Abstract

Organic materials have gained enormous popularity as electronics device component. The rising demand of organic materials is mainly because of certain advantages like flexibility, low cost and ease of operation as compared to inorganic materials. In the following research work design and electrical characterization of single organic molecule-based device has been emphasized. For the said purpose 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) molecule was used as active molecule between two electrodes in a two terminal device structure. Bidirectional multiple negative differential resistance (BM-NDR) was observed from a single DDQ molecule at room temperature when the device was studied by using density functional theory (DFT) in association with non-equilibrium Green's function (NEGF). The BM-NDR effect was also verified experimentally by studying the scanning tunneling spectra (STS) of single DDQ molecule. The carrier transport in the device occurs mainly through the transmission channel corresponding to the highest occupied molecular orbital (HOMO) of the molecule and a commensurate change in the magnitude of transmission peak was observed at the peak and valley voltages. The reason for the NDR is proposed to be due to the two competing factors involved namely, the reduction of the molecule and the interface resistance between the molecule and the electrodes. The involvement of both the factors is validated from the molecular projected self-consistent Hamiltonian (MPSH) and the local device density of states (LDDOS) of the device at the corresponding peak and valley voltages.

The super-molecular structure of DDQ molecule in the form of self-assembled monolayer (SAM) has been studied with the help of scanning tunneling microscope (STM) as well. The following study suggests conversion of analog signal into digital signal at atomic scale where individual molecule act as a flip-flop unit and entire SAM act as an electronic counter. These DDQ molecules reduce the size of the counter by two orders. The output of the counter was obtained by tracking the translational motion of a group of molecules which are oscillating about the average value concerning the applied bias. Sixteen new spatial locations are obtained corresponding to sixteen distinct analog inputs (bias voltage) to the flip-flops. The translational motion of the molecules in the self-assembled system was correlated with the conformational change of the molecule. So, unconventional conversion of an analog signal to ultra-digital (UD) signal is possible by using an n-bit counter consisting of as many numbers of flip-flops and thus can become a system for the conversion of A/UD signal.

The rectifiers and memory storage devices are very essential components of electronics from the point of view of digital information processing and storage. With numerous configurations of rectifiers nearly all complex Boolean functions can be expressed. A Polydentate Schiff's base ligand has been synthesized and characterized for the first time at molecular level with the help of STM. The ligand molecule shows both rectification as well as memory switching behavior when it is characterized with tungsten tip. The proposed conduction and switching mechanism for both rectification as well as memory switching is because of the formation and breakdown of coordination bonds between tungsten tip and ligand molecule and change in the conformation of ligand molecule under bias conditions. The ligand has duo of three sets of lone pairs on each oxygen and nitrogen atoms. Because of high electronegativity of both oxygen and nitrogen atoms the ligand acquires partial negative charge while the charge on tungsten atom can be adjusted by means of external biasing. From electrical characterization of single molecule, it has been observed at positive biasing on tip that metal-ligand complex forms dative bonds for a finite biasing value and thus breaking the coordination bond at zero biasing and even in negative biasing. Change in the conformation of molecule at positive bias leads to switching behavior. So, a single metal-ligand complex can perform dual operations of rectification as well as memory switching.

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