Negative Differential Resistance at SAM of Oligo (Phenylen Ethynylene) on Au (111) Surface

Hyungjun Kim¹, Seung Soon Jang² and William A. Goddard III¹

¹Materials and Process Simulation Center (MC 139-74)
California Institute of Technology, Pasadena, CA 91125

²School of Materials Science and Engineering
Georgia Institute of Technology, Atlanta, GA 30332-0245

Recently, negative differential resistance (NDR), which is one of the most peculiar phenomena occurred in nanoelectronic devices, has been frequently reported studied. Especially, Professor Richard Kiehl’s group observed a well-defined NDR characteristic from the metal–oligo (phenylene ethylene) –metal junction. Although many theoreticians and experimentalists has studied the NDR phenomena of oligo (phenylene ethylene) SAM system, two important features observed in the Kiehl’s experiments—a dependency of amplitude of NDR on sweeping rate and an existence of hysteresis loop—are not clearly explained. We propose an electric field induced conformational change mechanism, which understands NDR characteristics as a phase transition of two states, a planar conformation state and a twisted conformation state induced by voltage gradient between two electrodes. We investigated the energetics of those two possible conformations using QM and FF calculations. Furthermore, a Lattice Monte Carlo simulation based on the results of QM and FF calculations successfully regenerates main features experimentally observed.