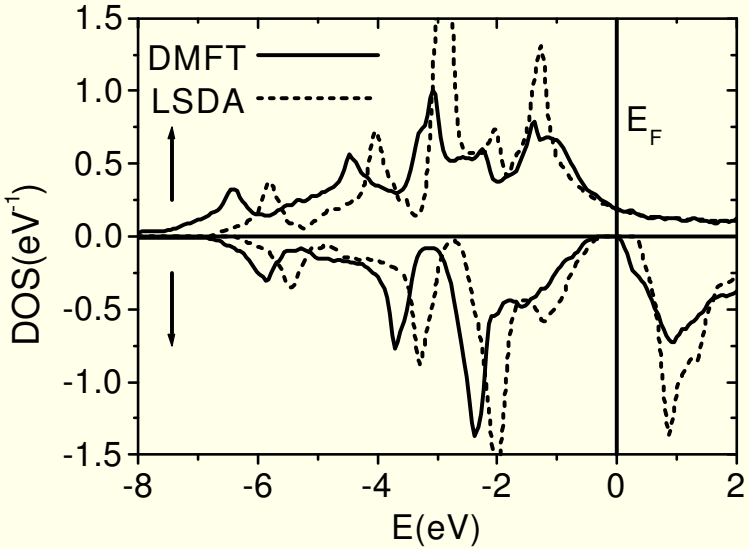
- DMFT self-consistency:

$$S^{\mathrm{eff}} = -\int_0^{\beta} d\tau \int_0^{\beta} d\tau' c^{\dagger}_{\sigma}(\tau) \mathcal{G}^{-1}_{\sigma}(\tau - \tau') c_{\sigma}(\tau') + U \int_0^{\beta} d\tau n_{\uparrow}(\tau) n_{\downarrow}(\tau)$$

$$S^{\mathrm{eff}} \rightarrow \mathrm{QMC} \rightarrow G_{\sigma} \rightarrow \mathcal{G}_{\sigma} = i\omega + \mu - t^2 G_{\sigma} - \frac{1}{2}\sigma\Delta$$

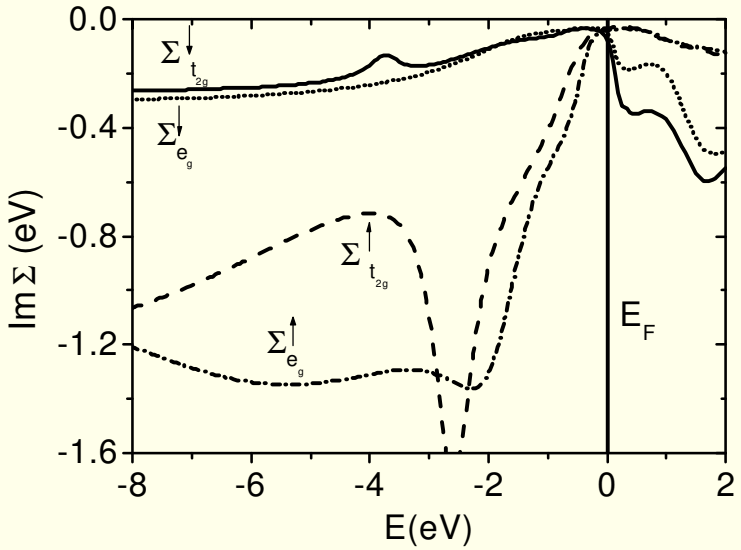
L. Chioncel et al., Phys. Rev. B 68, 144425 (2003)

NiMnSb: prototypical half-metal, almost fully polarized; transport?




LDA+DMFT self-consistency:
$U = 3$ eV, $J = 0.9$ eV (on Mn)
$T = 300$ K; $M = 3.96\ \mu_B$ !

$$\Sigma^{\sigma}(i\omega) = \sum_{\sigma'} W^{\sigma\sigma'} \cdot G^{\sigma'}$$



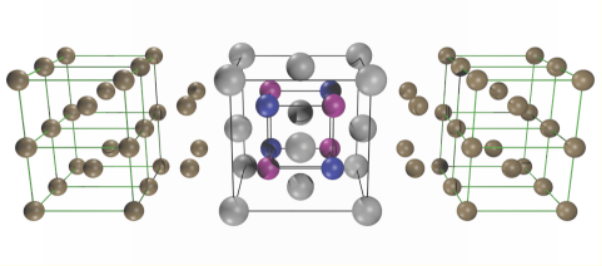

$\mathrm{Im}\,\Sigma_{\uparrow}(E) \sim (E - E_F)^2$
↑-electrons: Fermi liquid

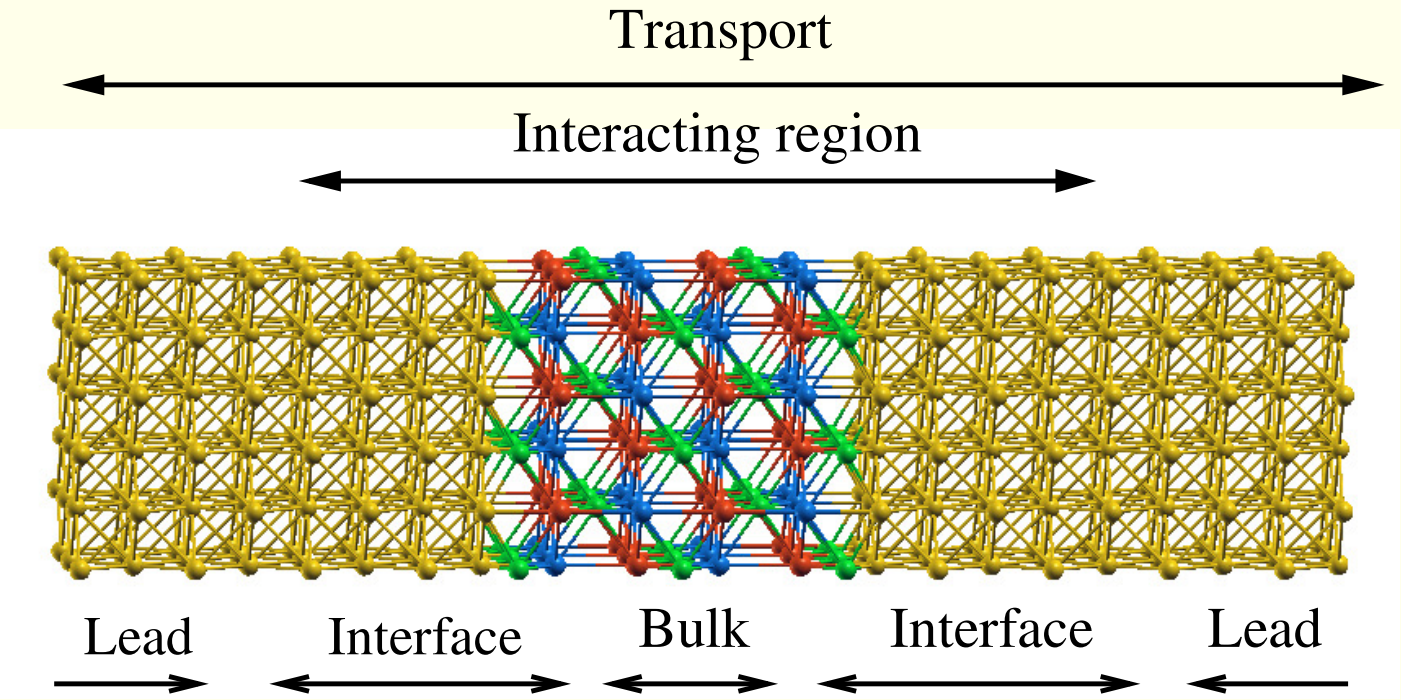
$\mathrm{Im}\,\Sigma_{\downarrow}(E) \sim (E - E_F)^x$ , x < 2

↓-electrons: Non-Quasi-Particle states

L. Chioncel et al., Phys. Rev. B 68, 144425 (2003)

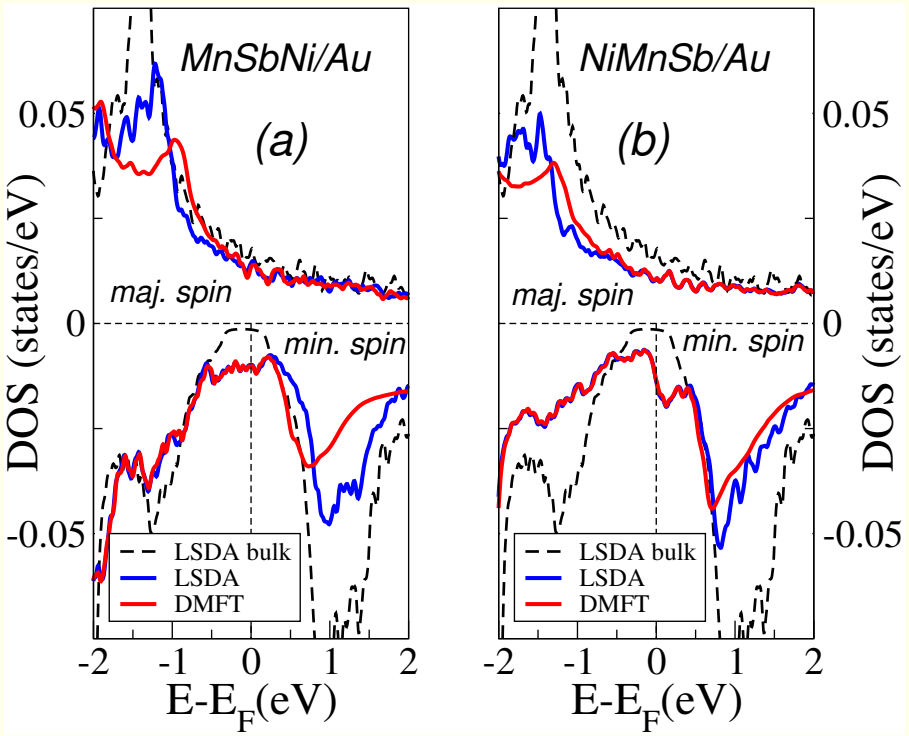
# Transport through Au-NiMnSb-Au






Favorable configuration: Ni terminated (001) interface

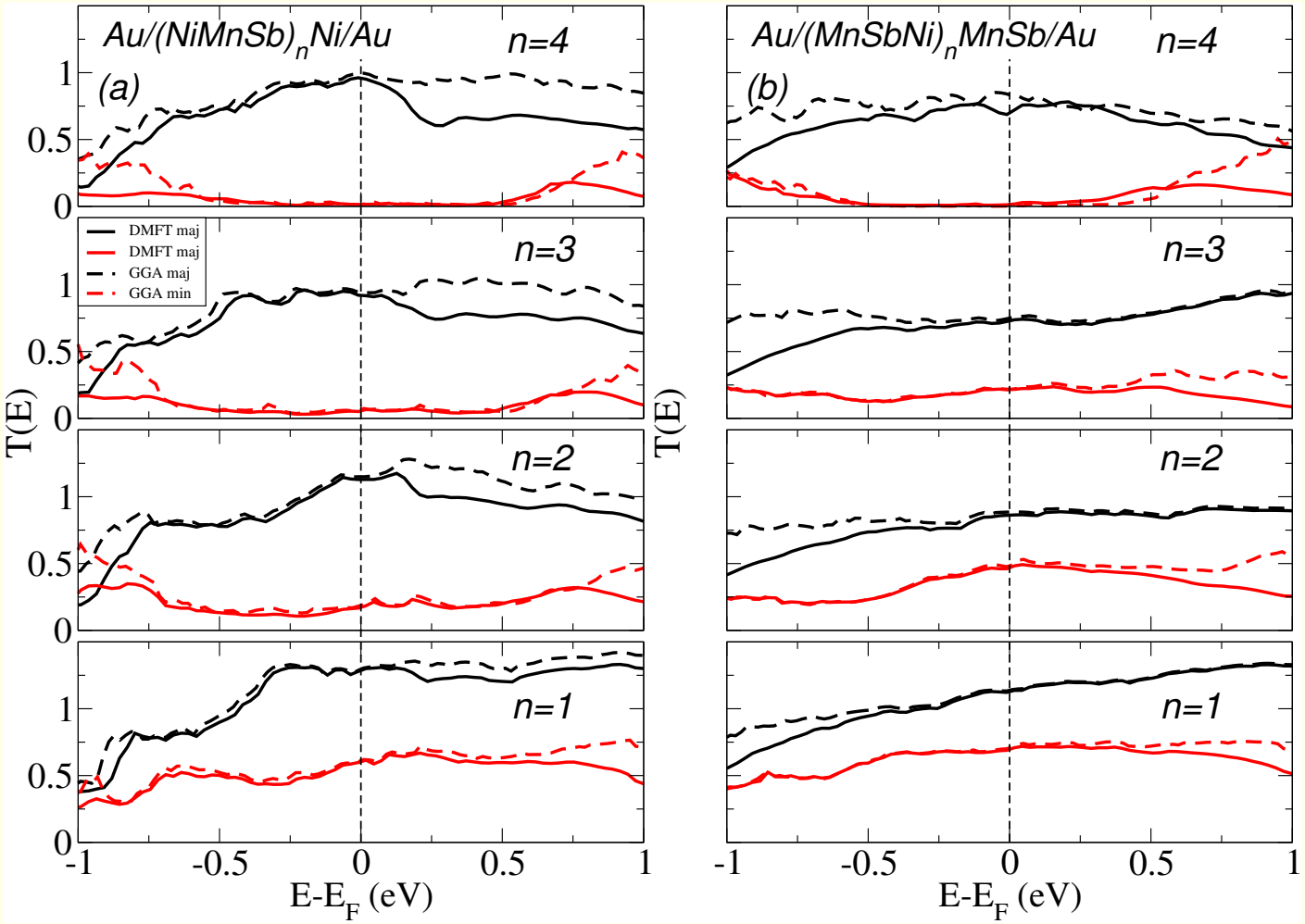
# States near interfaces: DOS




Total DOS for the Au-$(NiMnSb)_2$-Au slab. (a) Ni termination, (b) MnSb termination. Solid-blue line: LSDA; solid-red line: LSDA+DMFT ($U = 3$ eV, $J = 0.6$ eV)

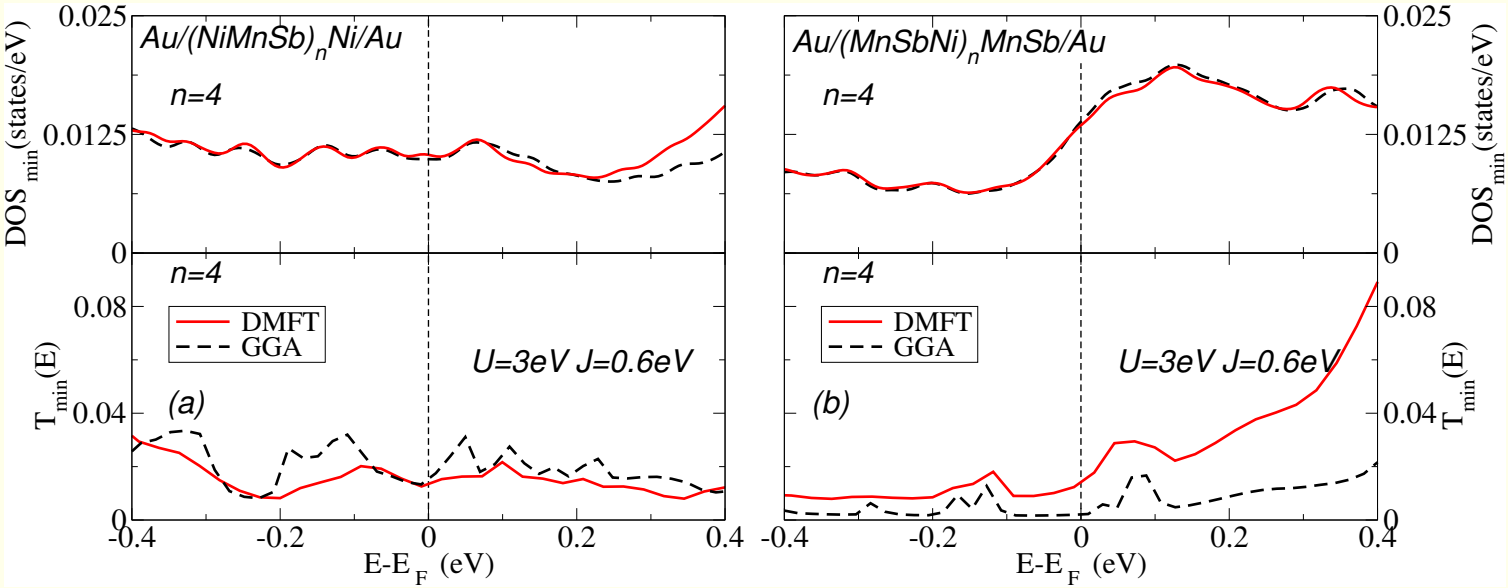
♣ DOS polarization not significant, due to strong hybridization of states near interfaces !

# Spin-polarized transmission




Spin-resolved transmissions. The dashed lines represent the GGA and the solid lines the GGA+DMFT results. Black lines: majority spin transmission; red lines: minority spin transmission. (a) Ni-termination, (b) MnSb-termination

# DOS versus transmission: minority spin




Comparison of the minority spin density of states (upper panel), and the minority spin transmission (lower panel): (a) Ni-terminated structure, (b) MnSb-terminated structure

♣ Significant spin polarization in transmission despite electronic correlations !



# Thank you for your attention !

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