Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Quantitative analysis of molecular spintronics ZHANYU NING, YU ZHU, JIAN WANG, HONG GUO, McGill University, HONG GUO TEAM, JIAN WANG TEAM — We report quantitative analysis of nonequilibrium spin injection from Ni contacts to octanethiol molecular spintronic system. Our calculation is based on carrying out density functional theory within the Keldysh nonequilibrium Green's function formalism. The first principles results allow us to establish a clear physical picture on how spins are injected from the Ni contacts through the Ni-molecule linkage to the molecule, why tunnel magneto-resistance is rapidly reduced by the applied bias in an asymmetric manner, and to what extent *ab initio* transport theory can make quantitative comparisons to the corresponding experimental data. We found that extremely careful sampling of the two-dimensional Brillouin zone of Ni surface is crucial for accurate results.

Zhanyu Ning
McGill University

Date submitted: 15 Nov 2007 Electronic form version 1.4