Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles theory of nonequilibrium vertex correction:disordered magnetic tunneling junction YOUQI KE, KE XIA, HONG GUO, McGill University, HONG GUO TEAM, KE XIA TEAM — The Keldysh Non-equilibrium Green's Function (NEGF) formalism has been developed Within DFT to calculate the electronic structure of disordered system at finite bias based on TB-LMTO+ASA combined with Coherent Potential Approximation. The conditionally averaged NEGF is evaluated by including the vertex correction. The disordered Fe/Va/Fe tunneling junctions are investigated with present first principle method, the vertex correction shows important role in both the electronic structure and transport calculations. The bias dependence of Tunneling Magnetoresistance (TMR) in the disordered Junctions and the disordered dependence of TMR at a finite Bias were illustrated.

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Date submitted: 15 Nov 2007 Electronic form version 1.4