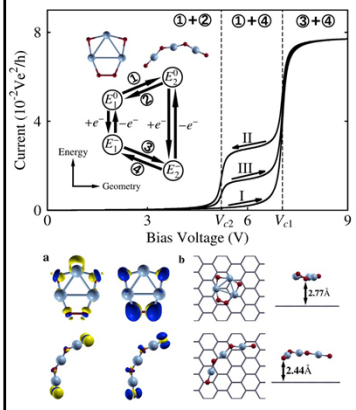
Conformational Electroresistance and Hysteresis in Nanoclusters



Top: I-V curves and hysteresis for a Zn_3O_4 nanocluster. Conformation dependent charging and discharging processes are labeled by circled numbers. Bottom: Stable geometries for the neutral (top row) and charged (bottom row) states without (a) and with (b) substrates.

Work was performed at University of Florida and the Center for Nanophase Materials Sciences, Materials Sciences and Engineering Division

Scientific Achievement

Coulomb blockade voltage and electroresistance of small molecules and nanoclusters is predicted to be sensitive to their geometric shapes and to cause large electroresistance and strong hysteresis.

Significance and Impact

Conformational dependence of the Coulomb charging energy exists in a broad spectrum of nanoclusters and small molecules, where electroresistance may offer a new mechanism for designing nanoscale applications.

Research Details

- Electron charging energy for Zn_3O_4 nanocluster is calculated from first principles as a function of geometric shape
- Charging and discharging currents and induced shape change are simulated by a transport model
- Large electroresistance and hysteresis found
- Substrates found to enhance the effect

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Narrative Highlight Text:
The existence of multiple thermodynamically stable isomer states is one of the most fundamental properties of small clusters. This work shows that the conformational dependence of the Coulomb charging energy of a nanocluster leads to a giant electroresistance, where charging induced conformational distortion changes the blockade voltage. The intricate interplay between charging and conformation change is demonstrated in a Zn_3O_4 nanocluster by combining a first-principles calculation with a temperature-dependent transport model. The predicted hysteretic Coulomb blockade staircase in the current–voltage curve adds another dimension to the rich phenomena of tunneling electroresistance. The new mechanism provides a better controlled and repeatable platform to study conformational electroresistance.

Reference

"Conformational Electroresistance and Hysteresis in Nanoclusters"
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