Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Molecular quantum-dot cellular automata–from molecular structure to circuit dynamics YUHUI LU, CRAIG LENT, Univ. of Notre Dame — Quantum-dot cellular automata (QCA) [1] provides a transistor-less paradigm for molecular electronics. In the QCA approach, binary information is stored in the charge configuration of single cells, and transferred via Coulomb coupling between neighboring cells. Single-molecule QCA cells can be realized by using as quantum dots the localized states of mixed-valence complexes. Several candidate QCA molecules have been synthesized and shown to have the required field-induced switching properties [2]. We report progress towards a hierarchic dynamic theory of QCA circuits. We use *ab initio* techniques to calculate the relevant molecular electronic structure, and extract parameters for a simpler Hamiltonian to describe switching behavior. We then apply a coherence vector formalism to model interaction with the thermal environment and generate a circuit-dynamic description. [1] C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, Nanotechnology, vol. 4, pp. 49, 1993. [2] H. Qi, S. Sharma, Z. Li, G. L. Snider, A. O. Orlov, C. S. Lent, and T. P. Fehlner, J.Am.Chem.Soc., vol. 125, pp. 15250, 2003.

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Date submitted: 27 Nov 2007 Electronic form version 1.4