

MAR05-2004-001681

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

**A Full-Potential Linearized Augmented Plane-Wave Method for Calculating Transport Properties:
Application to Fe/MgO/Fe Tunnel Junctions**

STEFAN BLUEGEL, IFF, Forschungszentrum Juelich, D-52425 Juelich, Germany

In order to calculate on the basis of the single particle picture as provided by the density-functional theory (DFT), the spin-dependent tunneling through barriers and interfaces of materials with increasing chemical and structural complexity, an extension of the full-potential linearized augmented plane-wave method (FLAPW) as realized in the FLEUR code is introduced. The volume in which the electrons scatter is sandwiched between two semi-infinite leads. The leads and the scattering volume are described by an embedding Green function formalism. Different scenarios of electron transport such as sequential and coherent tunneling is formulated and will be compared. Several applications will be presented. The method is used to understand the spin-polarized scanning tunneling microscope. For a three-layer heterosystem $\text{SrRuO}_3/\text{SrTiO}_3/\text{SrRuO}_3$, the effect of different orbital characters of the states at the Fermi level on the tunneling conductance was investigated. The main focus is on the Fe/MgO/Fe system for which we show that very small changes at the interface can have drastic effects on the conductance.