Spin polarized transport properties in Fe/NaBr(001) based heterojunctions

E. Burzo and P. Vlaic

Faculty of Physics, Babes-Bolyai University
Cluj-Napoca

1. Computing method
2. Ground state electronic and magnetic properties
4. Interlayer exchange coupling
5. Spin-polarized transport properties
6. Conclusions

1. Computing method

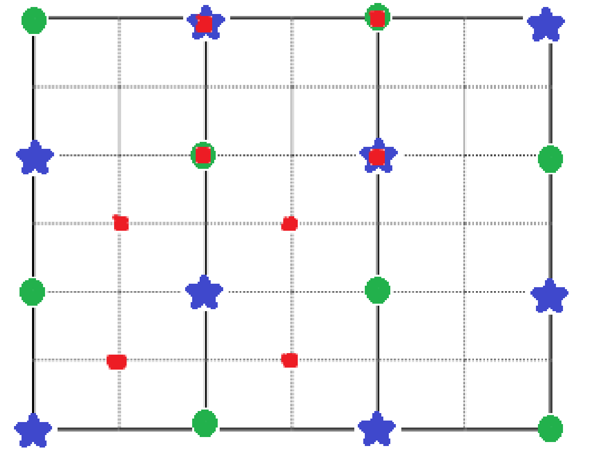
Ground state electronic structure and magnetic properties of semi-infinite Fe(001)/nFe/mNaBr(AgBr)/nFe(001)/semi infinite Fe(001) studied by:

- first-principles, scalar-relativistic and spin polarized surface Green's function technique implemented within the TB-LMTO method in ASA approximation.
- exchange correlation potential considered in the LSDA by means of Vosko-Wilk-Nusair parameterization.
- spin-resolved ballistic conductances in the CPP geometry at T = 0 K and zero-bias, calculated within TB-LMTO-CPA formalism and including the vertex corrections.
- tunneling magnetoresistance ratios TMR = $(\sigma_{FM}-\sigma_{AFM})/\sigma_{AFM}$ expressed by the asymmetry of FM and AFM conductances

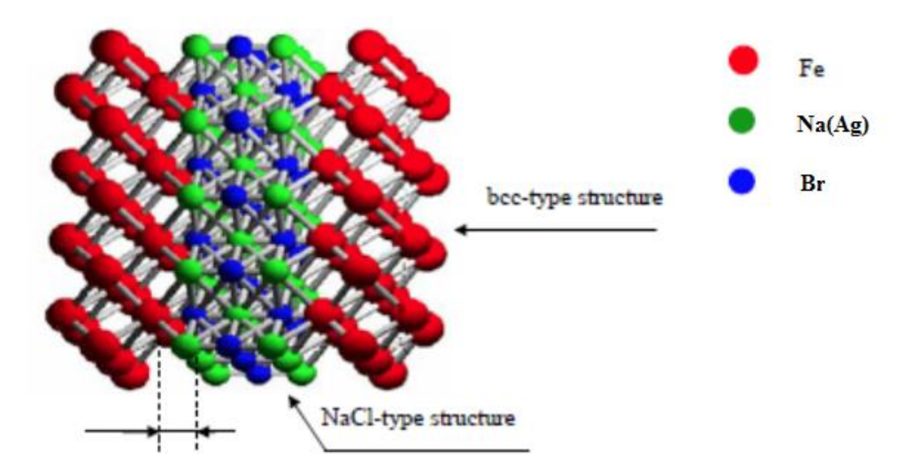
2. Structure

Model interfaces:

Calculations: lattice parameters epitaxially fixed at lattice spacing of iron $a_{NaBr} \simeq 2\ a_{Fe}$, $a_{AgBr} \simeq 2a_{Fe}$
NaBr, AgBr epitaxially fit bcc Fe structure



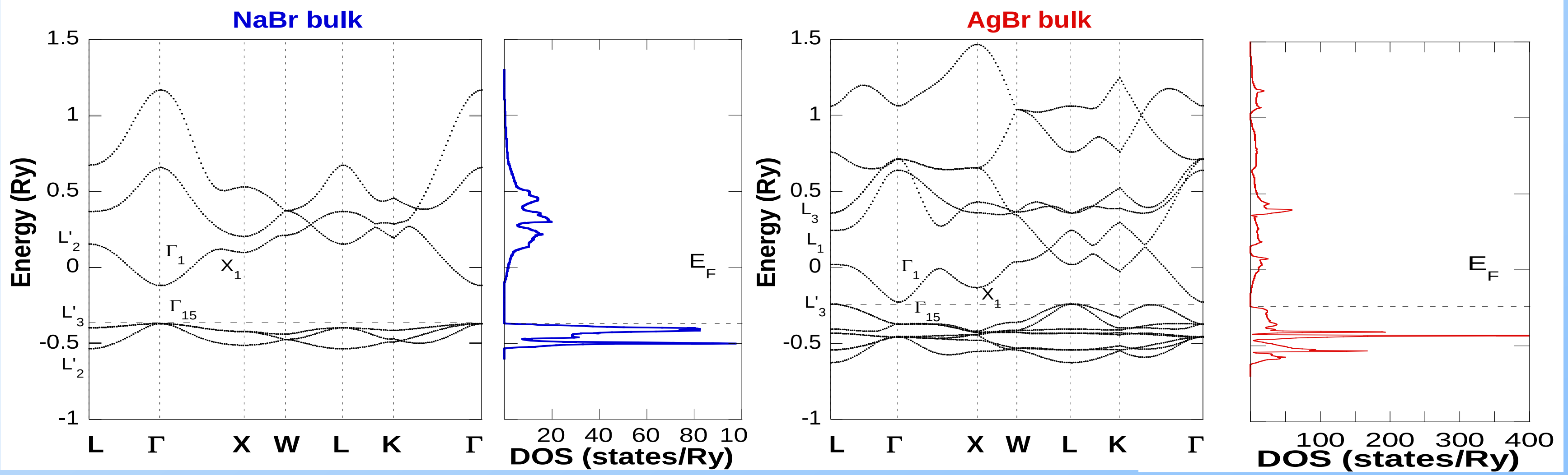
Model interfaces
C1:Fe sitting a top Ag(Na) and Br positions
C2: Fe atoms located above the hollow sites between Ag(Na) and Br.



Lattice constant:
NaBr a_{exp}=5.97 Å, a_{calc}=5.68 Å
AgBr a_{exp}=5.64 Å, a_{calc}=5.58 Å

Open structure: to fulfill ASA space filling
Fe/AgCl C1 interface: two empty spheres were introduced.

Band structures NaBr and AgBr



NaBr	Eg:7.1 eV (exp):	3.6 eV (calc)
AgBr	Eg: 2.68 (exp)	0.9 eV (calc)

Due empty sphere planes introduced between adjacent NaBr(AgBr): spacers are non-symmetric

Symmetric junctions

(even number of atomic monolayers)

$\Downarrow$

Non symmetric electrodes (n, n+1) iron layers

6Fe/9NaBr/7Fe

Atomic monolayers

I, I-1, I-2 magnetic slab

I, I+1, I+2 barrier

Ground state electronic and magnetic properties

- Electronic states: 6Fe/9NaBr/7Fe

Charge transfer

C1 interface

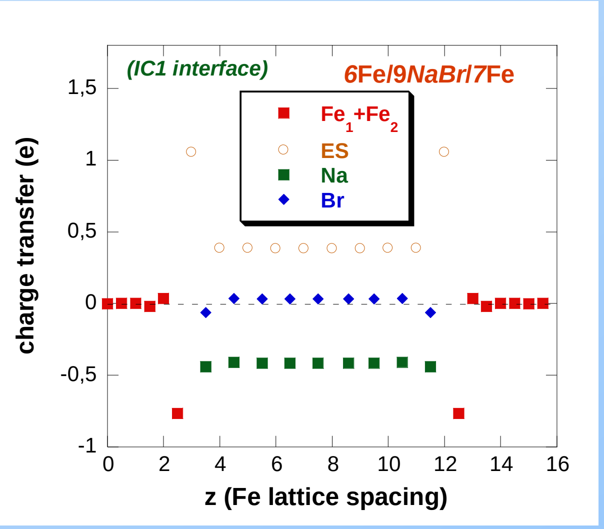
Br decreases by ≅ 0.03 e⁻

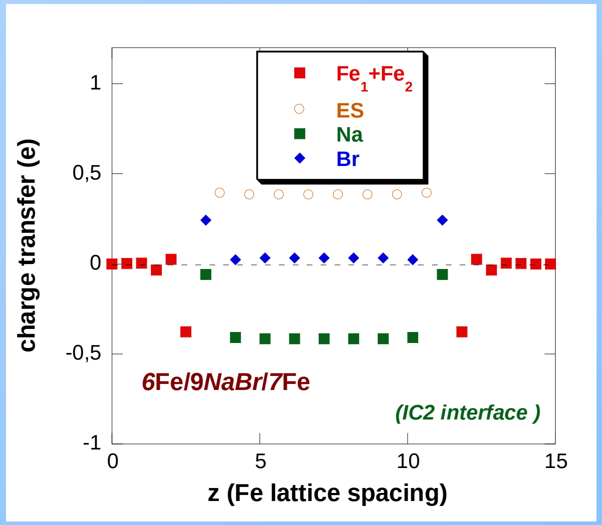
Na decreases by ≅ 0.02 e⁻

C2 interface

Br increases by ≅ 0.22 e⁻

Na increases by ≅ 0.35 e⁻



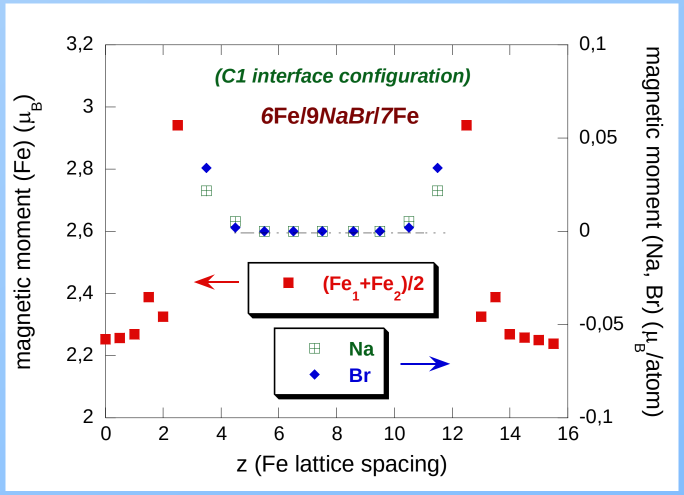


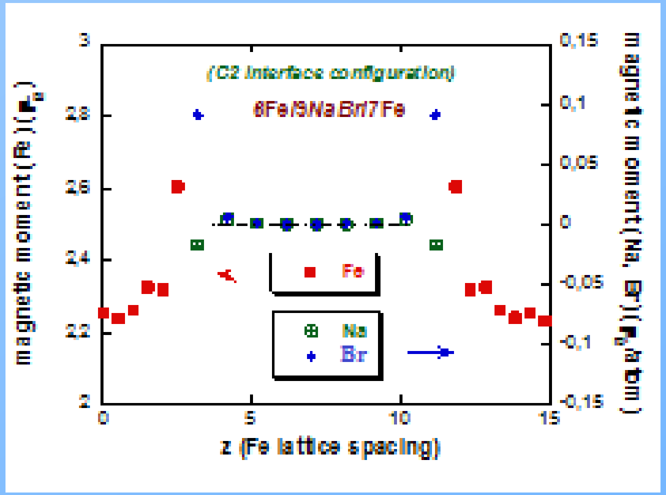
- Magnetic moments

Interfacial iron moments enhanced over bulk value:

C1 Fe $M_{Fe} \cong 2.94\ \mu_B$

C2 Fe $M_{Fe} \cong 2.60\ \mu_B$





Small polarizations induced on Na and Br:

C1 $M_{Na}=0.02\ \mu_B$

$z=3,\ 12$

$M_{Br}=0.03\ \mu_B$

$M_{Na},\ M_{Br}=0\ \mu_B \quad 4 \leq z \leq 11$

C2 $M_{Na}=-0.02\ \mu_B$

$z=3,\ 12$

$M_{Br}=+0.09\ \mu_B$

$M_{Na}=M_{Br}=0\ \mu_B \quad 4 \leq z \leq 11$

Similar behaviour for AgBr spacer

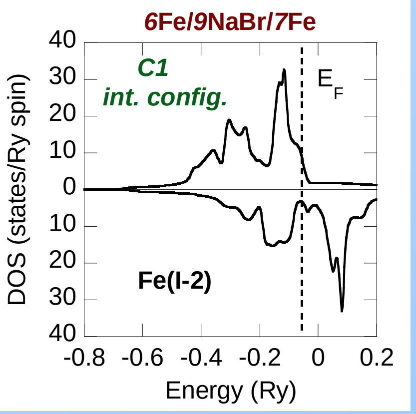
Layer and atom-resolved spin-polarized DOS
6Fe/9NaBr/7Fe

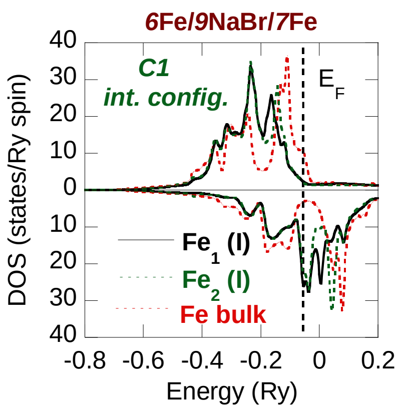
C1 configuration:

- Away from interface, Fe(I-2),

DOS of Fe: bulk like with partially filled majority-spin 3d sub-band

E_F located at a dip in the minority-spin 3d sub-band.





- Interface, (FeI)

DOS modified: lower coordination number of Fe atoms and interaction with NaBr interfacial layer
minority spin band, nearly fully occupied
majority spin band, nearly empty

Metal induced gap states (MIGs)

- **C1 interface:**

Iron metal induced gap states:

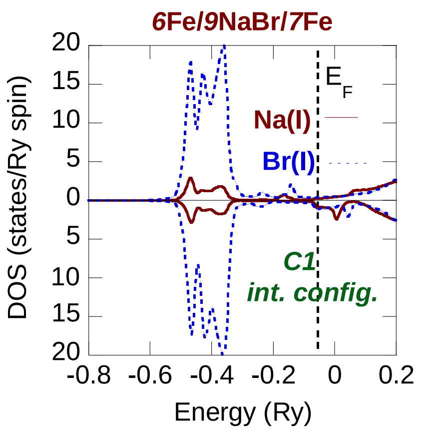
in NaBr barrier near the interfaces on both Na and Br

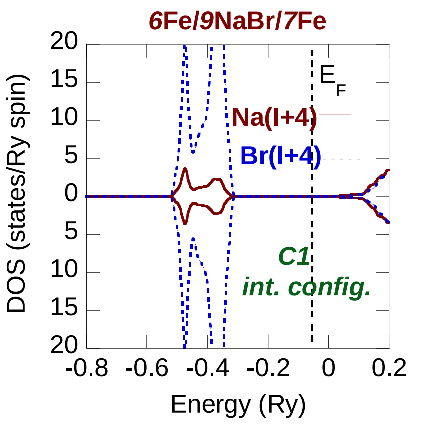
Fe/NaBr(001) interfaces practically metallic

Departing from interfaces:

isolating character recovered

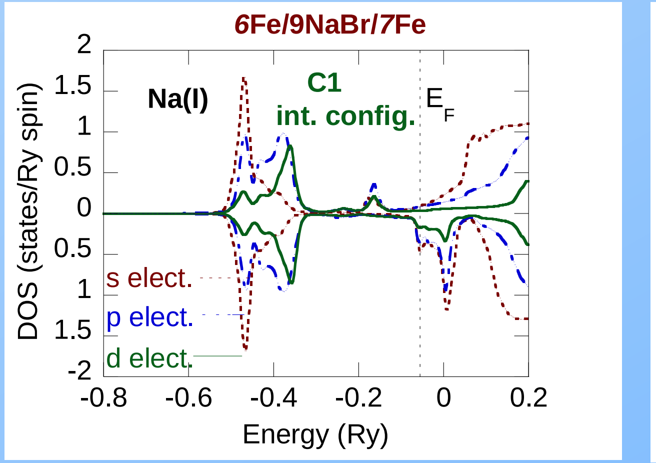
- C2 interface: near the same behaviour

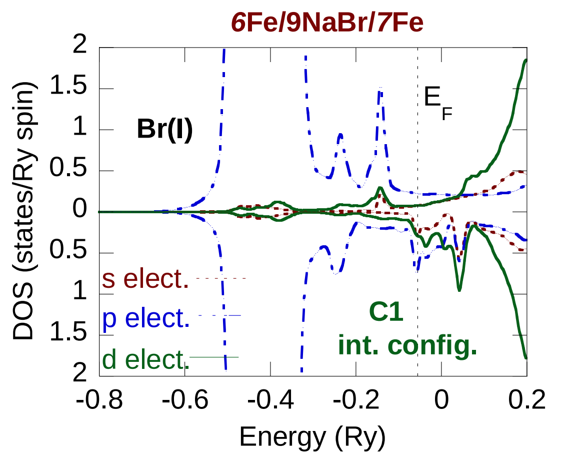




Induced gap states

contributions from d, p and s electrons





Interlayer exchange couplings (IEC)

Exchange coupling between Fe(001) magnetic slabs and the NaBr and AgBr spacers:

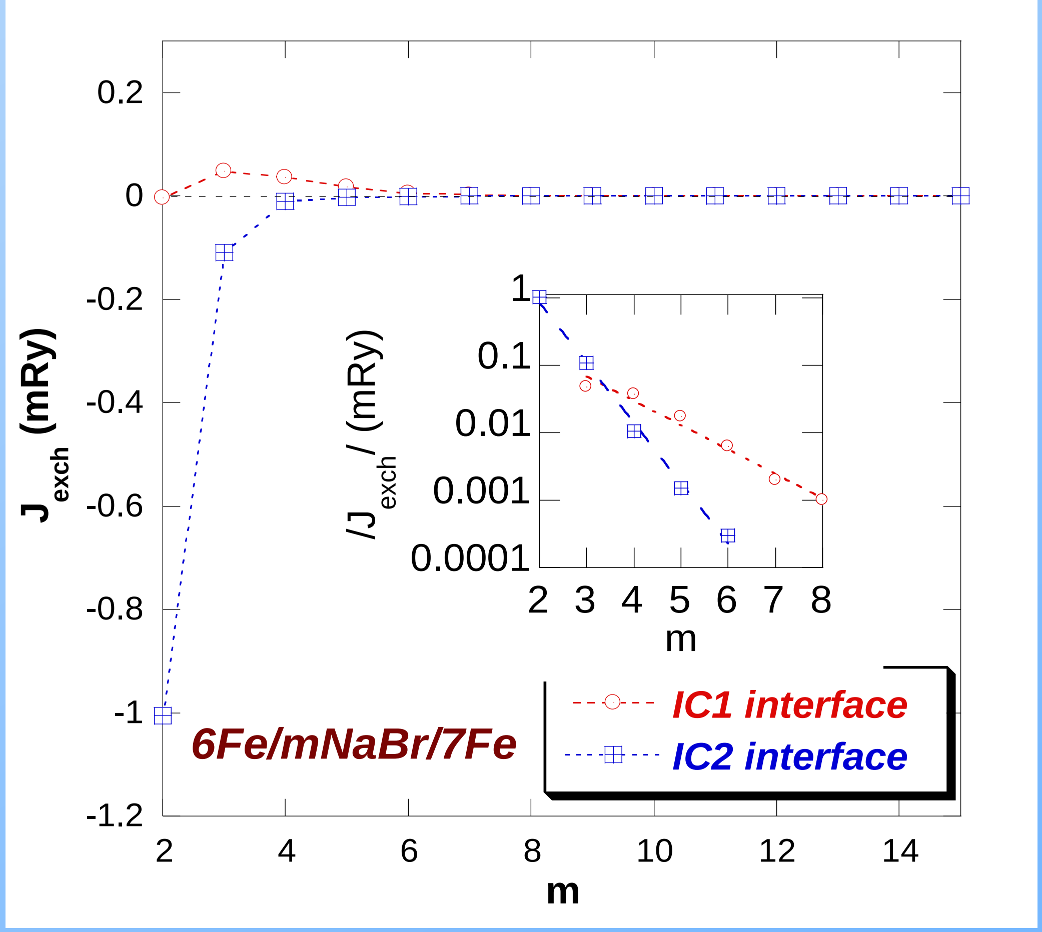
Fe/mNaBr(AgBr)/Fe

⇓

NaBr C1 interface small positive, $3 \leq m \leq 8$

exponential decay

C2 interface negative, $m \leq 6$



IEC

Negative $k_F^2 < k_F^{\uparrow} k_F^{\downarrow}$

Positive $k_F^2 > k_F^{\uparrow} k_F^{\downarrow}$

k_F in the barrier

$k_F^{\uparrow}, k_F^{\downarrow}$ vawe vector in magnetic electrode (Fe)

$k_F^2 \propto \sqrt{U_{eff}}$; depends on barrier height

k_F high in C1 interfaces

small in C2 interfaces

AgBr oscillatory:

thin barrier m < 2 C1 interfaces

m < 4 C2 interfaces

J_{exch}

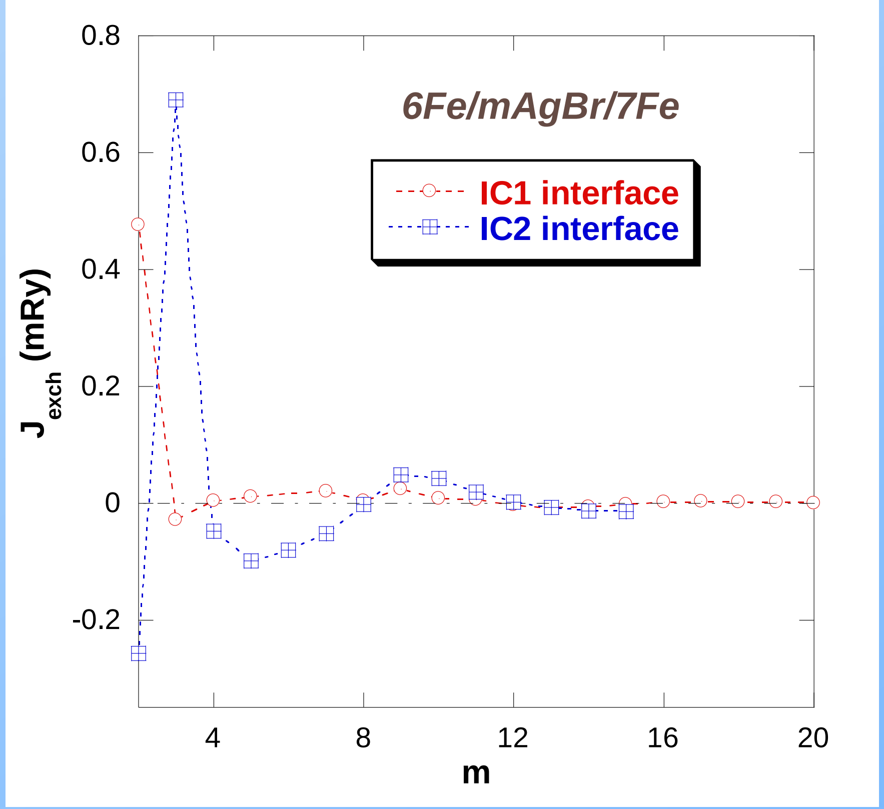
⇓

positive

Larger amount of MIGs near interfaces

Damped oscillations:

related: small barrier height



Spin dependent transport properties

6Fe/mNaBr/7Fe

Exponential decay with barrier thickness:

Dominant contributions

C1 interface

FM (spin down) with change in slope m=8

C2 interface

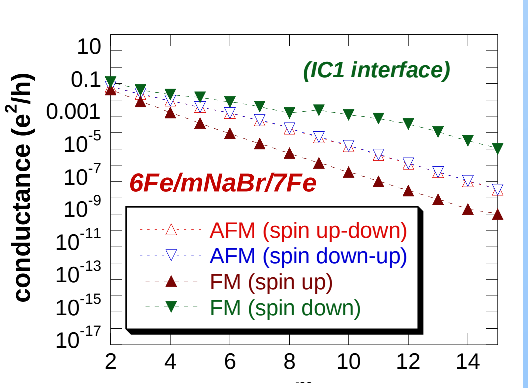
near the same contributions for all spin channels

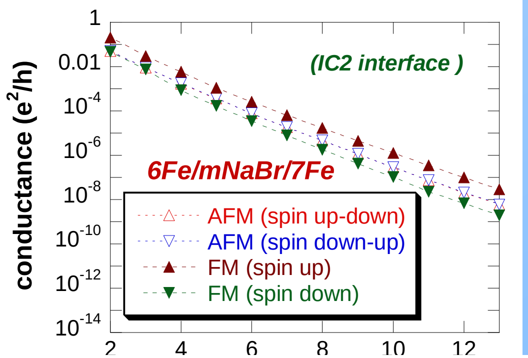
Tunneling magnetoresistance:

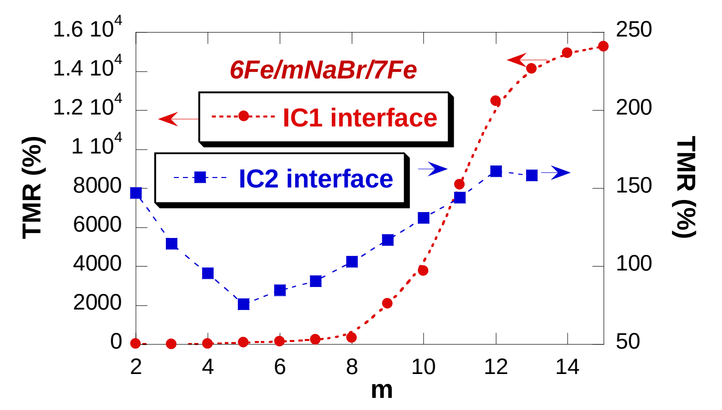
High TMR

C1 interface, m > 11, $\cong 10^4$ %

C2 interface $\cong 10^2$ %







$k_{||}$-resolved conductances

Transmission across a planar junction described by complex band structure of barrier

$\Downarrow$

Interface: wave vector split in: $k_{||}$ conserved during scattering

k_z along the transmission direction

Inside barrier band gap $k_z = q+i$; the imaginary part i describes exponential decay of the corresponding evanescent state.

Transmission probability for $k_{||}$ $T \propto \exp(-2kd)$, d –barrier thickness.

Presence of tunneling across the NaBr(AgBr) barrier: confirmed by exponentially decay of conductances in the asymptotic region.

Conductances

- Majority spin (up) conductances

FM conductances: free electron-like with broad and large transmission maximum at $\overline{\Gamma}$ point.

Conduction determined by Δ_1 states

NaBr: conduction band minium, at the center of Brillouin zone occurs at Γ_1 point, while the top valence band occurs at the Γ_{15} point

$\Downarrow$

Bottom of the conduction band and the top of valence band will be connected by purely imaginary band with Δ_1 symmetry

$\Downarrow$

lower Δ_1 decay parameter

States with other symmetrical decay much faster(negligible contribution to tunneling)

Δ_1 channel: only direct tunneling channel across NaBr(AgBr) barriers

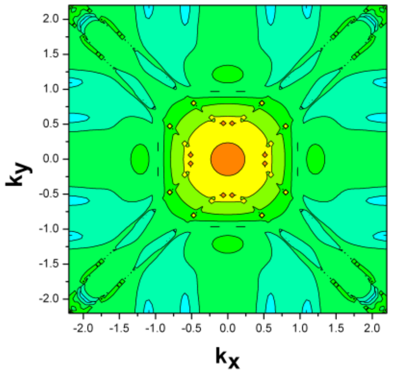
- Minority-spin FM and AFM conductances

Dominated by hot-spots or spike-like peaks around $\overline{\Gamma}$ point

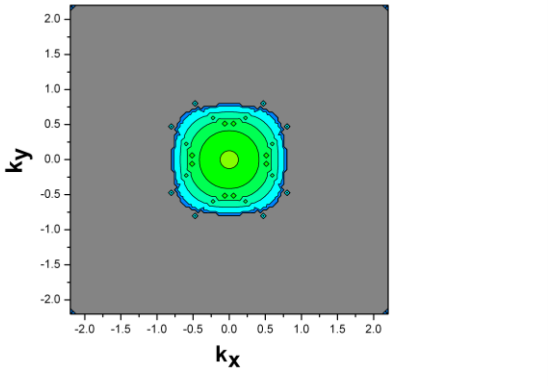
Spikes:

- originate from the minority-spin interface resonant states
- increase the transmission by resonant tunneling

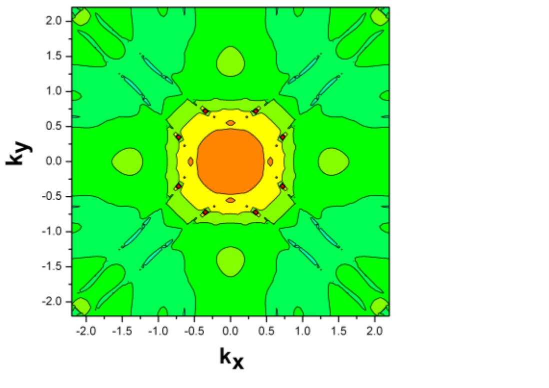
6Fe/5NaBr/7Fe (IC1 int.) (FM spin up)



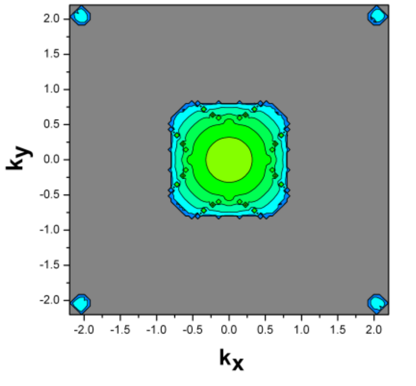
6Fe/9NaBr/7Fe (IC1 int.) (FM spin up)



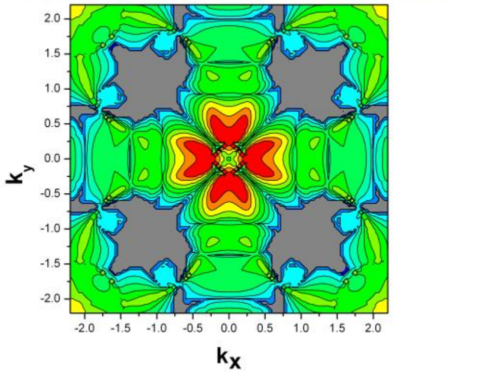
6Fe/5NaBr/7Fe (IC2 int.) (FM spin up)



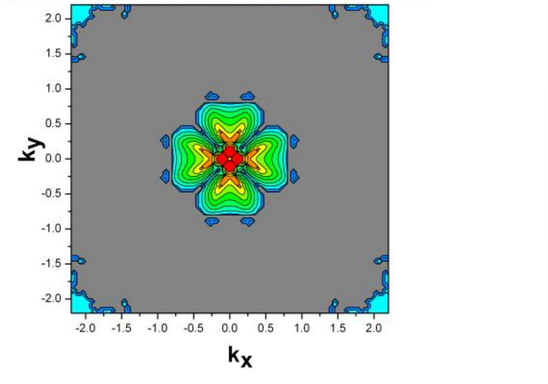
6Fe/9NaBr/7Fe (IC1 int.) (FM spin up)



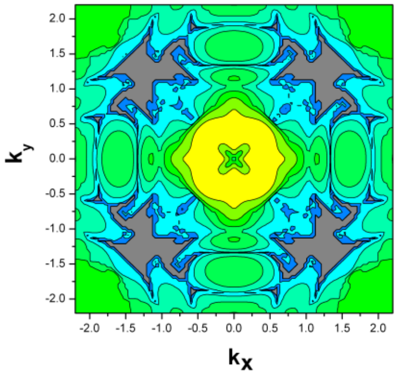
6Fe/5NaBr/7Fe (IC1 int.) (FM spin down)



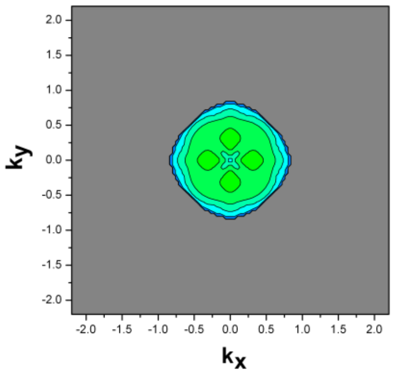
6Fe/9NaBr/7Fe (IC1 int.) (FM spin down)



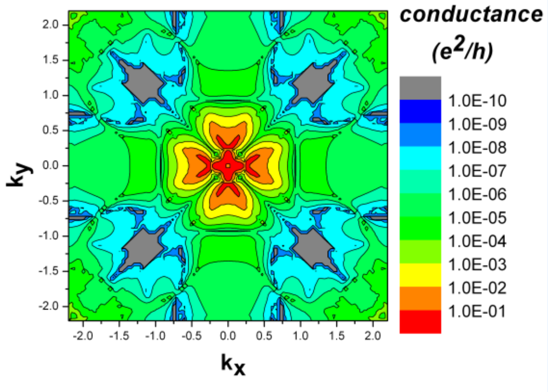
6Fe/5NaBr/7Fe (IC2 int.) (FM spin down)



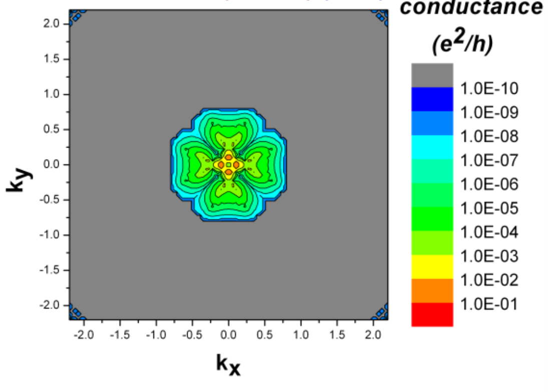
6Fe/9NaBr/7Fe (IC2 int.) (FM spin down)



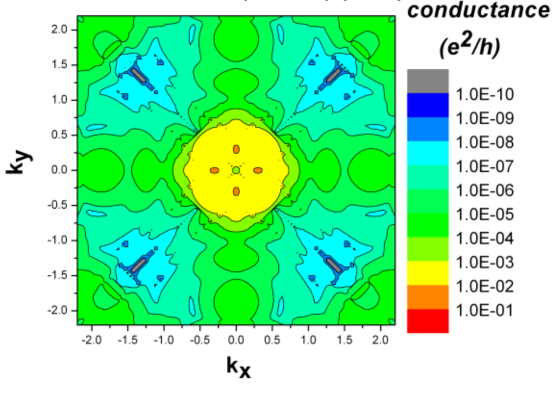
6Fe/5NaBr/7Fe (IC1 int.) (AFM)



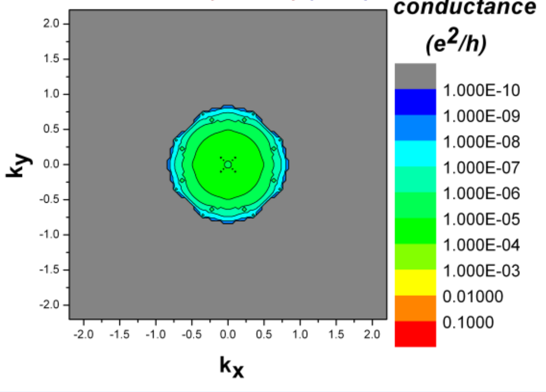
6Fe/9NaBr/7Fe (IC1 int.) (AFM)



6Fe/5NaBr/7Fe (IC2 int.) (AFM)



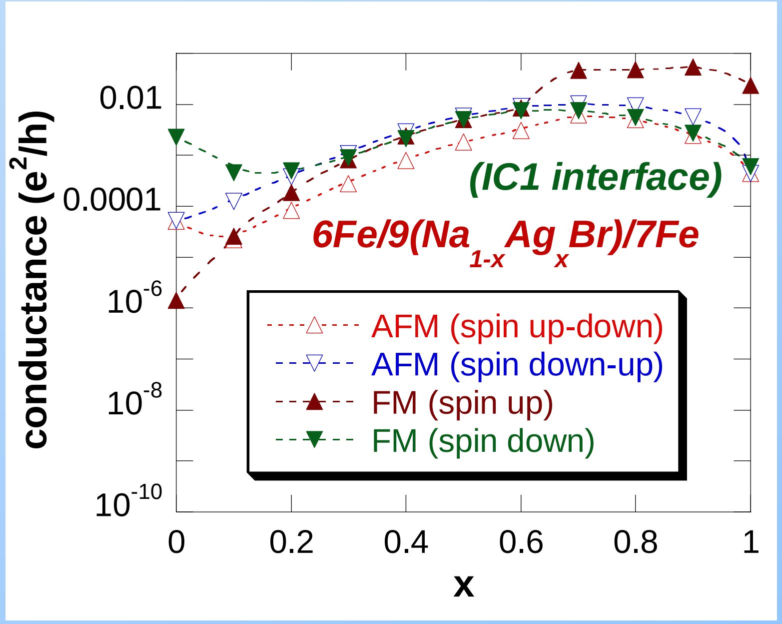
6Fe/9NaBr/7Fe (IC2 int.) (AFM)



Transport properties of Fe/Na$_{1-x}$Ag$_x$Br/Fe MTJ

C1 interface

Conductances

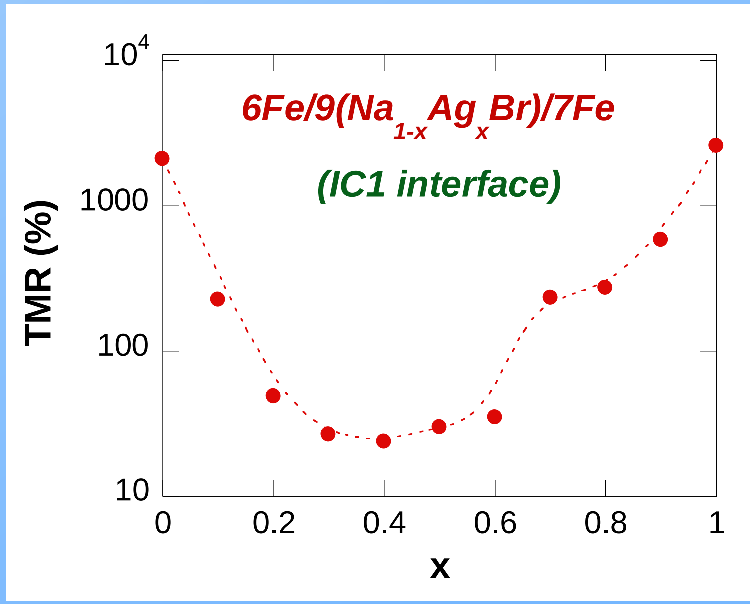


FM conductances

spin down, dominates at x < 0.2

spin up, dominates at x > 0.8

Intermediate region near the same for spin down and spin up



TMR

>10^3 % for x =0 or 1

decrease in intermediate region

CONCLUSIONS

- Fe/NaBr(001) and Fe/AgBr(001) interfaces are stable both for C1 and C2 interfaces
- Interfacial iron’s magnetic moment enhanced over bulk value
- Exchange coupling along a barrier
  - 6Fe/mNaBr/7Fe C1 and C2 interfaces
    - decrease up to m=6. From m>6 is nill
  - 6Fe/mAgBr/7Fe C1 and C2 interfaces
    - oscillatory
- Spin dependent transport properties

resonant tunneling mechanism

TMR	6Fe/mNaBr/Fe	C1: $5\cdot10^4$ %	for m > 12
		C2: $1.5\cdot10^2$ %	for m > 10
	6Fe/mAgBr/Fe	C1: $3\cdot10^3$ %	for m > 8
		C2: $2\cdot10^2$ %	

- Attractive in the context of magnetoelectronics.

ACKNOWLEDGMENTS

This work was supported by the Romanian Ministry of Education and Research (UEFISCDI), grant no. PN-II-ID-PCE-2012-4-0028.

Thank you very much for your attention