The structural, electronic and magnetic properties of Fe/LiF(LiBr)/Fe(001) magnetic tunnel junctions, MTJs, are theoretically studied by means of first principles Green’s function technique. LiF and LiBr alkali halides crystallize in a rock-salt type structure having lattice constants of 4.02 Å and 5.5 Å, respectively. Both compounds epitaxially fit bcc Fe structure. LiF and LiBr, are insulators with direct band gaps of 13.6 eV and 8 eV, respectively. The geometry of Fe(001)/nLiF(LiBr)/Fe(001) heterostructures is presented in Fig.1.

Total energy calculations evidenced that Fe/LiF(001) interfaces with Fe atoms located atop F ones and Fe/LiBr(001) interfaces with Fe atoms located above Li and Br sites are the most stable ones. The interfacial iron’s magnetic moments are of ≈ 3 μB, enhanced over the bulk value. No exchange coupling evidenced in case of Fe/nLiF/Fe heterostructure, case of Fe/nLiBr/Fe one, there is a small ferromagnetic coupling, decreasing exponentially with barrier thickness. The predicted tunneling magnetoresistance (TMR) of Fe/nLiBr/Fe MTJ, for n of 3·10^4 %, while this is only 4·10^2 % in Fe/nLiF/Fe Fig.2. Spin dependent transport properties of Fe/nLiBr/Fe MTJ are characterized by a resonant tunneling mechanism.

The effects of Li-F and Li-Fe interdiffusion studied in correlation with the evolution of tunneling magnetoresistance.

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