

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Spin states and their relaxation in transition-metallorganic self-assembled molecules**<sup>1</sup> ZHI-GANG YU, SRI International, 333 Ravenswood Avenue, Menlo Park, CA 94025 — The coexistence of spins localized on transition-metal ions and mobile charges on the  $\pi$ -conjugated ligands in transition-metallorganic self-assembled molecules (TMSAMs) makes these molecules attractive for molecular spintronic devices and quantum computing. We present our theoretical results on the spin states localized on the transition-metal ion in a TMSAM using both the first-principles approaches and the ligand-field theory. Then we construct a spin Hamiltonian to calculate spin lifetimes and identify the dominant spin relaxation mechanisms in the molecule. We also discuss the relation between the spin states on the transition-metal ion and the charge transport along the  $\pi$ -conjugated ligand in the molecule.

<sup>1</sup>This work was supported by the Office of Basic Energy Sciences, Department of Energy.

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Date submitted: 20 Nov 2006

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