

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Charge and spin transport in porphyrin-based molecular junctions**<sup>1</sup> ZHENFEI LIU, Molecular Foundry, Lawrence Berkeley National Lab, SUJUN WEI, Department of Chemistry, Columbia University, OLGUN ADAK, Department of Applied Physics and Applied Mathematics, Columbia University, HONGSIK YOON, Department of Chemistry, Yonsei University, Korea, LUIS M. CAMPOS, Department of Chemistry, Columbia University, WOO-DONG JANG, Department of Chemistry, Yonsei University, Korea, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University, JEFFREY B. NEATON, Molecular Foundry and Materials Sciences Division, Lawrence Berkeley National Lab, and Department of Physics, UC-Berkeley — We study weak-bias charge and spin transport behavior of four metal-porphyrin molecules in molecular junctions, using a combination of break-junction experiments and a self-energy corrected first-principles approach based on density functional theory. Some of the molecules are open-shell, and they are of potential interest to spin filtering and solar energy conversion. Optimally-tuned range-separated hybrid functionals are used in combination with a correction for static polarization effects to yield accurate level alignment between Fermi level and dominating conducting orbital energies in the junction. We find that the conductance can change by up to a factor of two when different metal cations are used. Our calculations of low-bias conductance generate similar trends and are in quantitative agreement with experimental measurements. Implications for spin transport are discussed.

<sup>1</sup>This work is supported by DOE and computational resources are provided by NERSC.

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Date submitted: 13 Nov 2013

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