

# Proof of Half-metallicity by Electron Spin Dynamics: application to $\text{Fe}_3\text{O}_4$

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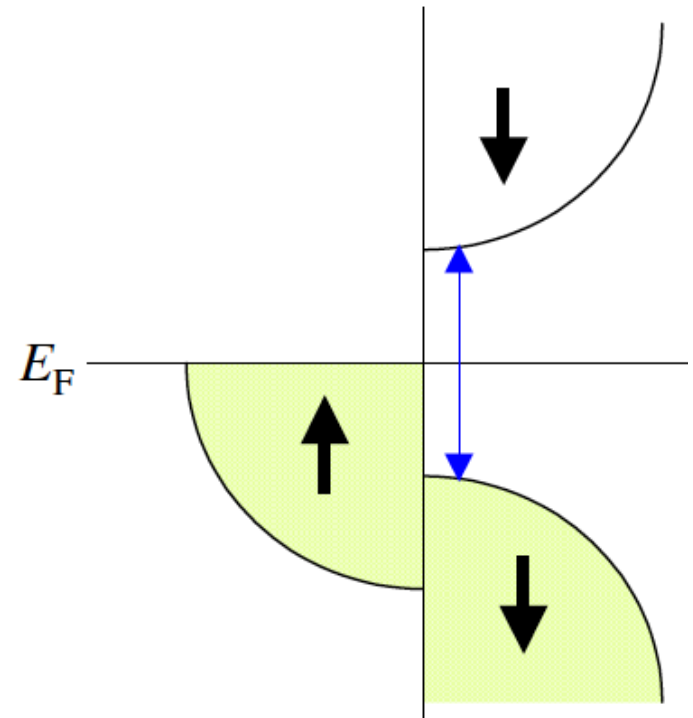
- **half-metals**
- **theoretical model**
- **spin- and time- resolved ARPES**
- **conclusions**

# half-metals

some alloys: metals as well as insulators at the same time,  
**depending on the spin direction**

# half-metals

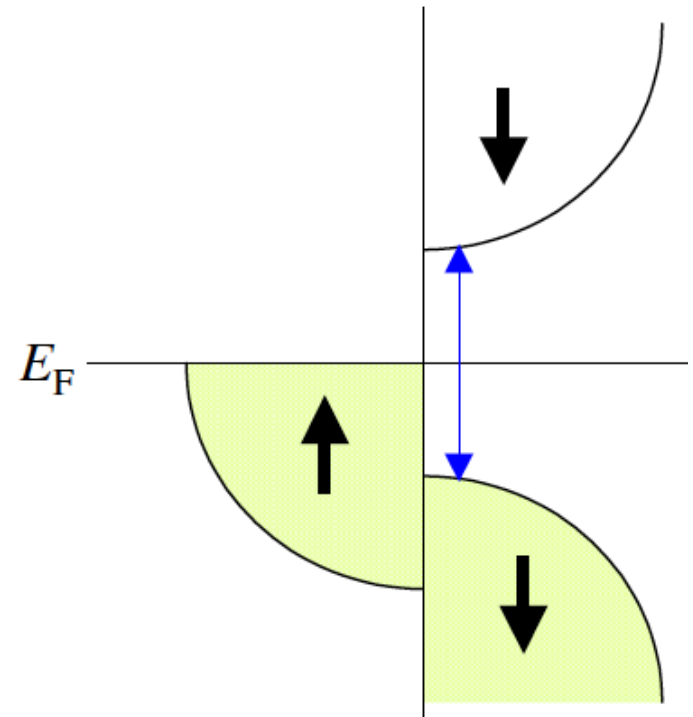
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# half-metals

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**depending on the spin direction**

100% spin polarization hypothetical at T=0 K



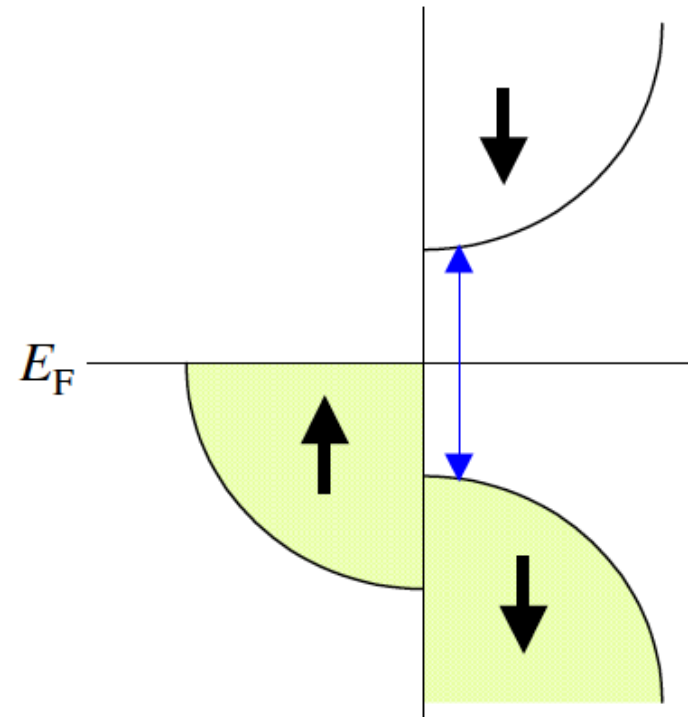
# half-metals

- Mn-based Heussler alloys (NiMnSb) **de Groot, PRL 50, 2024 (1983)**
- $\text{Fe}_3\text{O}_4$  **Yanase J. Phys. Soc. Jpn., 53, 312 (1984)**
- $\text{CrO}_2$  **Schwartz, J. Phys.F 16, L211 (1986)**
- manganites ( $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ ) **Pickett PRB 53, 1146 (1996)**

• transition metals with fully polarized d-like bands: hybridization with oxygen 2p, the 4s are shifted above the Fermi level

100% polarized material can be formed

**“half-metallic ferromagnet”**



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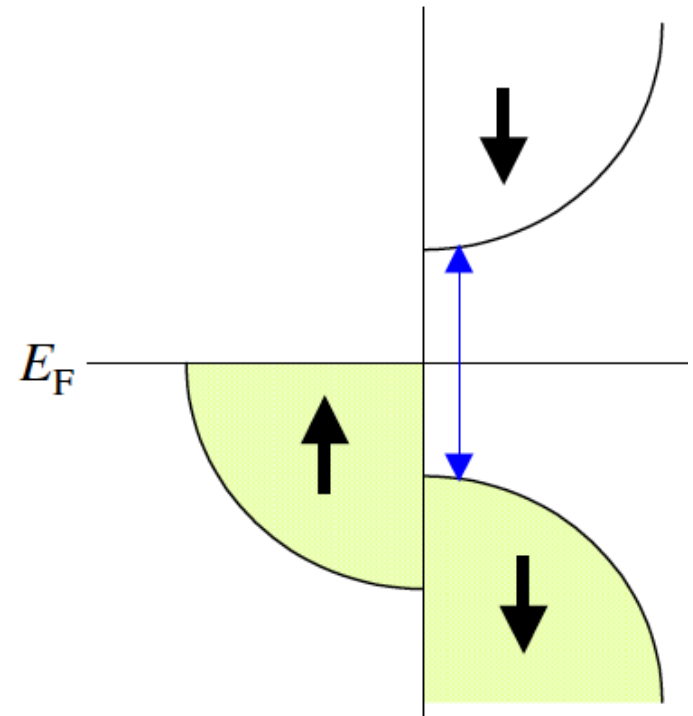
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**“half-metallic ferromagnet”**

- several physical interactions **spin, charge, lattice, and/or orbital** are simultaneously active (colossal magnetoresistance, high-temperature superconductors...)

- applications: **oxide-based electronics**



# determination of spin polarization

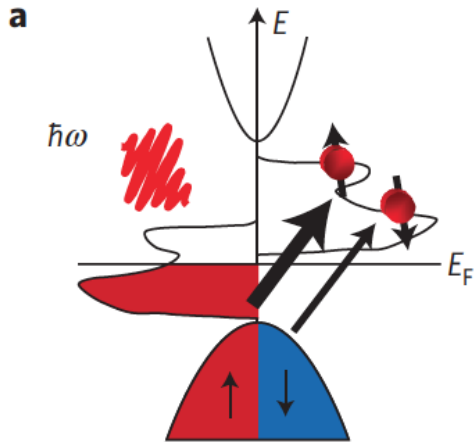
**NO “smoking gun” experiment to prove half metallicity**



# determination of spin polarization

NO “smoking gun” experiment to prove half metallicity

- density of states (photoemission) (a)

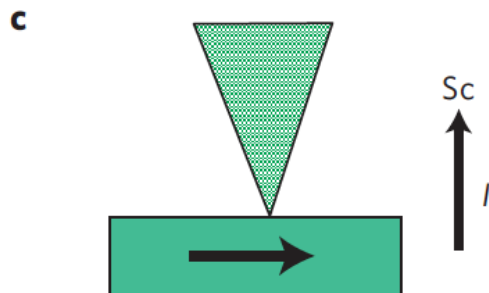
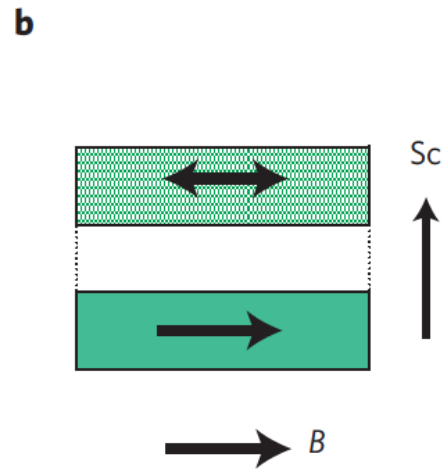
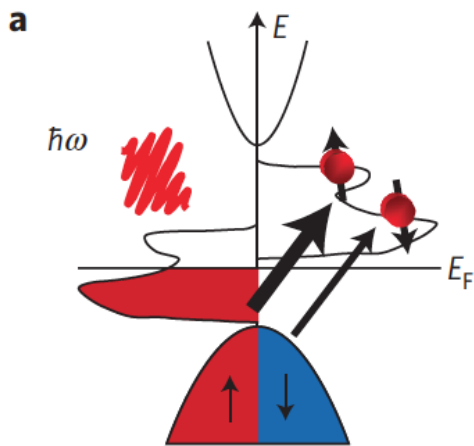


# determination of spin polarization

**NO “smoking gun” experiment to prove half metallicity**

- density of states (photoemission) (a)
- spin currents (spin-transport devices)

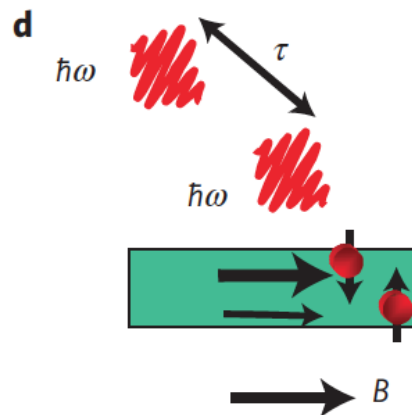
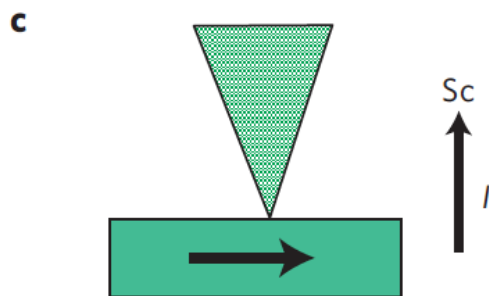
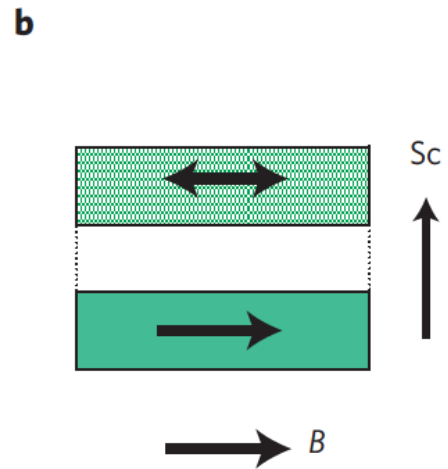
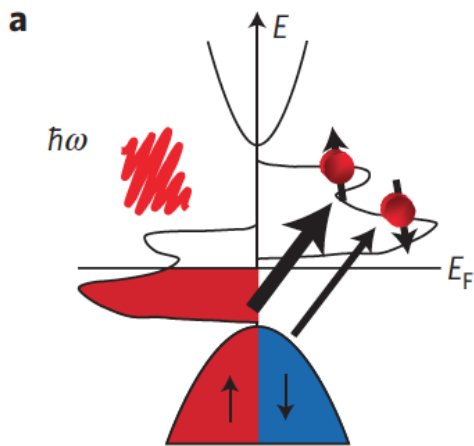
(b) Meservey-Tedrow  
(c) Andreev reflection



# determination of spin polarization

**NO “smoking gun” experiment to prove half metallicity**

- density of states (photoemission) (a)
  - spin currents (spin-transport devices) (b)
  - pump-probe (Kerr rotation) (c)
  - spin-resolved positron annihilation (d)
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# determination of spin polarization

**NO “smoking gun” experiment to prove half metallicity**

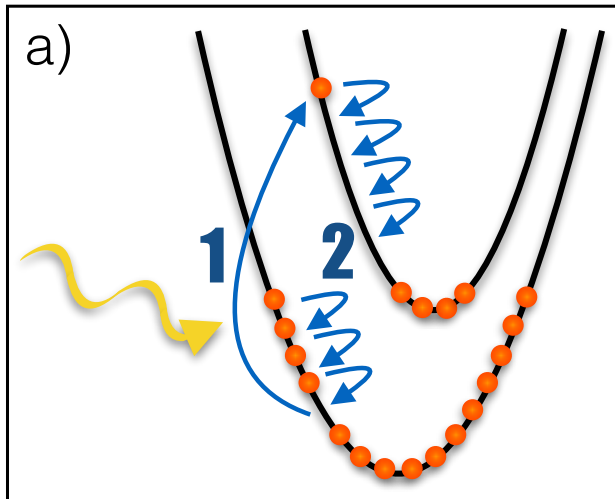
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- pump-probe (Kerr rotation) (d) (c) Andreev reflection
- spin-resolved positron annihilation

**we propose a new method (applied here to  $\text{Fe}_3\text{O}_4$ ) :**

recognising a very peculiar fingerprint of the HM's bulk band structure  
on the **sub-picosecond dynamics of spin polarisation**

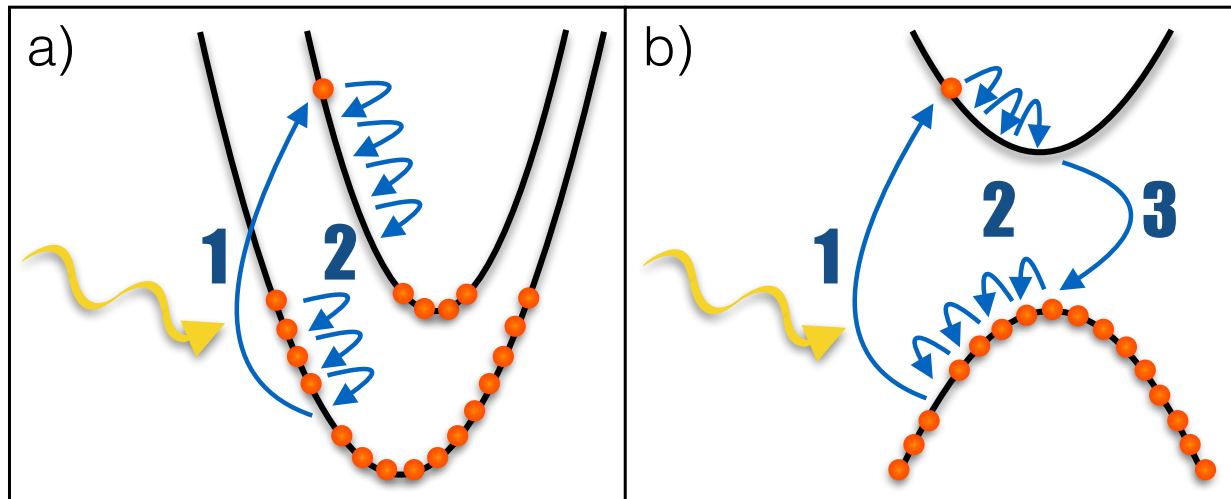
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# relaxation processes



metal

# relaxation processes

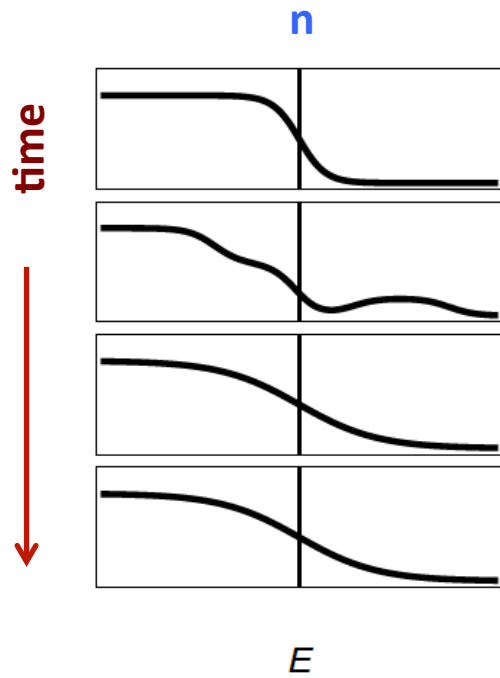


**metal**

**semiconductor**

# relaxation processes

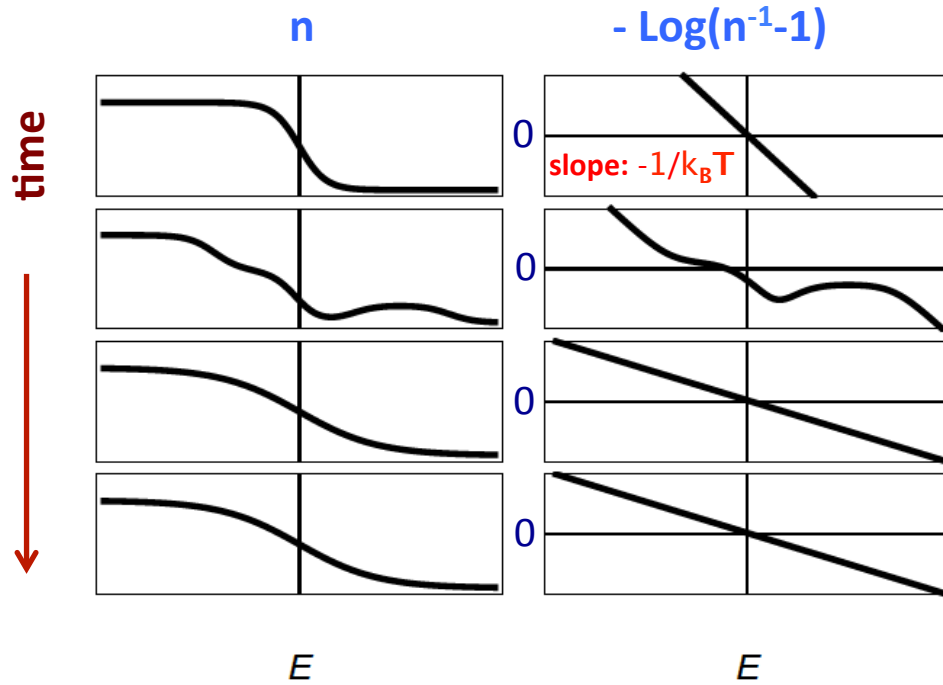
metal





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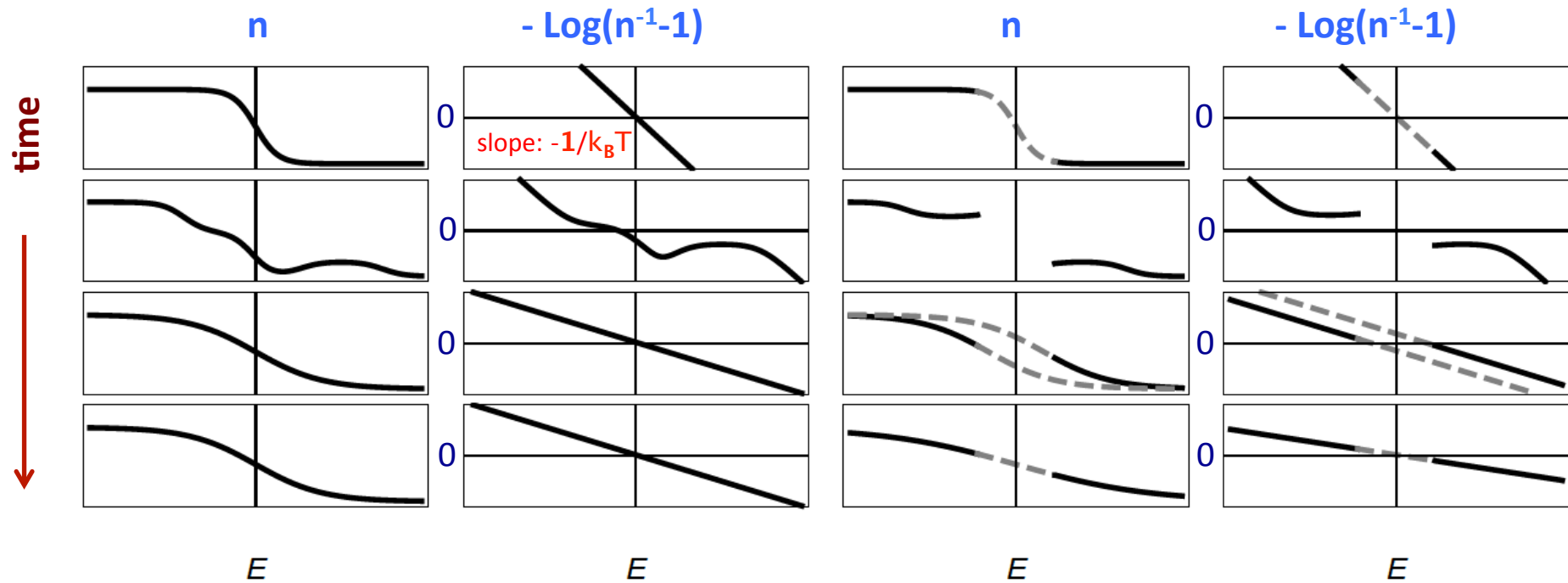
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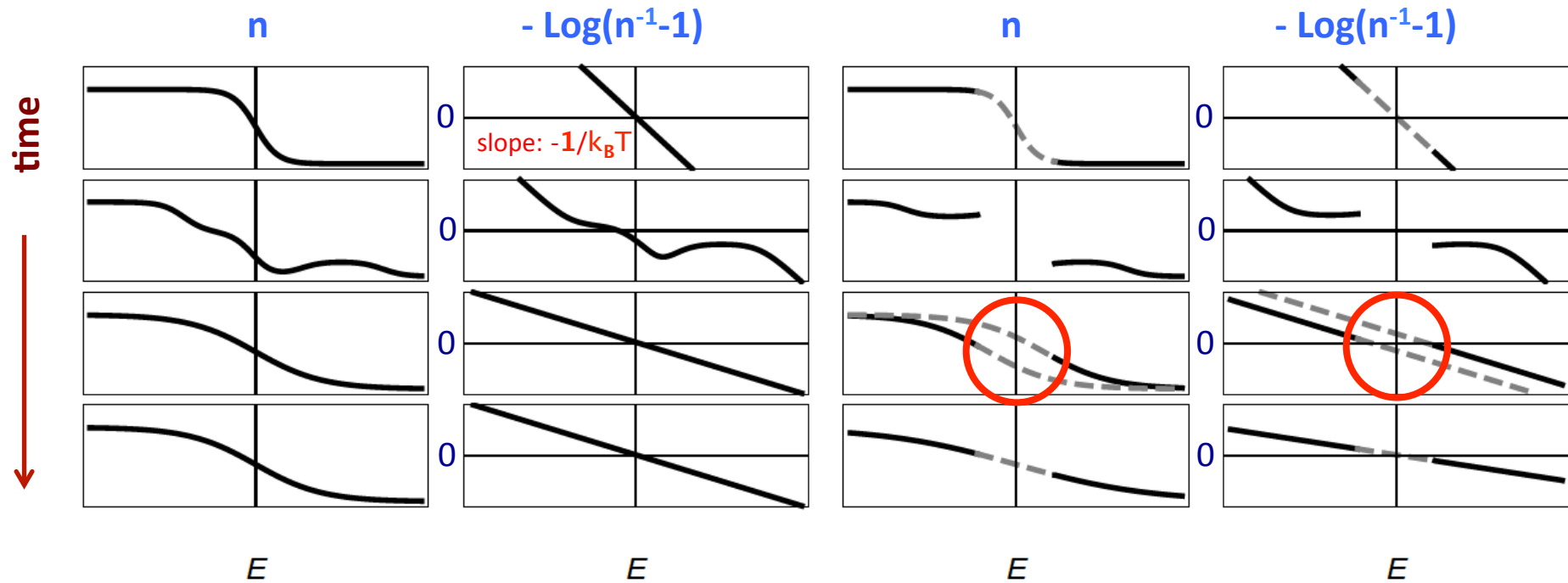
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# relaxation processes

metal

semiconductor



# electron dynamics calculations : $\text{Fe}_3\text{O}_4$

thermalization process:

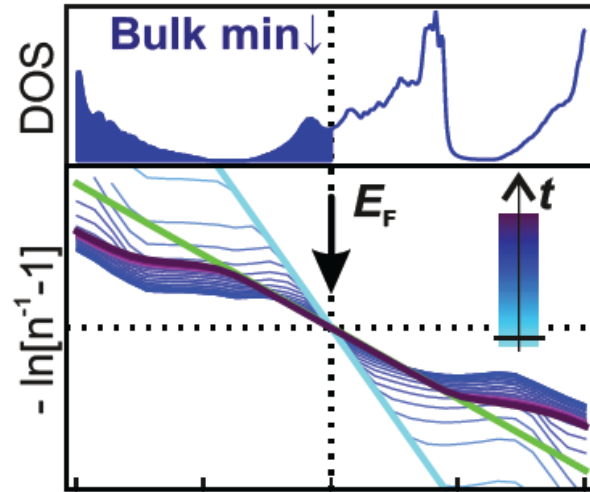
solving numerically the Boltzmann equation

for electron-electron scattering in a spin-dependent density of states

electrons with different spins can scatter with each other,  
total spin is preserved

spin-flip scatterings are ignored

# electron dynamics calculations : $\text{Fe}_3\text{O}_4$



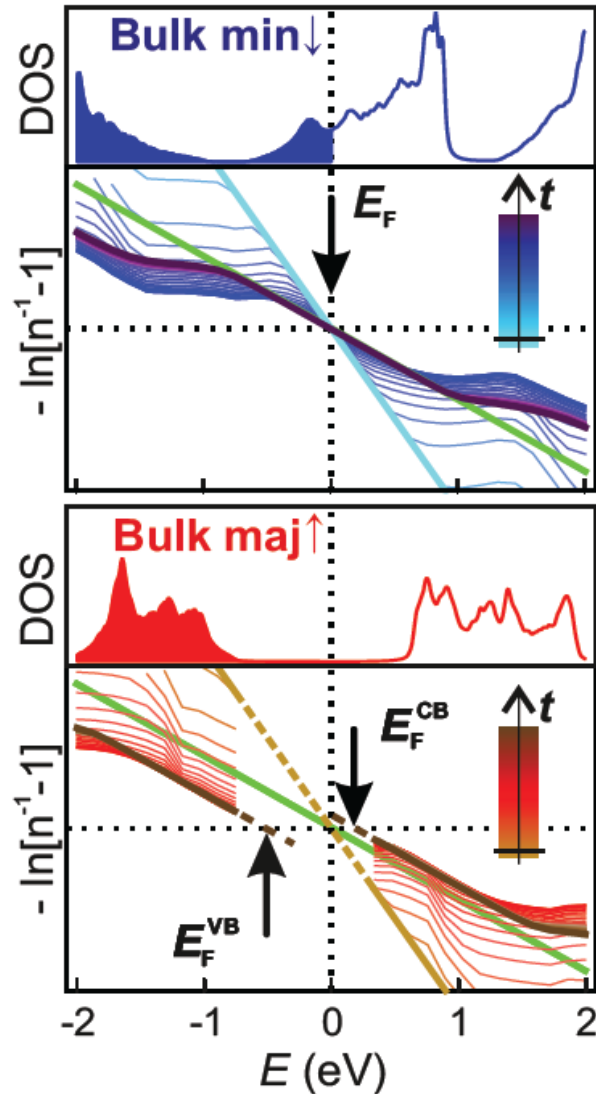
$\text{Fe}_3\text{O}_4$  spin-resolved DOS computed from first principles

SPR-KKR package

- Green's function formalism within the multiple scattering theory
- Dirac equation: all relativistic effects

H. Ebert, D Ködderitzsch, J Minar  
Rep. Prog. Phys. 74, 096501 (2011)

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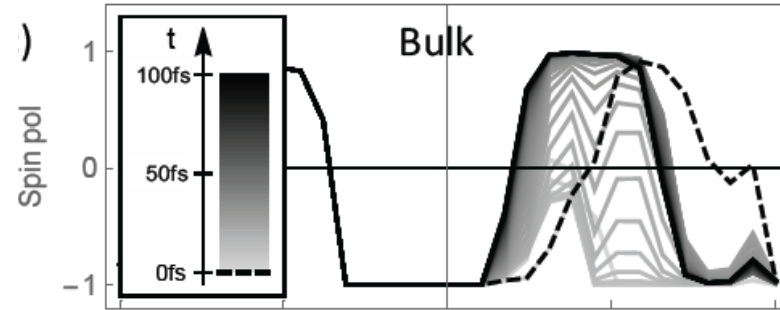
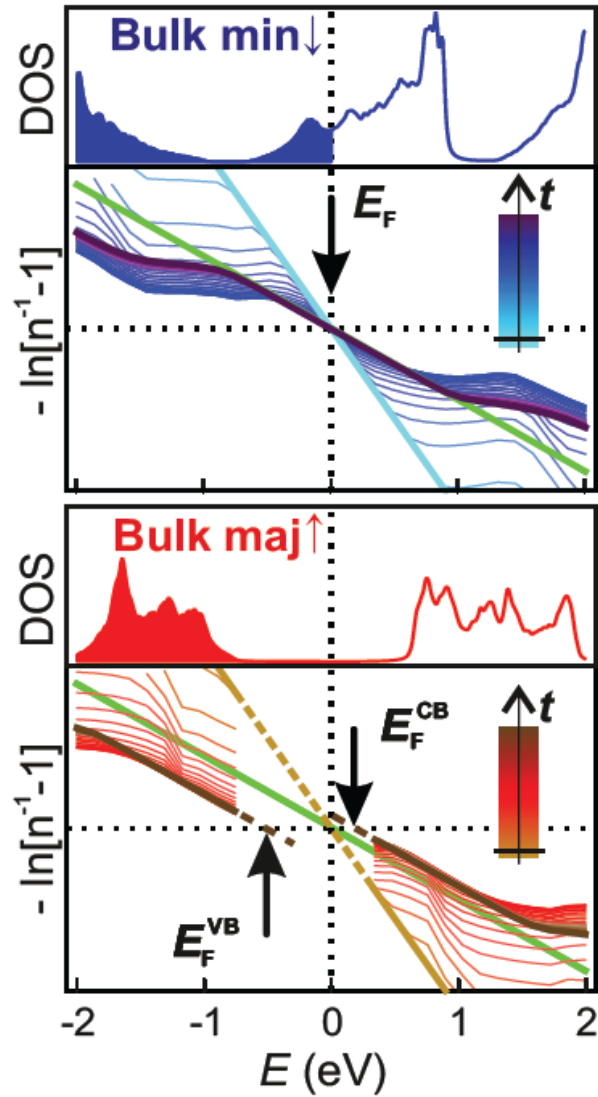
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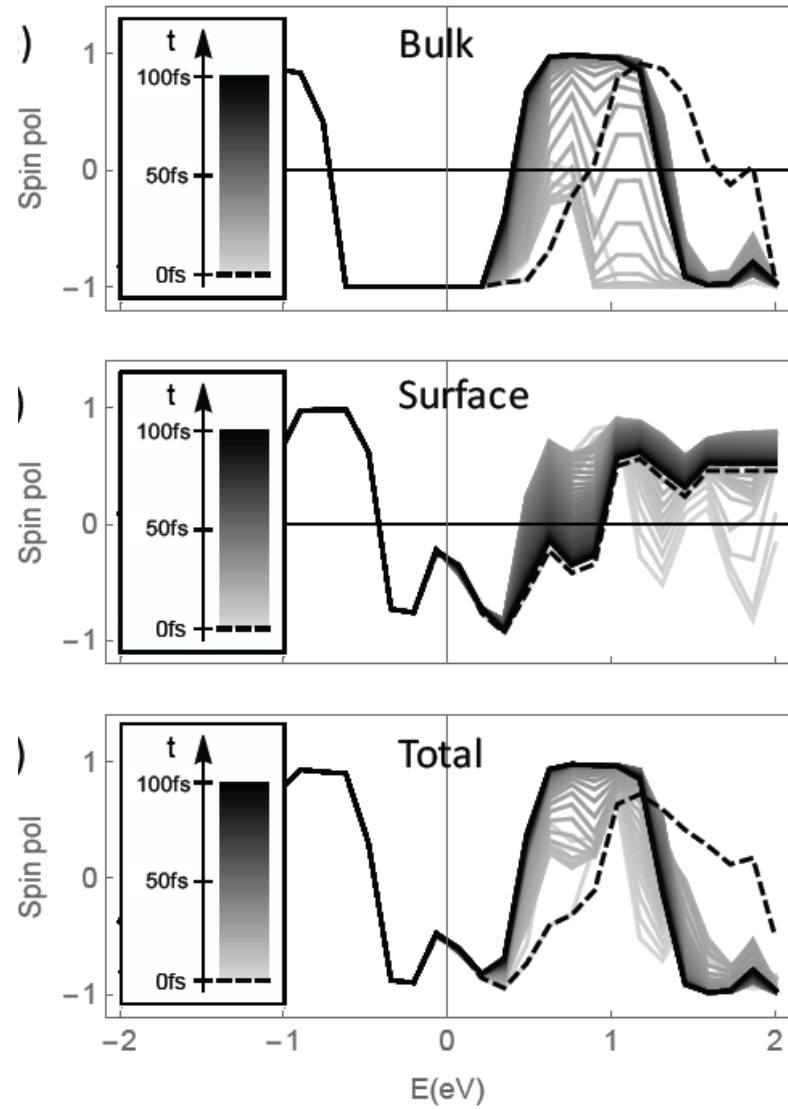
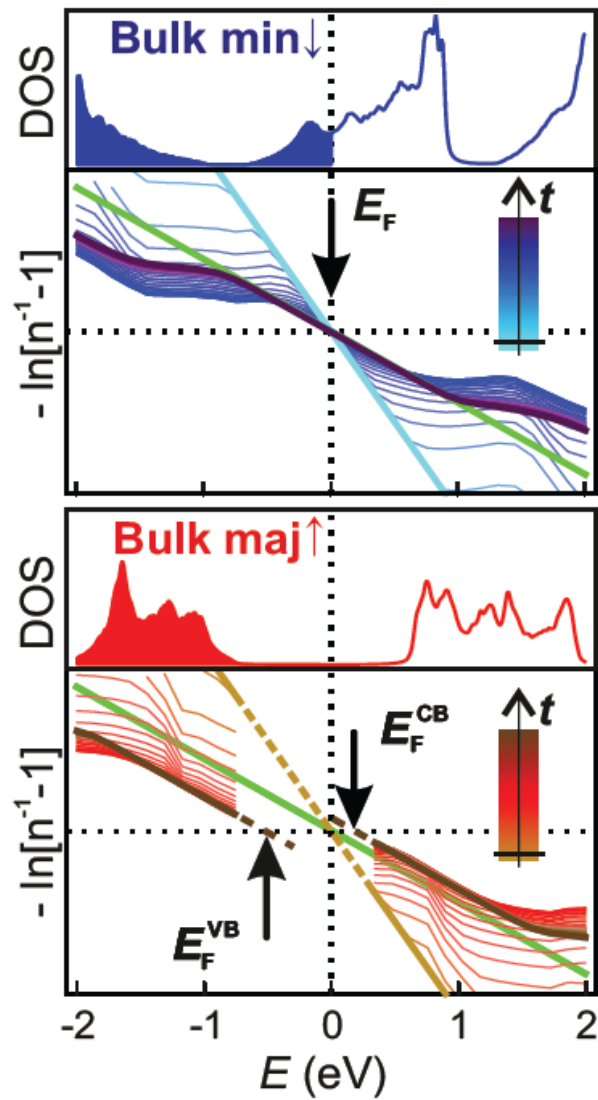
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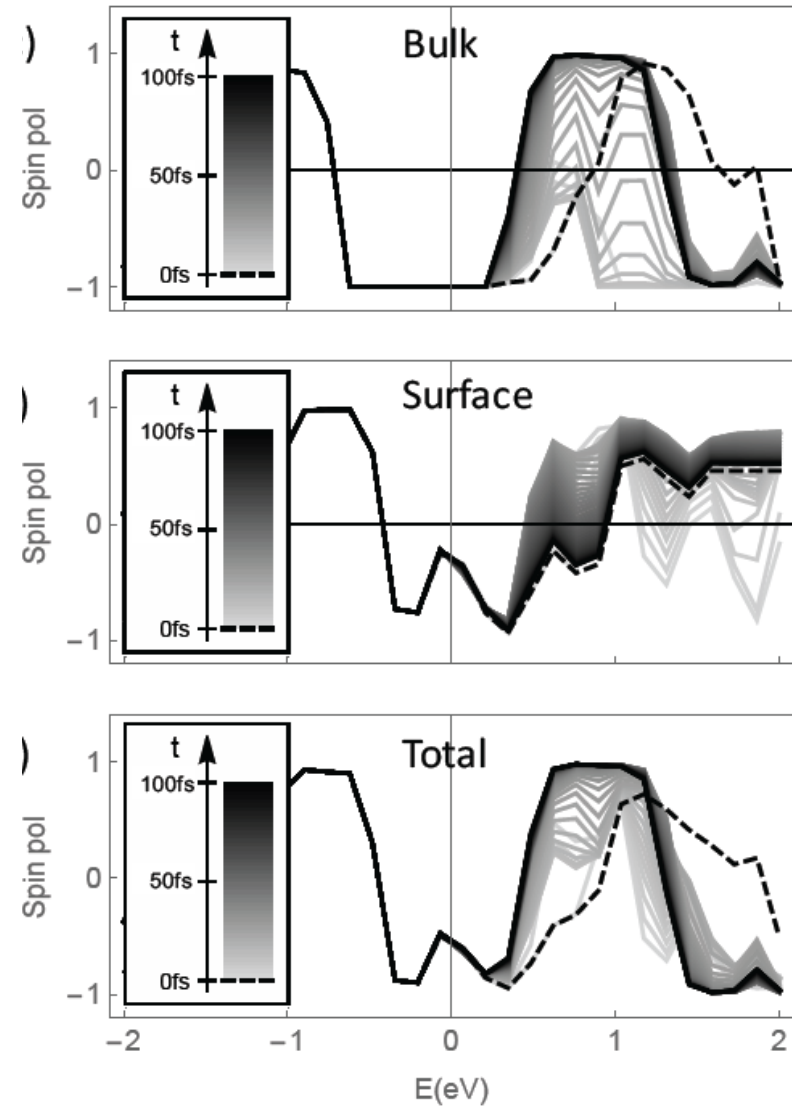
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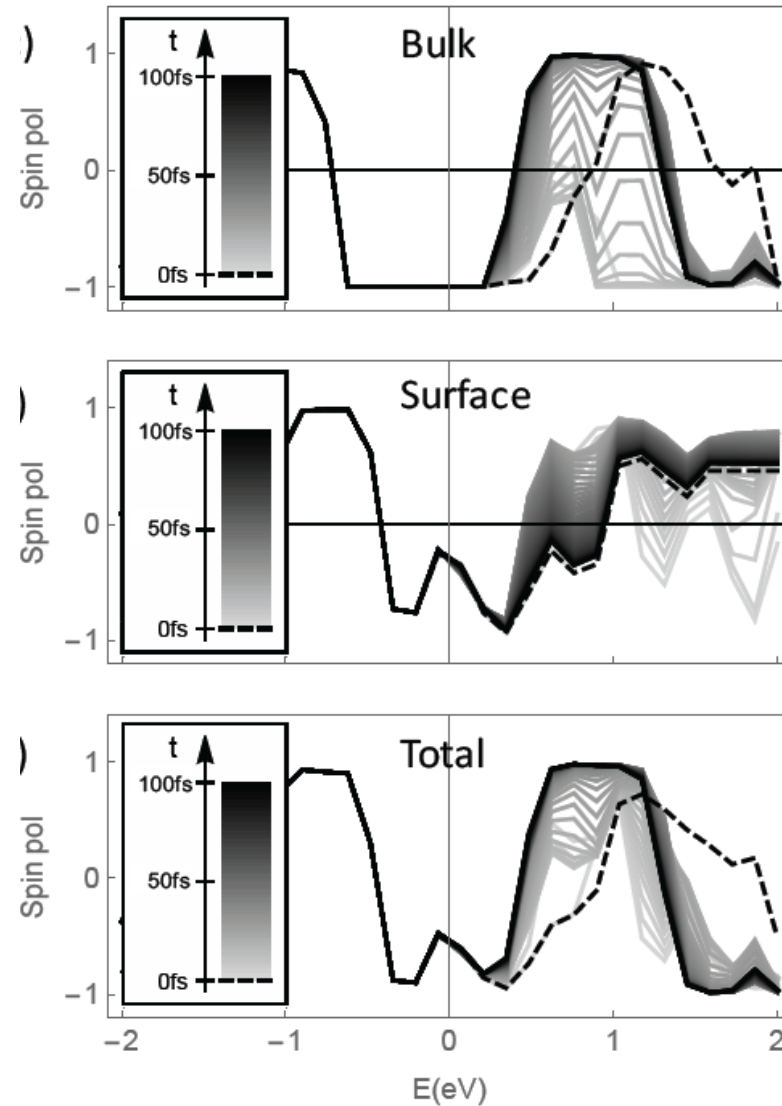
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fingerprint on the  
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dynamics  
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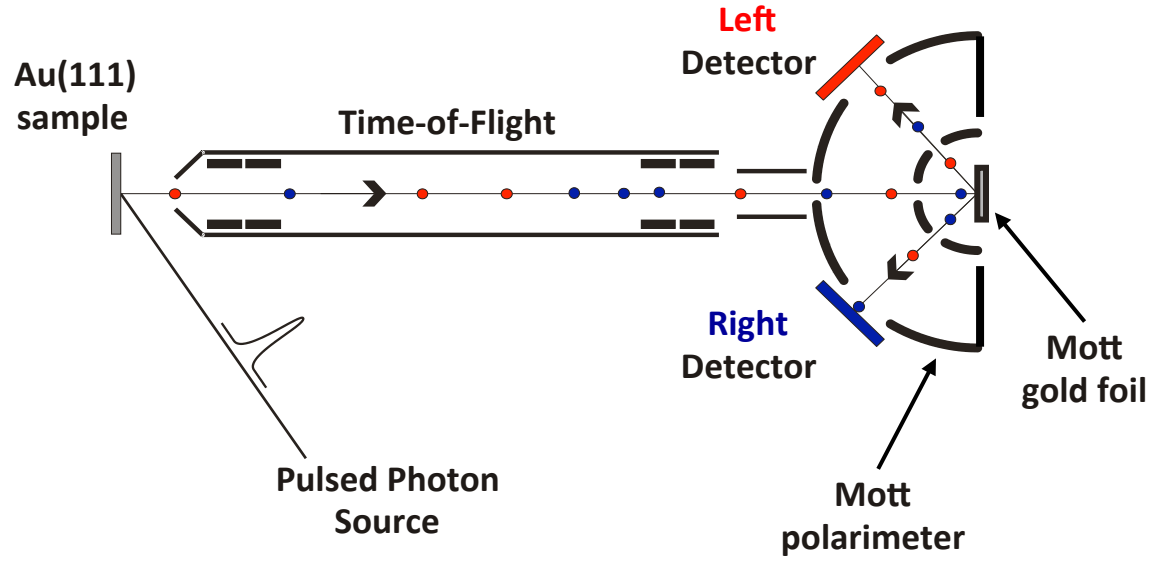
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spin dynamics is resilient  
to the presence of metallic  
surfaces

- half-metals
- theoretical model
- **spin- and time- resolved ARPES**
- conclusions

# TOF experimental setup with spin detection



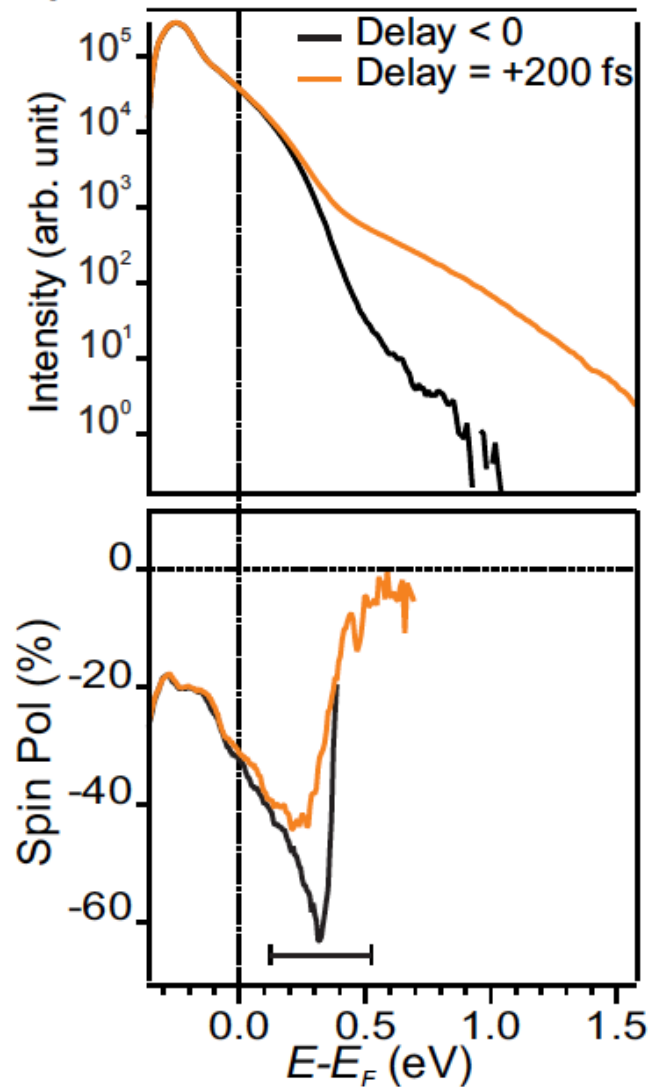
C. CACHO Rev.Sci.Instrum. 80, 043904 (2009)

Ti:sapphire laser (Coherent)  
photon pulses with a repetition rate of 250 kHz,  $\Delta t = 150$  fs

pump-probe experiments

P(800 nm) = 70 mW (0.7 mJ/cm<sup>2</sup>)  
P(266 nm) = 3 mW

# spin polarisation dynamics



## *Spin-resolved EDC*

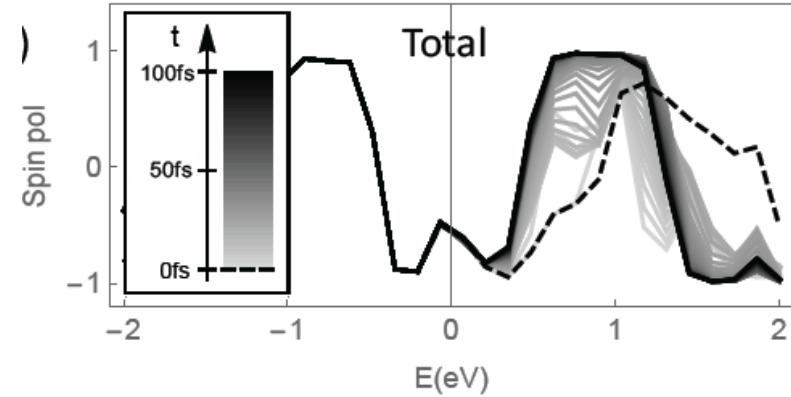
$$E_{\text{photon}} = 4.65 \text{ eV}$$

Delay = -400 fs to 1 ps

*Variation of the spin polarisation with the pump-probe time delay.*

- reduction of the spin polarization above  $E_F$ , no variation at higher binding energy
- no sign of demagnetization is observed, Fermi spin variation is attributed to the electron dynamics.

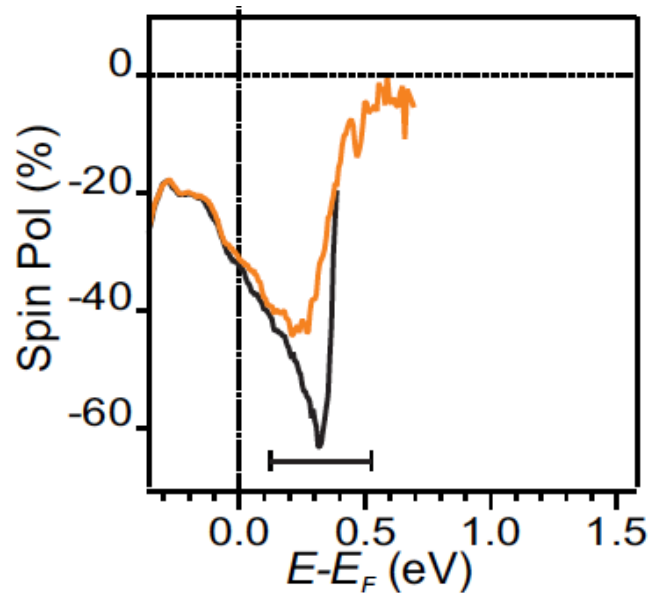
# spin polarisation dynamics



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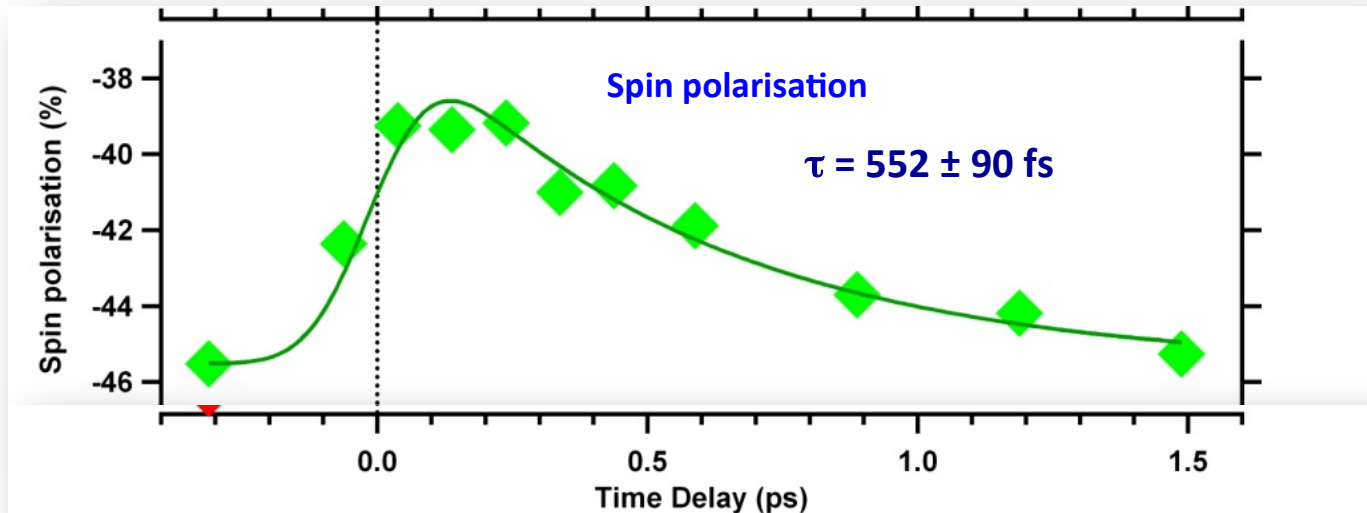
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# spin polarisation dynamics



# Conclusions

new approach allowing to test **half-metallicity**

- very peculiar fingerprint of the HM's bulk band structure on the **sub-picosecond dynamics of spin polarisation**
- spin dynamics is resilient to the presence of metallic surfaces and interfaces