Electroresistance in nanoclusters through conformational changes

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A considerable number of experiments have observed the tunnelling electroresistance (TER) effects in various junctions and several theories have also been proposed to explain it. Here, we introduce a new process that are responsible for the large TER effect in nanoscale systems through investigating the charging energy of neutral and charged systems. First-principles calculations demonstrate that some nanoscale systems will undergo conformational change upon charging or discharging, which creates a large quantum capacitance difference between neutral and charged states. In the nano-size quantum dots junctions, one can exploit TER through Coulomb blockade effect by modulating the bias voltage and reversing the electric field direction. Detailed analysis on small cluster Zn_3O_4 shows a 25% in quantum capacitance difference between neutral and charged states, which can be further enhanced to 65% by placing the cluster above a dielectric surface, opening up new avenues for novel nanoscale materials design.