Alternative Barrier Materials for Symmetry based Magnetic Tunnel Junctions

M. Chshiev, P. R. LeClair and W. H. Butler

MINT Center, The University of Alabama

Abstract

We show that magnetic tunnel junctions with alternative barrier materials to MgO may be used to obtain coherent spin-dependent tunneling and high tunneling magnetoresistance (TMR). Using the Vienna Ab-initio Simulation Code (VASP), we have calculated the wave function character of each band in an epitaxial Fe(100)|LiF(100) structure.

It is shown that:

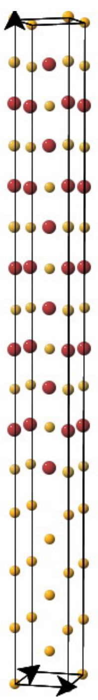
(a) wave functions in Fe near E_F of different symmetry decay differently in the LiF;

(b) wave functions of the wrong symmetry cannot propagate in Fe

LiF and the alkali halides in general also satisfy several experimental criteria

- nearly ideal insulating characteristics
- relatively simple crystal structure well-matched to important magnetic transition metals and alloys,
- bandgaps ranging from ~6eV (CsI) to ~14eV (LiF)
- lattice parameter varying from ~0.4 - 0.7nm
- single valence → phase stability
- strongly ionic → strong desire to form non-polar (100)-terminated surfaces
- extremely low chemical reactivity → good interfaces (?)

These properties combined with more detailed electronic structure considerations make them ideal insulators in spin-dependent tunneling devices.



LiF (11 layers)

Fe (7 layers)

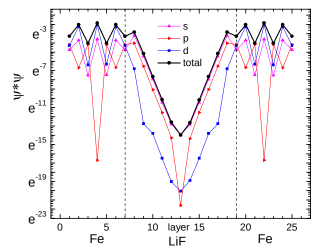
Properties of selected alkali halides and transition metals

	a (Å)	a/√2 (Å)	E_g(eV)	Str.
LiF	4.03	2.84	13.6	NaCl
LiCl	5.13	3.63	9.4	NaCl
LiBr	5.50	3.89	7.6	NaCl
NaF	4.63	3.28	11.6	NaCl
NaCl	5.64	3.99	8.5	NaCl
KF	5.34	3.78	10.7	NaCl
KCl	6.29	4.45	8.4	NaCl
MgO	4.13	2.92	7.9	NaCl
Fe	2.86	4.04	--	bcc
Co	2.83	4.00	--	bcc*
Al	4.04	5.71	--	fcc
Cr	2.88	4.07	--	fcc

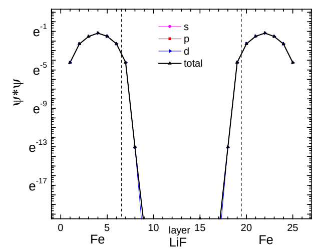
← Fe(100)|LiF(100) supercell used in calculations.

• We have evaluated the spd- and site projected wave function character of bands with different symmetries for parallel (Fe|LiF) and anti-parallel (Fe↑|Fe↓) spin configuration

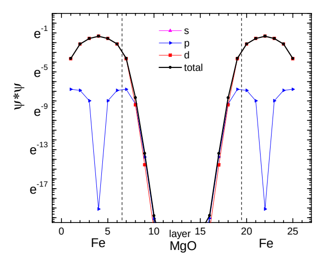
Fe (100) Bloch states of different symmetry decay at different rates in LiF.



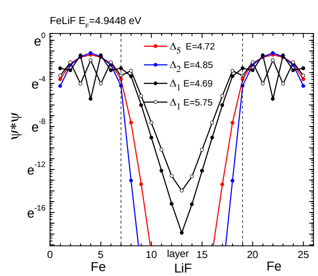
- This panel shows Δ_1 band for Fe(100)↑ |LiF(100)| Fe(100)↑.
- Note slow decay in LiF.



- Band with Δ_2 symmetry
- Note much faster decay than Δ_1
- Fe(100)↑ |LiF(100)| Fe(100)↑



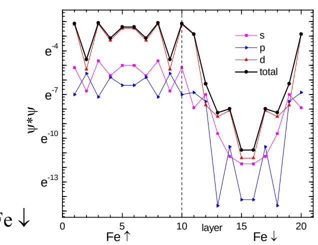
- Band with Δ_5 symmetry
- Decay rate is intermediate between Δ_1 and Δ_2.
- Fe(100) ↑ |LiF(100)| Fe(100) ↑



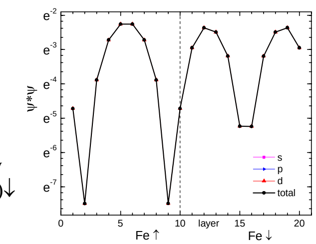
- Propagation of bands with Δ_1, Δ_2 and Δ_5 symmetry into LiF

Bloch states with "wrong" symmetry cannot propagate.

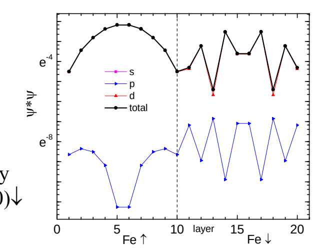
Δ_1 state cannot propagate at Fermi energy of minority Fe.



- Band with Δ_1 symmetry
- Fe10(100)↑ | Fe10(100)↓
- Note exponential decay in Fe ↓



- Band with Δ_2 symmetry
- Fe10(100)↑ | Fe10(100)↓



- Band with Δ_5 symmetry
- Fe10(100)↑ | Fe10(100)↓

Conclusion:

- Bloch states of certain symmetries are better able to propagate through the LiF.
- Bloch states with the wrong symmetry cannot propagate in a metallic electrode.