Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

Design and Simulation of Single-Electron Molecular Devices

By

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This work presents a study of molecular single-electron devices that may be used as the basic building blocks in high-density resistive memories and hybrid CMOS/nanoelectronic integrated circuits. It was focused on the design and simulation of a molecular two-terminal nonvolatile resistive switch based on a system of two linear, parallel, electrostatically-coupled molecules: one implementing a single-electron transistor and another serving as a single-electron trap. To verify the design, a theoretical analysis of this “memristive” device has been carried out, based on a combination of *ab-initio* calculations of the electronic structures of the molecules, Bardeen's approximation for the rate of tunneling due to wavefunction overlap between source/drain electrodes and the molecular device, and the general theory of single-electron tunneling in systems with discrete energy spectra. The results show that such molecular assemblies, with a length below 10 nm and a footprint area of about 5 nm^2, may combine sub-second switching times with multi-year retention times and high ($> 10^3$) ON/OFF current ratios, at room temperature. Moreover, Monte Carlo simulations of self-assembled monolayers (SAM) based on such molecular assemblies have shown that such monolayers may also be used as resistive switches, with comparable characteristics and, in addition, be highly tolerant to defects and stray offset charges. An important and unexpected finding in this work was that the simulated *I-V* curves in a few molecular junctions may exhibit negative differential resistance (NDR) with the origin so fundamental, that the effect should be observed in most molecular junctions where the sequential single-electron transfer limit is valid. Another important by-product of this work was a more complete understanding of some shortcomings of the existing density functional theory software packages, including their advanced versions such as ASIC SIESTA.

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