Electronic properties of Fe/LiF(LiBr)/Fe magnetic tunnel junctions

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1. Computing method

Ground state electronic structure and magnetic properties of semi-infinite Fe(001)/nFe/mLiF(LiBr)/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, together with CPA in order to describe the disorder effects like the intermixing at interfaces.
- 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 $TMR = (\sigma_{FM}-\sigma_{AFM})/\sigma_{AFM}$ expresed by the asymetry of FM and AFM conductances

2. Structure

- BCC structure considered for Fe electrodes
- rock salt structure for LiF and LiBr

a_{LiF} = 4.02 Å, a_{LiBr} = 5.5 Å $a_{LiBr} = 2a_{Fe}$

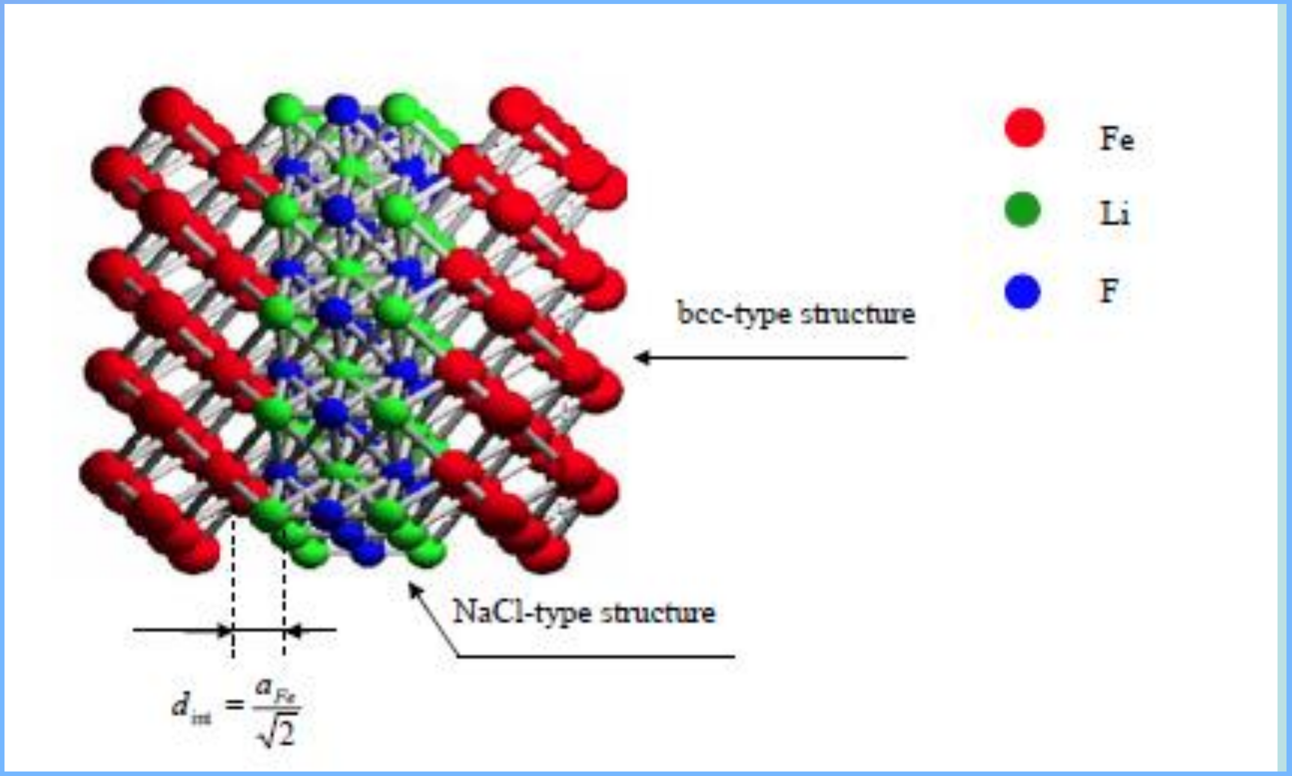
$a_{LiF} = \sqrt{2}a_{Fe}$

LiF, LiBr epitaxially fit bcc Fe structure

LiF insulator direct band gap 13.6 eV

LiBr insulator direct band gap 8 eV

Fe/LiF(LiBr)/Fe MTJ feasible heterostructures for spintronic applications

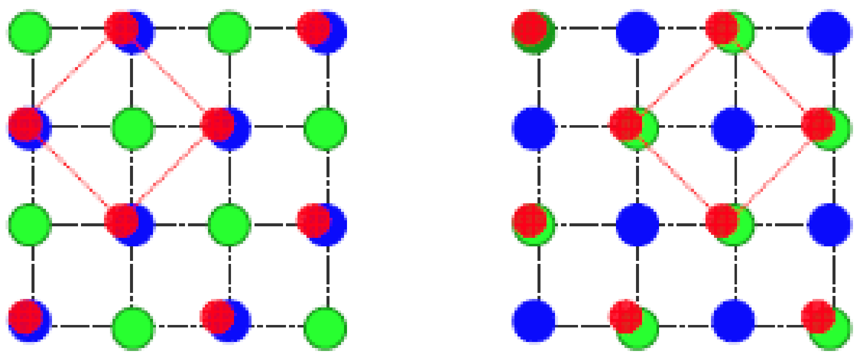


Due to open structure of LiF, to fulfil ASA space filling requirement two empty spheres (ES) at interstices positions at Fe/LiF (100) interface; Fe located atop of F

Model interfaces

Fe atoms located above Li(Br) sites

Fe atoms located above F atoms

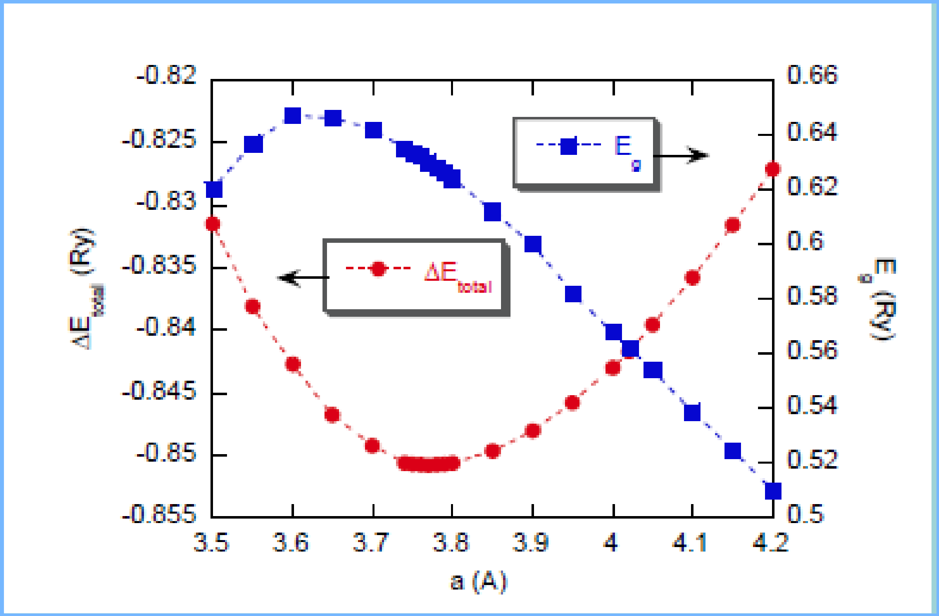


$IC_{Fe\text{-}F}$ $IC_{Fe\text{-}Li}$

Band structure LiF

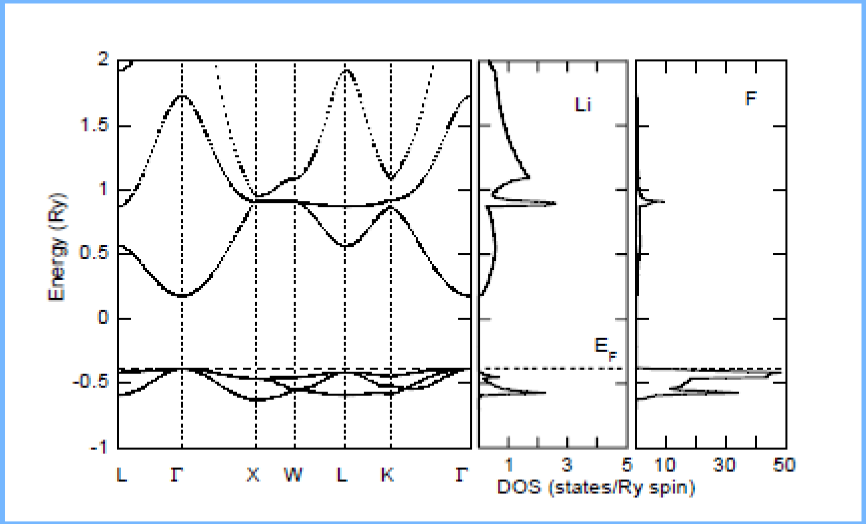
Stable configuration

Equilibrium lattice constant 3.78 Å smaller by 5.3 % than experimental value 4.02 Å



Band structure for equilibrium lattice parameter

LiF



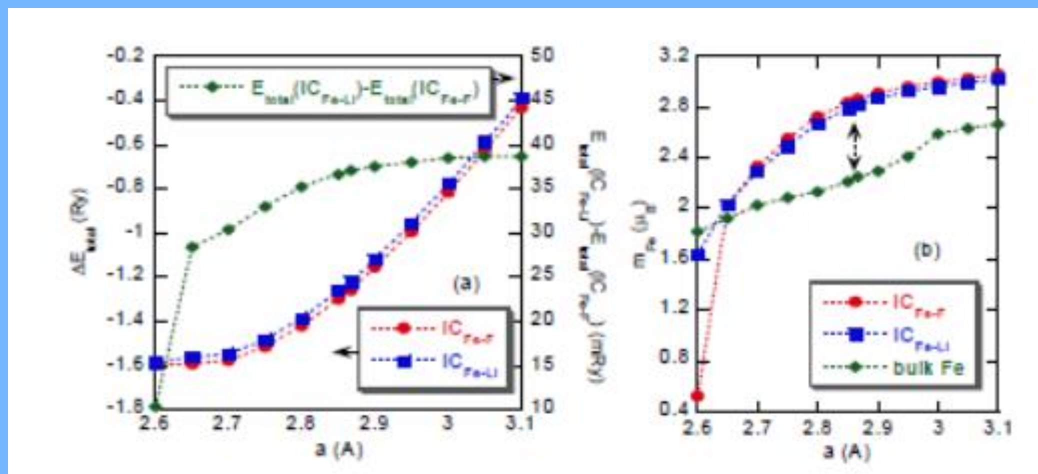
Direct band gap E_g = 9 eV

Interface stability

Fe/LiF (001)

Relative to Fe lattice constants

$IC_{Fe\text{-}F}$, $IC_{Fe\text{-}Li}$ interface configurations



most stable

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$IC_{Fe\text{-}F}$ Fe/LiF (001) interface with Fe atoms located atop F ones – Fig.a

Fe magnetic moments at interface: enhanced over the bulk value – Fig.b.

Fe/LiBr(001) interface

Stable for Fe atoms located both above Li and Br sites

Interface stability as effect of mixing

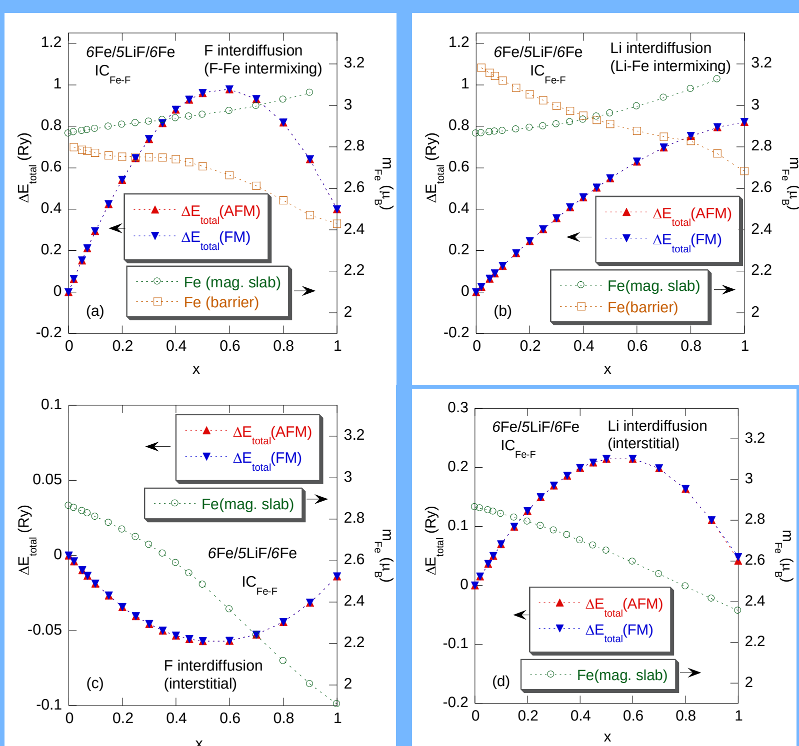
Interdiffusion of Li and F, respectively at Fe/LiF interfaces

- $IC_{Fe\text{-}F}$ interface

Interfacial layers having compositions

$$Fe_2(Fe_1)_{1-x}F_x/F_{1-x}Fe_xLi;\ Fe_2(Fe_1)_{1-x}Li_x/Li_{1-x}Fe_xF$$

Configuration 6Fe/5LiF/6Fe



F-Fe intermixing: Fe interdiffusion: E_{tot} (AFM, FM): increase up to x = 0.6 and then decrease

Li-Fe intermixing: Li interdiffusion: E_{tot} (AFM, FM): increases

F interdiffusion (interstitial): E_{tot} (FM, AFM) decreases at x < 0.5 and then increases

Li interdiffusion (interstitial): E_{tot} (FM, AFM) increases up to x = 0.6 and then decreases

Magnetic properties:

- F and Li interdiffusion (interstitial)

Fe magnetic moments: decrease in the slab, when x increases

- Fe and Li interdiffusion (mixing)

Fe magnetic moments:

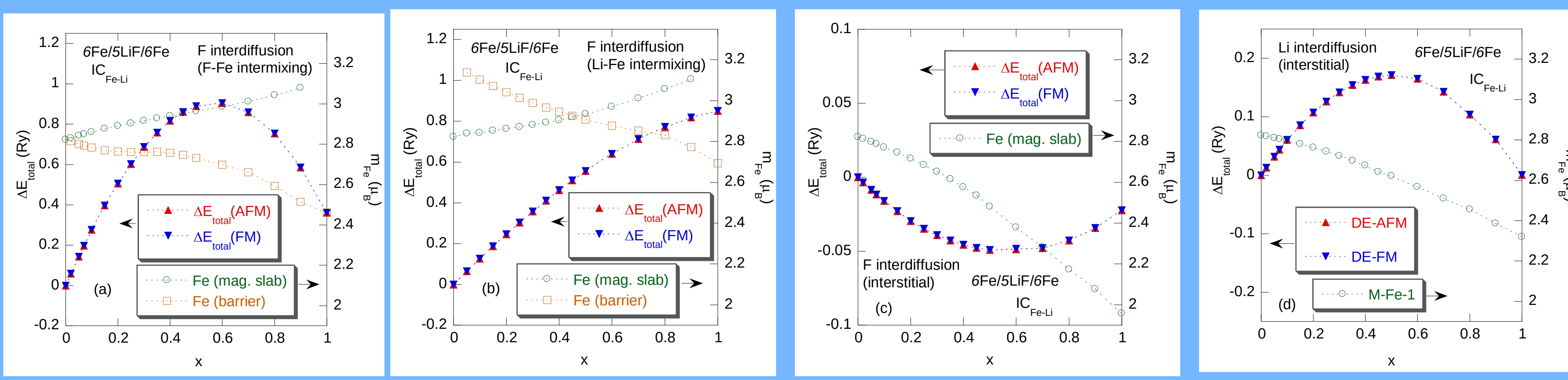
decrease at Fe barrier
increase in the Fe slab

when x increases

- $IC_{Fe\text{-}Li}$ interface

6Fe/5LiF/6Fe

$Fe_2(Fe_1)_{1-x}F_x/F_{1-x}Fe_xLi$ $Fe_2(Fe_1)_{1-x}Li_x/Li_{1-x}Fe_xF$



Decreasing total energy for both FM and AF configurations for $x < 0.5$

F interdiffusion (interstitial)

Increasing total energy both for AF and FM configurations

F interdiffusion (Li-Fe intermixing)

Fe interdiffusion (F-Fe intermixing) $x \leq 0.6$

Li interdiffusion (interstitial) $x < 0.5$

Magnetic properties

Interdiffusion (F-Fe, Li-Fe intermixing)

M_{Fe} at barrier decreases with x

M_{Fe} in the slab increases with x

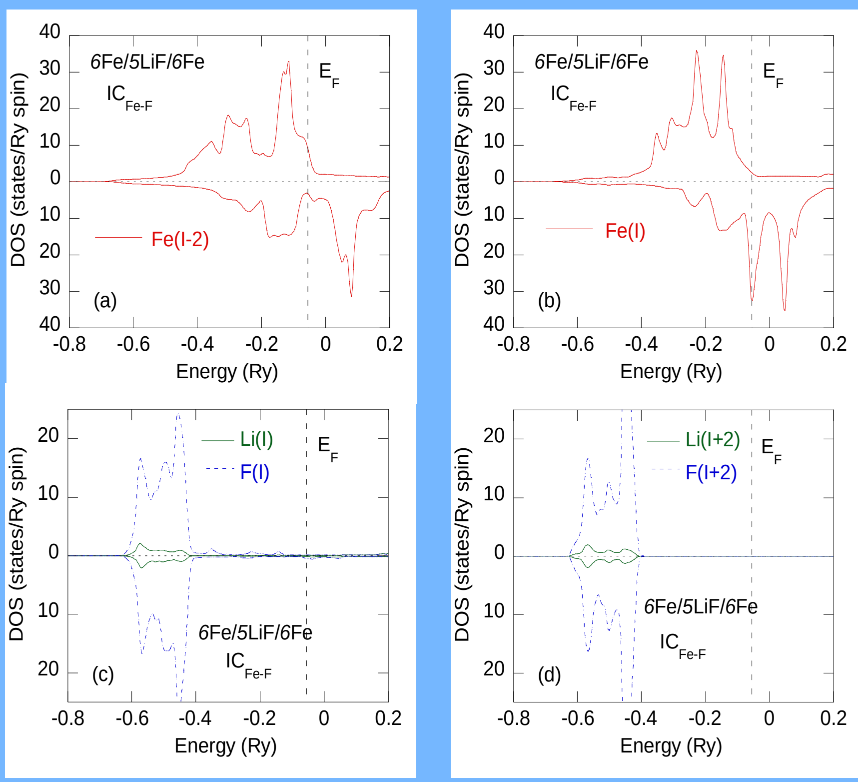
Interdiffusion (F and Li interstitial)

M_{Fe} decreases with x

3. Charge transfer and magnetic properties

Layered- and atom-resolved spin-polarized DOS 6Fe/5LiF/6Fe heterostructure

IC_{Fe-F} Fe/LiF(001)



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

At interface Fe(I):

DOS modified: lower coordination number of Fe atoms and interaction with LiF interfacial layer: majority-spin sub-bands almost fully occupied.

Metal induced gap states (MIGs) in LiF barrier near interfaces.

$IC_{Fe\text{-}Li}$ Fe/LiF(001)

- minority-spin interface states: slightly displaced at lower energy
- peak in DOS appears at E_F

Iron (metal) induced gap states (MIGs) in LiF barriers near interfaces on both Li, F ions

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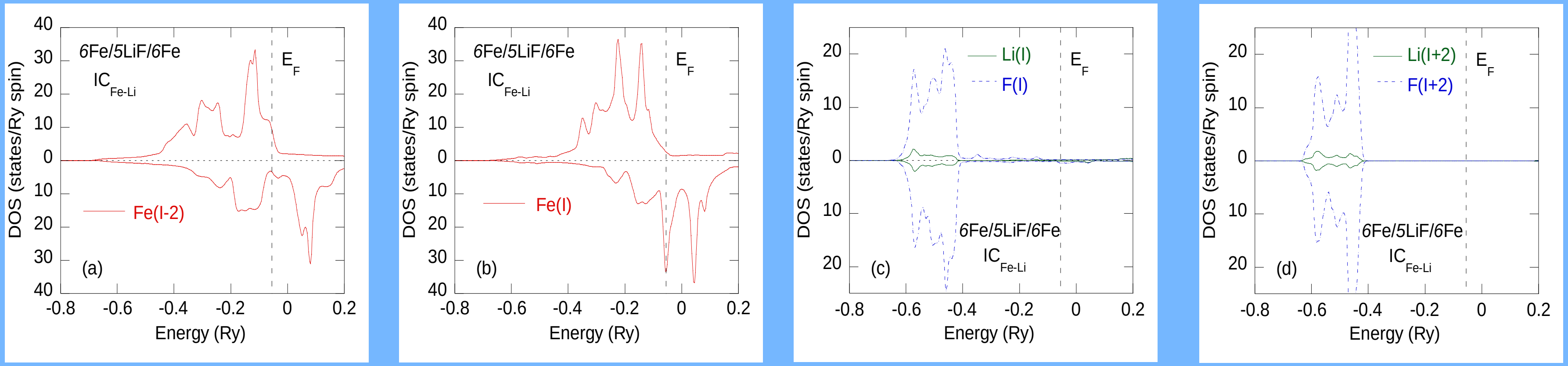
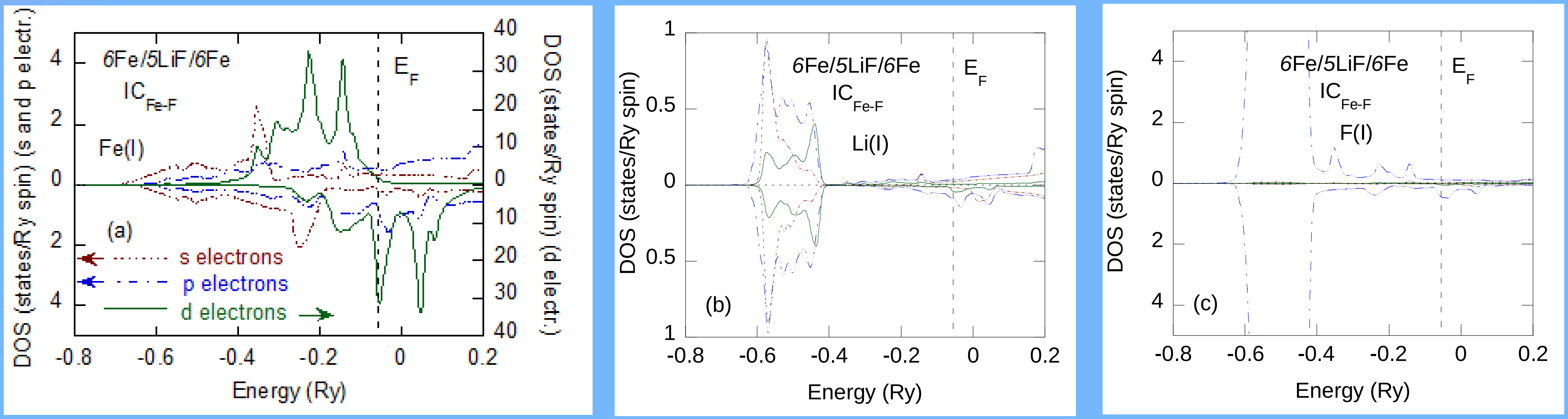
Fe/LiF (001) interfaces practically metallic

Departing from interface: isolating character recovered

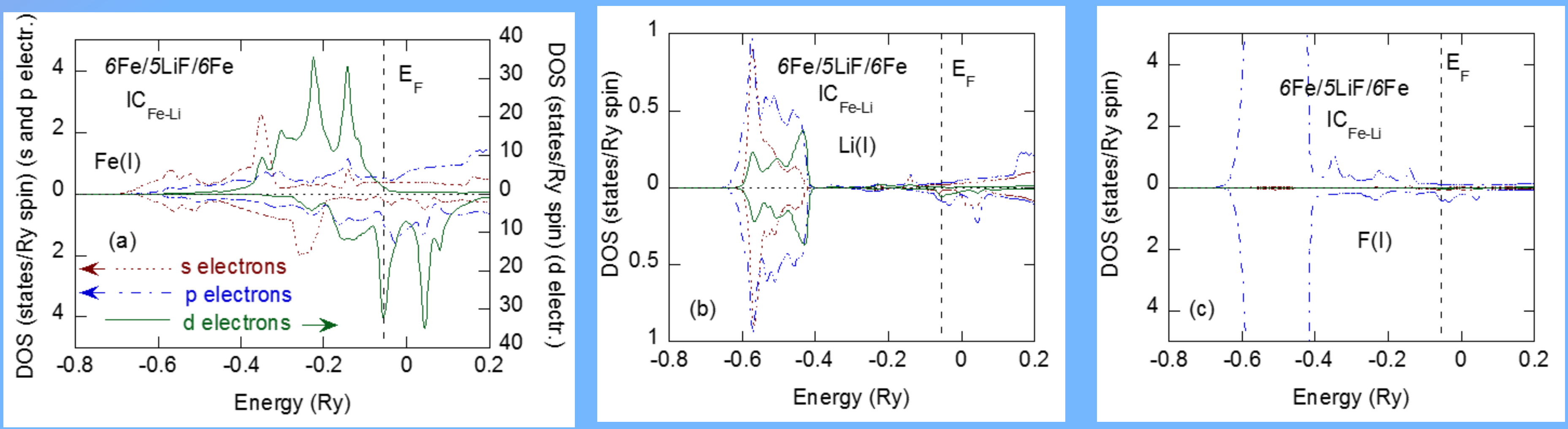


Atom and orbital resolved interfacial DOS at $IC_{Fe\text{-}F}$ and $IC_{Fe\text{-}Li}$ interfaces



MIGs:

- majority-spin state around E_F mainly due to s electrons of cationic sites and p electrons of anionic sites
- minority-spin state, more localized, peak around E_F largest contribution from p- and d-electrons



at interface

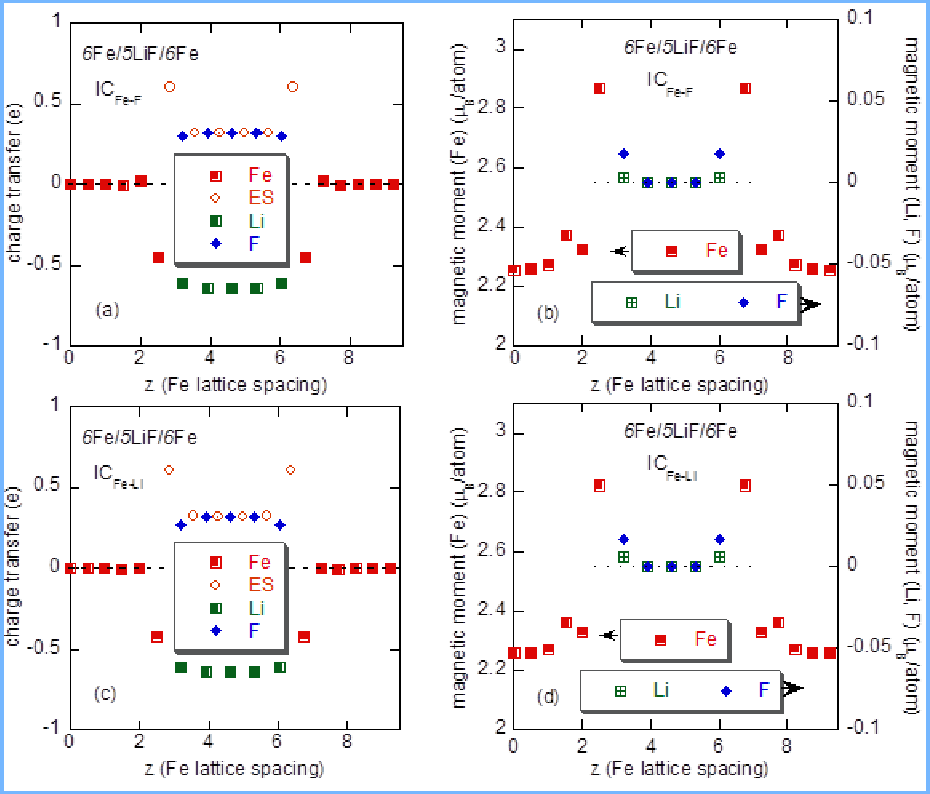
minority spin: predominantly: conduction band character for Li ions

valence band character for F ions

majority spin: valence band for both ions

Charge transfer and magnetization profiles

$IC_{Fe\text{-}F}$ and $IC_{Fe\text{-}Li}$ interfaces



Charge transfer

$IC_{Fe\text{-}F}$ Fe(I) – 0.46 e

$IC_{Fe\text{-}Li}$ Fe(I) – 0.41 e

difference: higher electronegativity of F

Charge modulation of interfacial Fe($IC_{Fe\text{-}F}$) atoms

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charge modulation in the interfacial iron layer

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stabilization of $IC_{Fe\text{-}F}$ interface

Barrier side

F ($IC_{Fe\text{-}F}$) decrease by 0.033 e from Δq(LiF) 0.325 e

F ($IC_{Fe\text{-}Li}$) decrease by 0.037 e from Δq(LiF) 0.315 e

Li ($IC_{Fe\text{-}F}$) increase by 0.02 e from -0.62 e

Li ($IC_{Fe\text{-}Li}$) increase by 0.03 e from -0.633 e

Magnetic moments

Interfacial iron moment: enhanced over bulk value

Fe ($IC_{Fe\text{-}F}$) $M_{Fe} = 2.85\ \mu_B$

Fe ($IC_{Fe\text{-}Li}$) $M_{Fe} = 2.81\ \mu_B$

Small positive polarizations induced on F and Li

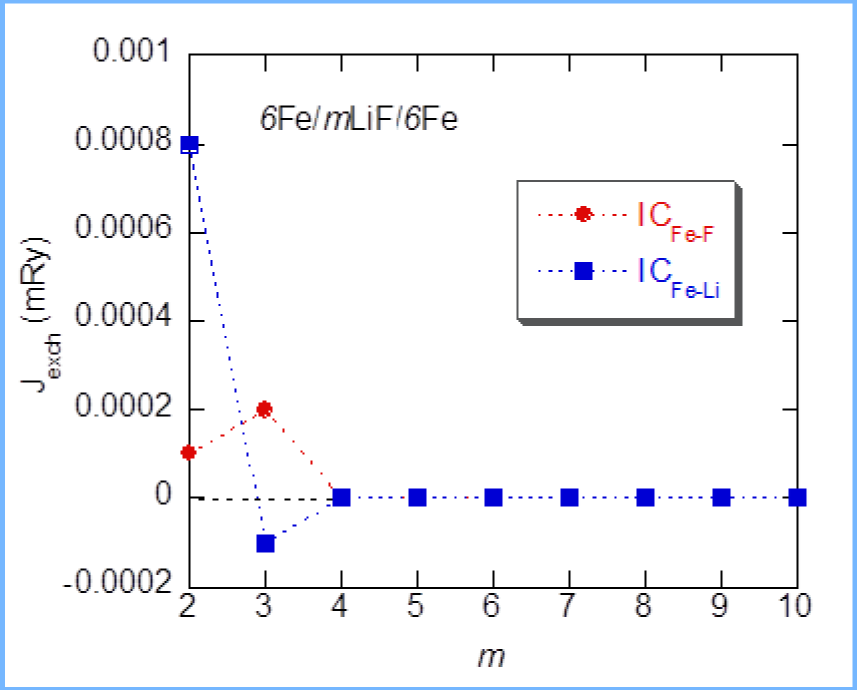
Li ($IC_{Fe\text{-}Li}$) $M_{Li} = 0.0075\ \mu_B$ } z = 3, 6

$M_F = 0.0185\ \mu_B$ } z = 3, 6

M_{Li}, $M_F = 0\ \mu_B$ $4 \leq z \leq 5$

4. Interlayer exchange coupling

$$J_{exch} = E_{tot}^{AFM} - E_{tot}^{FM}$$

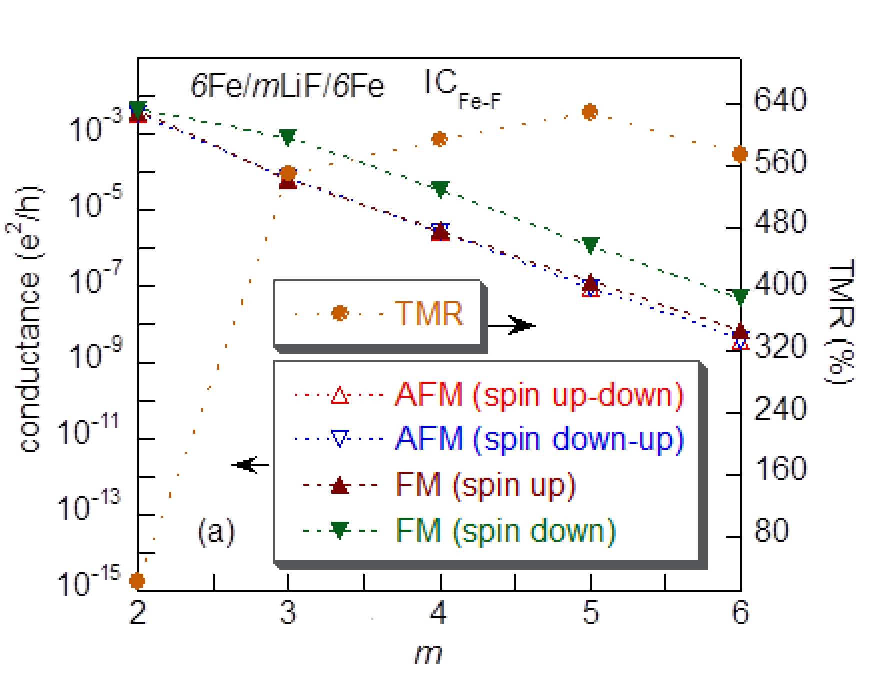


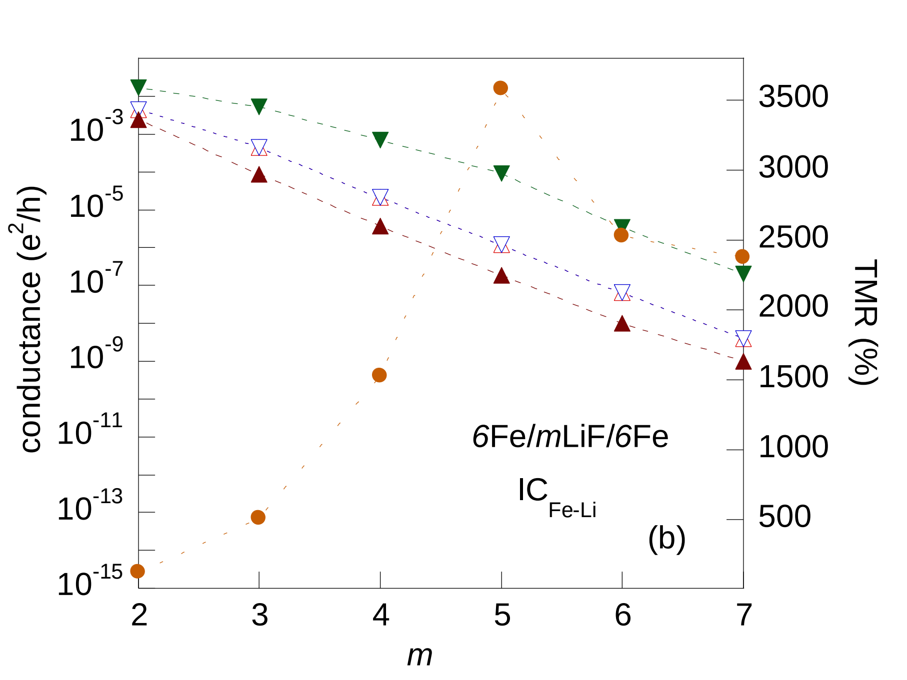
6Fe/mLiF/6Fe: no exchange coupling

6Fe/mLiBr/6Fe: small ferromagnetic coupling,decreasing exponentially with barrier thickness

5. Spin polarized electronic transport properties

6Fe/mLiF/6Fe heterostructure





IC_{Fe-F}, IC_{Fe-Li} interfacial configuration

Largest contributions: FM conductance with spin down electrons

IC_{Fe-F}, IC_{Fe-Li}; exponentially decay

Identical contributions: AFM conductances with spin-up and spin-down electrons

$IC_{Fe\text{-}F}$, $IC_{Fe\text{-}Li}$

Smallest contributions: FM conductance with spin-up electrons

$IC_{Fe\text{-}Li}$

All decrease exponentially with barrier thickness

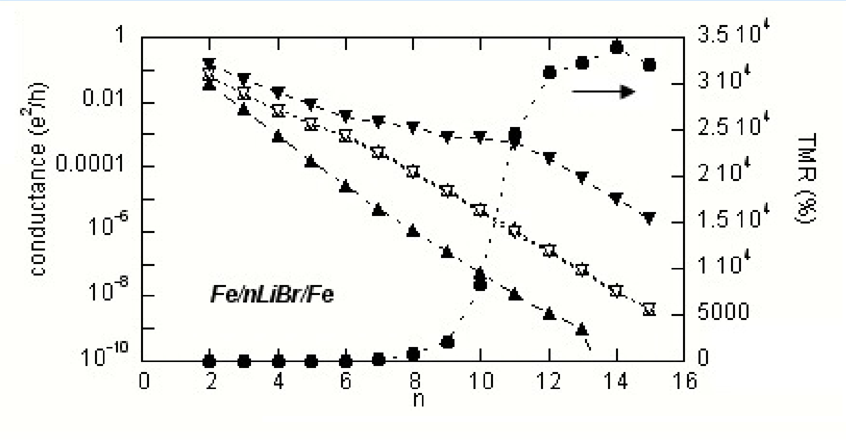
Tunneling magnetoresistance

$IC_{Fe\text{-}F}$: TMR increases with barrier thickness with change in slope at m = 3

$IC_{Fe\text{-}Li}$: TMR increases up to m = 5, followed by a decrease

TMR of 500 % predicted for $IC_{Fe\text{-}F}$ (most stable) interface

Fe/nLiBr/Fe heterostructure



Conductances:

largest contribution: FM with spin down electrons; decreases nearly exponentially with a change in slope at $n = 11$.

smallest contribution: FM with spin-up electrons

identical contributions: AFM with spin-up and spin-down electrons

High increase of TMR at $n = 11$

asymptotic region ($n > 11$) TMR $\cong 3.2 \cdot 10^4$

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

$\Downarrow$

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

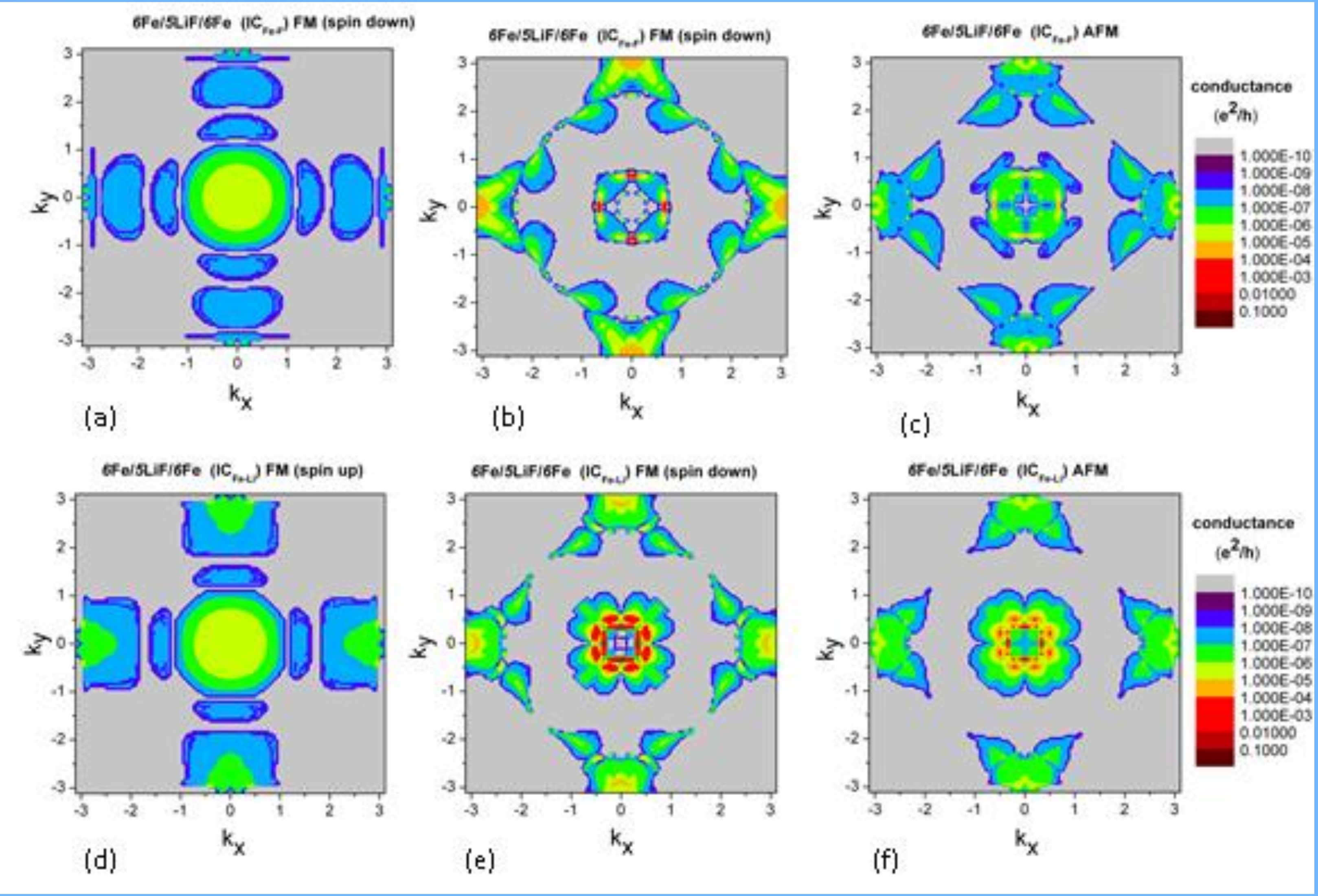
k_z along the transmission direction

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 LiF(LiBr) barrier: confirmed by exponentially decay of conductances

$k_{||}$ – partial resolved conductances of 6Fe/5LiF/6Fe ($IC_{Fe\text{-}F}$, $IC_{Fe\text{-}Li}$) Reciprocal vector $\pi/\sqrt{2}a_{Fe}$



Majority-spin FM conductances: free electron-like with broad peak and large transmission maximum at $\bar{\Gamma}$ point. Conductance determined by Δ_1 states.

At center of Brillouin zone

conduction band minimum of LiCl(LiBr) occurs at Γ_1 point, top valence band occurring at Γ_{15}

Bottom conduction band and top of valence band connected by purely imaginary band Δ_1 symmetry

$\Downarrow$

lower Δ_1 decay parameter

States with other symmetries decay much faster

$\Downarrow$

Δ_1 channel $\rightarrow$ only direct tunneling channel across LiF (LiBr) barriers.

Minority-spin FM and AFM conductances dominated by hot-spots or spike-like peaks around $\bar{\Gamma}$ point.

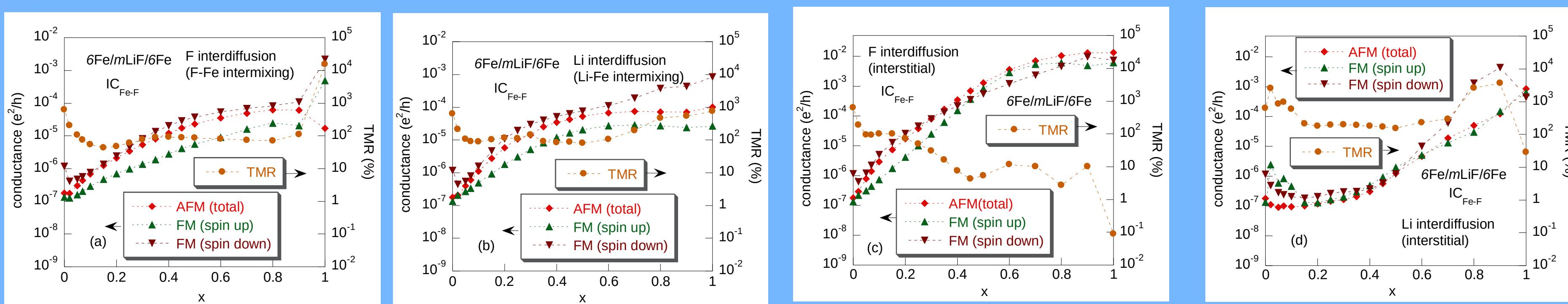
Spikes: originate from minority-spin interface resonant states; increase the transmission by resonant tunneling.

6. Interdiffusion at Fe/LiF/Fe interface

$IC_{F\text{-}Fe}$ interface

$Fe_2(Fe_1)_{1-x}F_x/F_{1-x}Fe_xLi$ interdiffusion

$Fe_2(Fe_1)_{1-x}Li_x/Li_{1-x}Fe_xF$ interdiffusion



F-Fe intermixing

FM, AFM conductances increase with x

TMR decrease up to x = 0.15; for x > 0.15 nearly constant

Li-Fe intermixing

FM (spin up), AFM increase up to x = 0.5; constant at x > 0.5

FM (spin down) increases with x

TMR decreases up to x = 0.15; x > 0.15 nearly constant

F interstitial

FM, AFM conductances increase

TMR decreases in irregular fashion

Li interstitial

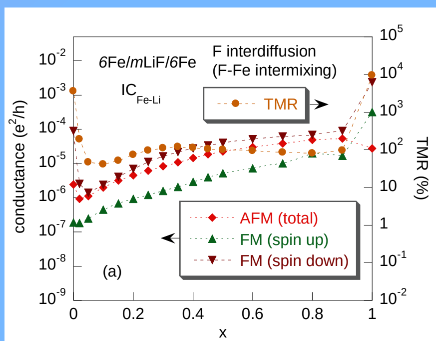
FM, AFM conductances decrease up to $x = 0.2$; $0.2 \le x \le 0.7$ nearly constant, $x > 0.7$ irregular variation

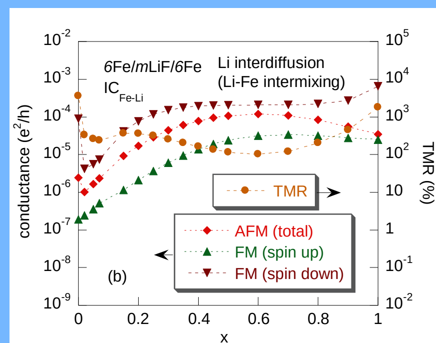
$IC_{Li\text{-}Fe}$ interface

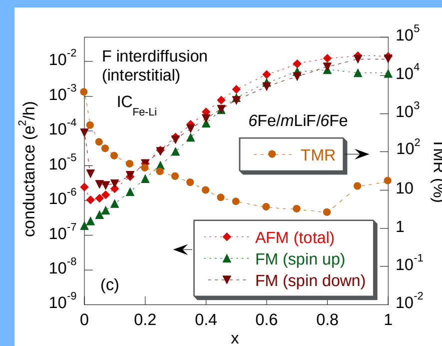
F-Fe or Li-Fe interdiffusion (intermixing, interstitial)

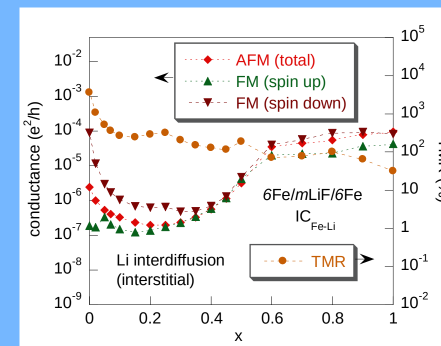
$Fe_2(Fe_1)_{1-x}Li_x/Li_{1-x}Fe_xF$

$Fe_2(Fe_1)_{1-x}F_x/F_{1-x}Fe_xLi$









F-Fe intermixing

FM conductances increase with x

AFM conductances, decrease up to x = 0.05 and then increase

TMR decreases up to x = 0.1 and then constant, TMR = 10^2

Fe-Li intermixing

FM and AFM conductances increase up to x = 0.3 and then nearly constant

TMR decreases for x < 0.1; x > 0.1 nearly constant

F interdiffusion (interstitial)

FM (spin-up) conductances increase with x

FM (spin-down, AFM total) conductances decrease up to x = 0.1, then increasing

TMR decreases gradually

Li interdiffusion (intestitial)

FM, AFM conductances decrease up to x = 0.2, increasing up to x = 0.6 and constant for x ≥ 0.6.

TMR decreases up to x = 0.15 and then is constant.

CONCLUSIONS

Most stable interfaces:

Fe/LiF (001) interfaces: Fe atoms located atop F ones.

Fe/LiBr (001) interfaces: Fe ones located above Li and Br sites.

Interfacial iron's magnetic moments enhanced over bulk value

Fe/LiF/Fe heterostructures: no exchange coupling.

Fe/LiBr/Fe heterostructure: small ferromagnetic coupling exponentially decreasing with barrier thickness.

TMR

Fe/LiF/Fe	rather small	$5 \cdot 10^2$ %
Fe/LiBr/Fe	high	$3.3 \cdot 10^4$ %

Spin dependent transport properties: resonant tunneling mechanism.

ACKNOWLEDGMENTS

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