Spin Dependent Electronic Structure and Transport Properties of Fe/CaS/Fe (001) Heterostructure

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In this contribution an ab initio study of electronic, magnetic and spin dependent transport properties of Fe/CaS/Fe (001) magnetic tunnel junction (MTJ) is presented. The 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 the atomic sphere approximation (ASA). The spin dependent transport properties in the current-perpendicular-to-plane (CPP) geometry are studied by means of linear response of Kubo approach implemented within TB-LMTO formalism and including vertex corrections. A small charge transfer mainly localized at Fe/CaS interfaces and interface induced futures are reveled. The interface iron magnetic moments are enhanced (m_{Fe}=2.9 μ_B) and a small antiferromagnetic coupling that rapidly decreases to zero is evidenced. In the ferromagnetic configuration the majority spin conductance dominated by electronic states close to $\mathbf{k}_{||}$=0 decays faster than the minority spin one and almost at the same rate as both conductances in the antiferromagnetic configuration. Tunneling magnetoresistence (TMR) ratios up to 400 % are evidenced.

9.7 cm

13.4 cm

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