Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Half-Metallic Sandwich Molecular Wires with Negative Differential Resistance and Sign-Reversible High Spin-filter Efficiency LU WANG, XIN YAN, JING ZHOU, JING LU, ZHENGXIANG GAO, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, XINGFA GAO, SHIGERU NAGASE, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki 444-8585, Japan, STEFANO SANVITO, School of Physics and CRANND, Trinity College, Dublin 2, Ireland, YUTAKA MAEDA, Department of Chemistry, Tokyo Gakugei University, Tokyo 184-8501, Japan, TAKESHI AKASAKA, Center for Tsukuba Advanced Research Alliance, University of Tsukuba, Ibaraki 305-8577, Japan, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266 — Using density functional theory and non-equilibrium Green's function method, we construct organometallic nanowires that consist of Fe or V atoms sandwiched between composite molecules (Cp^*FeCp^*, where Cp^* is $C_5(CH_3)_5$). For the first time, we demonstrate that half-metallicity, negative differential resistance, and sign-reversible high spin-filter capability can coexist remarkably in one organometallic nanowire ($FeCp^*$ wire). This renders $FeCp^*$ wire promising in electronics and spintronics.

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Date submitted: 21 Nov 2010 Electronic form version 1.4