NANO HIGHLIGHT

Field-effect switching of molecular charge for quantum-dot cellular automata

NSF Grant NSF CCF04-03760
PIs: Craig S. Lent, Thomas P. Fehlner, S.A. Kandel,
Gregory L. Snider, Marya Lieberman,
University of Notre Dame, Notre Dame, IN

Molecular quantum-dot cellular automata (QCA) is an approach to electronic computing at the single-molecule level which encodes binary information using the molecular charge configuration. This approach differs fundamentally from efforts to reproduce conventional transistors and wires using molecules. A QCA molecular cell has multiple redox centers which act as quantum dots. The arrangement of mobile charge among these dots represents the bit. The interaction from one molecule to the next is through the Coulomb coupling—no charge flows from cell to cell. Prototype single-electron QCA devices have been built using small metal dots and tunnel junctions. Logic gates and shift registers have been demonstrated in this system, though at cryogenic temperatures. Molecular QCA, by contrast could work at room temperature. By using molecules, not as current switches—but as structured charge containers, the QCA paradigm may offer a solution to fundamental problems of excess heat dissipation in computation.

Symmetric mixed valence QCA double-dot molecules, *trans*-[$(H_2NCH_2CH_2C''N)(dppe)_2Ru(C''C)_6$ $Ru(dppe)_2(N''CCH_2CH_2NH_2)$] 2 $[PF_6]_2$, **2**$[PF_6]_2$, have been synthesized and characterized spectroscopically, electrochemically, and with a solid-state single-crystal structure determination. The molecules are functionalized for binding to a silicon substrate. Measurement of the ac capacitance of the film as a function of voltage across the film demonstrates controlled electric field generation of the two stable mixed-valence forms differing in the spatial location of one electron, *i.e.*, switching between the two QCA-active states.

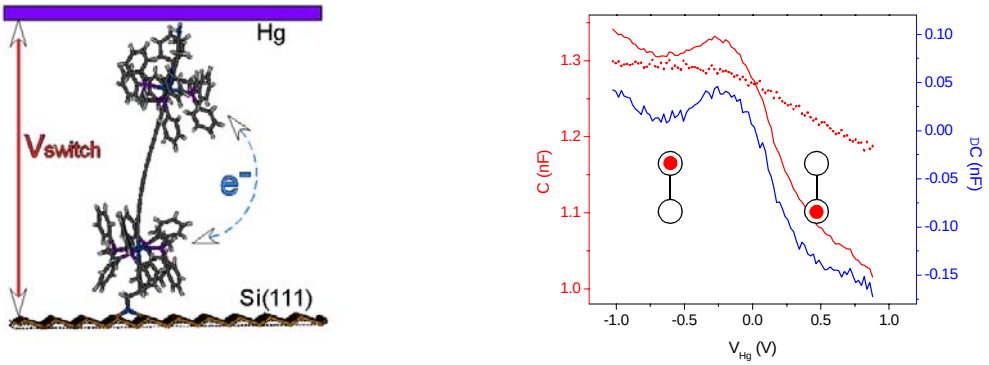

Figure. Capacitance measurements show single electron switching of QCA-active molecules. The measurement is the solid red line, the dotted red line is the control (unoxidized sample) and the blue line is the difference. The electron residing in the top or bottom dots represents a binary 1 or 0.

Reference: Qi, H.; Gupta, A; Noll, B.C.; Snider, G.L.; Lu, Y.; Lent, C.S.; Fehlner, T.P., accepted for publication in J. Am. Chem. Soc.