Modeling Electronic Detection of Molecular Switching

Grant Morgan and Craig S. Lent*
Department of Electrical Engineering, University of Notre Dame
Notre Dame, IN, *e-mail: lent@nd.edu

Quantum dot cellular automata (QCA) devices, store binary information encoded in the arrangement of charge among several quantum dots.[1] In molecular QCA, nonbonding orbitals in a mixed-valence molecule act as quantum dots. Different charge configurations represent a "1" or "0" bit, or a "null" state containing no information. [2] Electron through-bond tunneling allows the molecule to switch charge configurations in response to the local electric field. Intermolecular Coulomb interaction provides the device-to-device coupling which enables computation.

Appropriate mixed valence molecules have been synthesized and shown to have the bi-stable switching response to an applied field which is required for QCA devices. [3] Room temperature operation has been demonstrated both in molecular systems and in QCA cells composed of dots formed by silicon dangling bonds.[4,5] Several challenges in making QCA circuits at the molecular level are being investigated. One important issue is the measurement the charge-state switching of molecular-scale devices. Scanning probe measurements of individual molecules have been able to detect switching, [6] but for device application integrated electronic detection is an important criterion.

In prototype metal-dot QCA devices, electrometers comprised of single-electron transistors (SET) have been shown to be able to measure the motion of as little as 2% of an electronic charge.[7] Small changes in the electrostatic potential of the SET gate, caused by the motion of nearby charge, can be reliably measured through the tunneling current. Efforts are underway to adapt this approach to the single-molecule scale.

Here we construct a finite element electrostatic model to investigate the question of how small the gate of an SET electrometer needs to be in order to detect intermolecular charge transfer. Charge transfer in the molecular system is modeled simply as single-electron hopping between two dots. The effect of the grounded substrate is included, as is the detailed shape and geometry of the electrometer gate. The full capacitance matrix and voltage shifts are calculated from first principles.

ACKNOWLEDGEMENT

This research is supported by the National Science Foundation under NSF CHE-1124762 and by the Nanoelectronics Research Initiative.

REFERENCES

[1] C.S. Lent and P.D. Tougaw, A device architecture for computing with quantum dots, *Proc. of the IEEE* 85, 541 (1997).

[2] A.O. Orlov, I. Amlani, G.H. Bernstein, C.S. Lent, and G.L. Snider, Realization of a functional cell for quantum-dot cellular automata, *Science*, 277, 928 (1997).

[3] H. Qi, S. Sharma, Z. Li, G.L. Snider, A.O. Orlov, C.S. Lent, and T.P. Fehlner, Molecular quantum cellular automata cells. Electric field driven switching of a silicon surface bound array of vertically oriented two-dot molecular quantum cellular automata, *J. Am. Chem. Soc.*125, 15250 (2003).

[4] H. Qi, A. Gupta, B.C. Noll, G. L. Snider, Y. Lu, C.S. Lent, and T.P. Fehlner, Dependence of field switched ordered arrays of dinuclear mixed-valence complexes on the distance between the redox centers and the size of the counterions, *J. Am. Chem. Soc.*127, 15218 (2005).

[5] M.B. Haider, J.L. Pitters, G.A. DiLabio, L. Livadaru L, Mutus J.Y., R.A. Wolkow, Controlled coupling and occupation of silicon atomic quantum dots at room temperature, *Phys. Rev. Lett.* 102, 046805 (2009).

[6] Y. Lu, R. Quardokus , C.S. Lent, F. Justaud, C. Lapinte, A. Kandel, Charge localization in isolated mixed-valence complexes: An STM and theoretical study, *J. Am. Chem. Soc*. 132, 13519 (2010).

[7] I. Amlani, A.O. Orlov, G.L. Snider, C.S. Lent, and G.H. Bernstein, External charge state detection of a double-dot system, *Appl. Phys. Lett.*, 71, 1730 (1997).

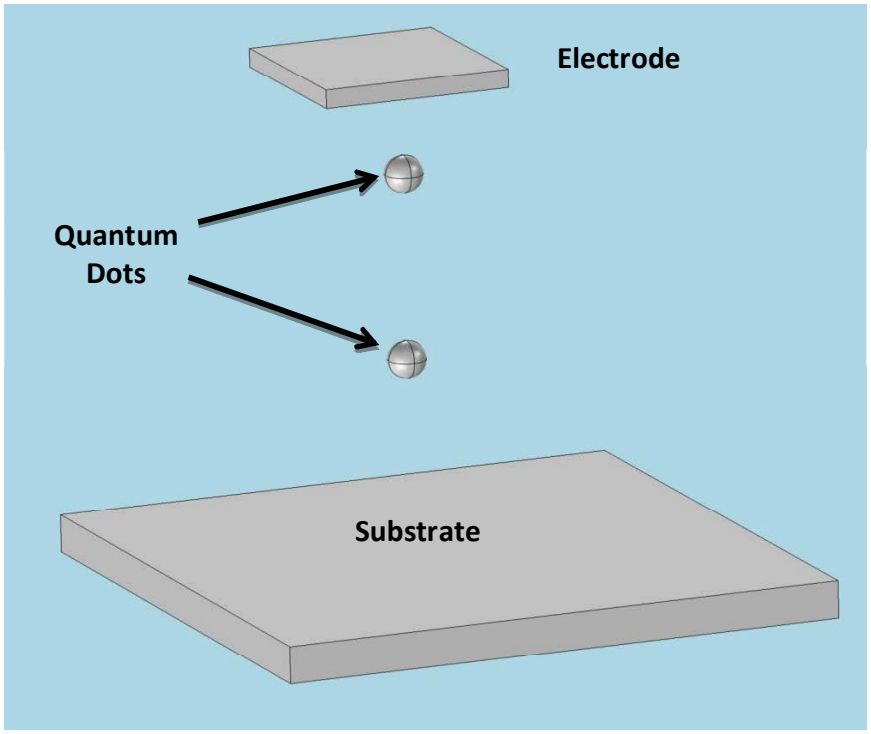

Figure 1: Basic construction of model for electronic detection of molecular switching. A charge arrangement is specified for the quantum dots, and surface charge on the electrode surface is detected.

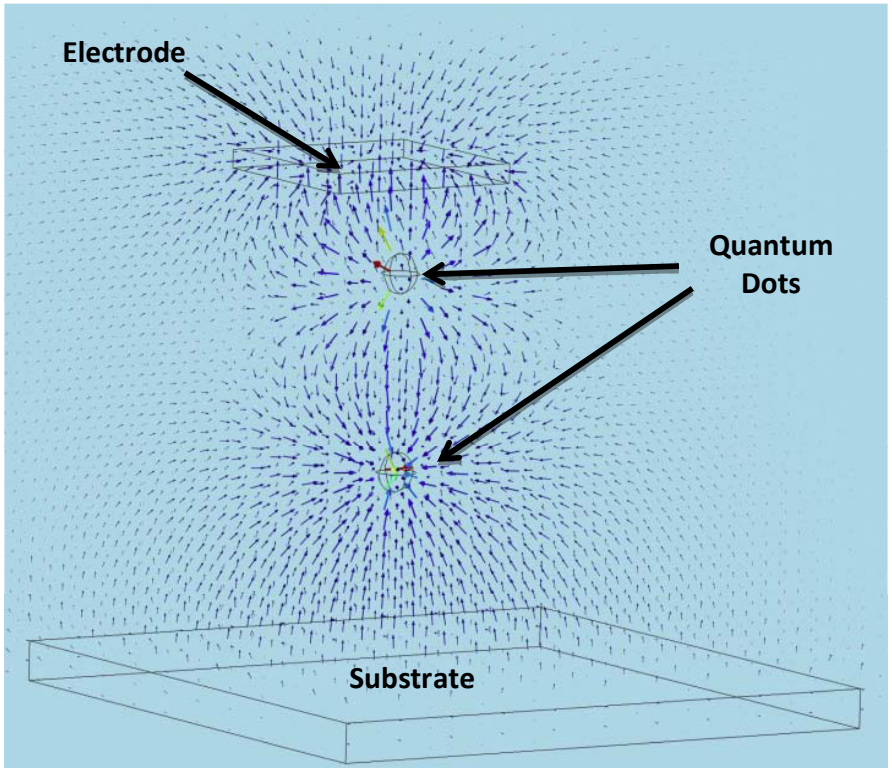

Figure 2: Electric field lines due to the charges in the model.