Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

What determines the sign of magnetoresistance in a molecular tunnel junction? SUBHASISH MANDAL, RANJIT PATI, Michigan Technological University — The recent observations of both positive and negative sign of tunneling magnetoresistance (TMR) in the same organic spin-valve structure has mystified researchers working in organic spintronics. In this article, we resolve this puzzle by exploring the role of interfacial metal-molecule coupling on TMR in a single molecular spin-valve junction. A planar organic molecule sandwiched between two nickel electrodes is used to build a prototypical spin-valve junction. A parameter-free, single particle Green's function approach in conjunction with a posteriori density functional theory involving a hybrid orbital dependent functional is used to calculate the spin-polarized current. The effect of external bias is explicitly included to investigate the spin-valve behavior. Our calculations show that only a 3% change in the interfacial distance at the metal-molecule junction can alter the sign of the TMR from a positive to a negative value.

Subhasish Mandal
Michigan Technological University

Date submitted: 20 Dec 2011 Electronic form version 1.4