## High Tunnel Magnetoresistance of Fe/NaBr/Fe Magnetic Junction P. Vlaic<sup>a</sup> and E. Burzo<sup>b</sup>

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A first-principles study of electronic, magnetic and spin dependent transport properties of Fe/NaBr/Fe (001) magnetic tunnel junction (MTJ) is presented. The ground state electronic structure calculations are performed by means of a self-consistent Green's function technique for surface and interfaces implemented within tight-binding linear muffin-tin orbital (TB-LMTO) method in its atomic sphere approximation (ASA) and in conjunction with the coherent potential approximation (CPA) in order to describe the interdiffusion at Fe/NaBr interfaces. The spin dependent conductances are calculated by means of linear response of Kubo approach implemented within TB-LMTO-CPA formalism and including vertex corrections. The results evidence the formation of sharp Fe/NaBr interfaces and the enhancement of magnetic moments of interfacial iron atoms  $(m_{Fe} \approx 2.95 \,\mu_B)$ . A small antiferromagnetic coupling that rapidly decreases to zero with increasing barrier thickness is observed. The main contribution to the conductance in the ferromagnetic state is given by the minority spin electrons. The tunneling magnetoresistance (TMR) ratio rapidly increases with the barrier width and reach values as high as 4000 % in the asymptotic regime. Finally, a comparative study between Fe/MgO/Fe, Fe/NaCl/Fe and Fe/NaBr/Fe, respectively, MTJs is presented.

-13.4 cm -

Subject category :

4. Spin Electronics and Magneto-Transport

**Presentation mode :** poster

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 $9.7~\mathrm{cm}$