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Electrode and substitutional effects on electronic transport properties of NiO nano devices

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ABSTRACT

The effect of electrodes plays a vital role in the construction of nano electronic devices. Two different electrodes are constructed with gold and platinum atoms and are attached with NiO nano wire in order to study the effect of electronic transport properties. In addition, in the NiO device N and Fe atoms are substituted and their electronic transport properties are also studied. From the observed results it is evident that the gold electrode NiO nano devices show better performance than that of the platinum electrode connected NiO nano device. The transmission and PDOS spectra show that in the gold electrode NiO devices N doped NiO nano device gives better performance than the other two. In the case of platinum connected NiO nano devices, Fe doped NiO nano device gives better performance than the other two.

Keywords: NiO nano device; electrode effect; doping effect; transmission spectrum.

INTRODUCTION

Metal oxide semiconductor nanostructures have recently attracted by many researchers since they have high potential applications in the field of nano electronics. In particular, they will be very useful for constructing molecular devices since they possess combined properties of metal oxide and the nano structured materials. One of the important aspects in the design of molecular devices is the selection of the electrode materials[1]. In general, in the design of a molecular device, it is necessary to elucidate the role of each part of a molecular device[2]. For a nano electronic device, linker atom, a functional group acts as a glue which connects the electrode and the device molecule. It also modify the electronic structure of the device and thereby the electronic transport property of the device[3,4]. Similarly many reports are available in the literature regarding the structural and transport properties of the device molecule[5-7]. However, very few reports are available which regards the importance of electrode in a molecular device[2,8]. This present study aims to describe the effect of different electrodes in a NiO molecular wire device. Two different electrode materials have been chosen for constructing the electrodes namely, Au and Pt. In addition to this, the effect of substitutional atom on the molecular device is also studied by one anioic and cationic substitution. The computational studies have been performed with the help of density functional analysis combined with non equilibrium green's function method(NEGF). Since this blended analysis(DFT+NEGF) reproduced the results almost equal to the experimental results[9], they have chosen for the present calculations. The effect of electrode materials are studied in terms of electron transmission, density of states(DOS) and V-I characteristics of the molecular device.

MATERIALS AND METHODS

COMPUTATIONAL DETAILS

The calculations are performed using pseudopotentials and numerical atomic orbitals (NAO) basis sets as implemented in SIESTA[10] package. Initially, the electrodes and the device molecule geometry are optimized individually, and thereby the total device structures are optimized by conjugate gradient(CG) technique. The generalized gradient approximation by Perdew-Burke-Ernzerhof(PBE)[11] is used for the exchange and

correlational functional. For expanding the wavefunction, triple zeta triple polarized(TZTP) basis function is used in this calculations for the better explanation of the surface states of Au,Pt and Ni atoms in the device. Brillouin zone sampling is done using Monkhorst-Pack scheme with $1 \times 1 \times 50$ mesh. The transport properties are studied using non-equilibrium green's function(NEGF) method combined with the DFT code implemented in the TranSIESTA[12], which is part of SIESTA package. The current through the device can be calculated using Landauer-Buttiker formula[13]

$$I(V_b) = G_0 \int_{\mu_R}^{\mu_L} T(E,V_b)dE \qquad \text{-----(1)}$$

where $G_0 = 2e^2/h$ is quantum conductance and $T(E,V_b)$ is the transmission probability under the bias voltage V_b. The transmission energy and the device density of states are calculated using TBTRANS[14], a post processing utility available in SIESTA package.

RESULTS AND DISCUSSION

The structures of the designed nano devices with different electrodes and substitutional atoms in the scattering region are shown in figures 1 and 2. For transport calculations, the electrode region is selected depends upon the material. For the gold and platinum electrode NiO nano devices, 36 atoms are taken into account on the both sides of the electrode by the corresponding Au and Pt atoms. The scattering region consists of NiO nanowire and the substitutional atoms of Fe and N, for the pristine and substitutional NiO nanowires respectively. In the case of Au and Pt electrode nano devices, the scattering region is connected to the electrode by means of sulphur atoms as a linker atom since the linker(sulphur) atom has high affinity with the gold, platinum and the NiO nano wire. The linker atom also modify the electronic structure of the device molecule and hence the transport properties also. The NiO nano device is designed along the (0 0 1) plane and the device scattering length is 10 Å. The Au and Pt electrodes are designed along (1 1 1) plane for better performance. The V-I characteristics are studied by varying the bias voltage from 0V to 1V in terms of 0.2V.

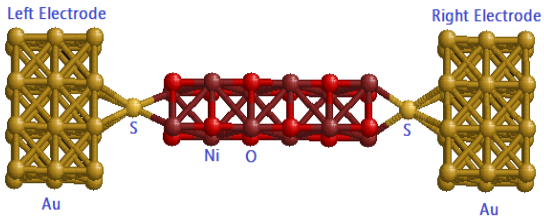

Fig 1(a) NiO nano device attached with golden electrodes

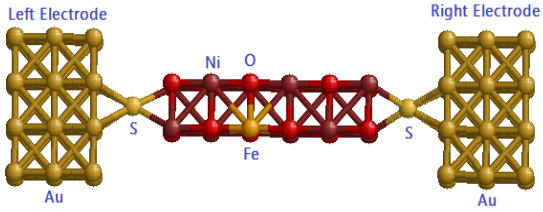

Fig 1(b) Fe doped NiO nano device attached with golden electrodes

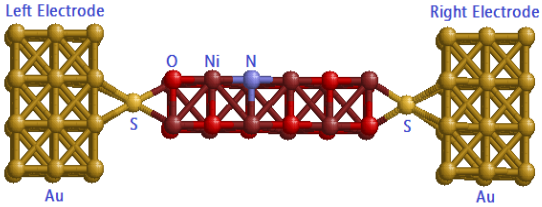

Fig 1(c) N doped NiO nano device attached with golden electrodes

Fig. 1 NiO nano devices with gold electrodes

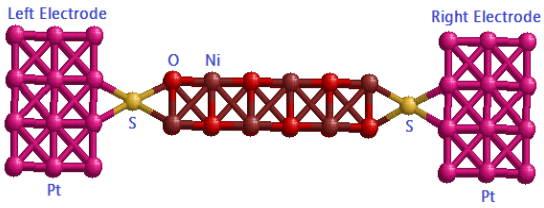

Fig 2(a) NiO nano device with platinum electrodes

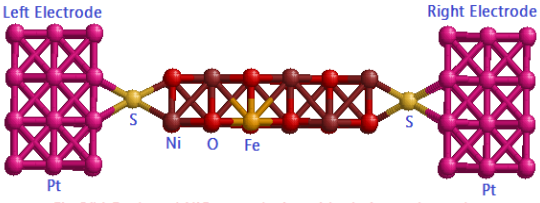

Fig 2(b) Fe doped NiO nano device with platinum electrodes

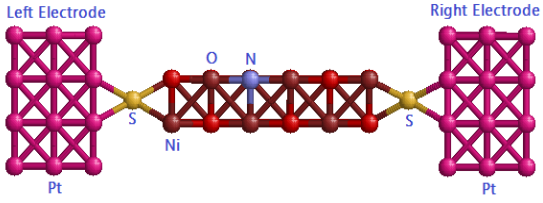

Fig 2(c) N doped NiO nano device with platinum electrodes

Fig. 2 NiO nano devices with platinum electrodes

Zero bias transport properties of NiO nanowire

Zero bias transmission and density of state spectra of the NiO nano device with Au and Pt electrodes are shown in Fig 3 and Fig 4.

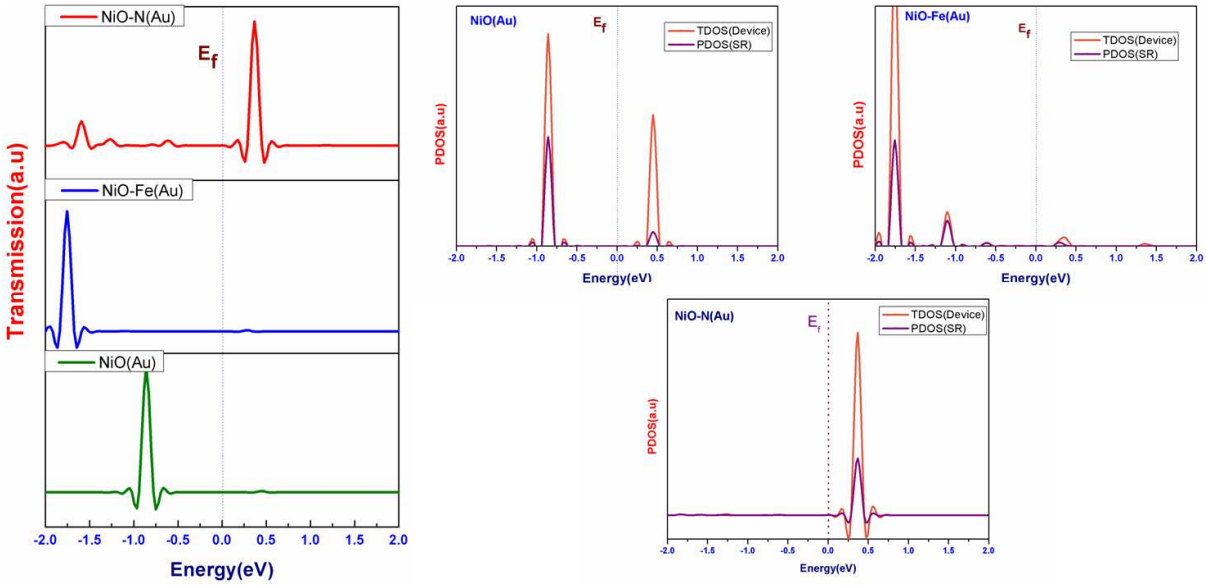

Fig.3 Zero bias transmission and PDOS spectra of NiO nano device with gold electrode

From the figure 3 it is seen that the transmission at zero bias for gold electrode connected NiO nano device, a strong transmission peak below the Fermi level is observed. The corresponding PDOS spectrum confirms this and this is majorly due to the electrode gold atoms. However, a strong peak below the Fermi level also contributed by a considerable amount in the PDOS due to the device region. Under the zero bias, the electrode and the device region combined effect makes the chemical potential across the device. For Fe doped NiO nano device, at zero bias, a strong peak is observed below the Fermi level which correspondingly due to the electrode gold atoms and the device scattering region. However a strong peak above the Fermi level in the corresponding PDOS shows the incorporation of the Fe atom in the device since Fe atom creates more states in the HOMO(below Fermi level) side. Similarly, in the case of the N doped NiO nano device, the transmission curve shows a strong peak above the Fermi level which

is due to the incorporation of N atom in the device. This is confirmed by the corresponding PDOS spectra of the device. The N incorporation creates more states in LUMO side of the NiO device and makes the chemical potential even there is no applied bias.

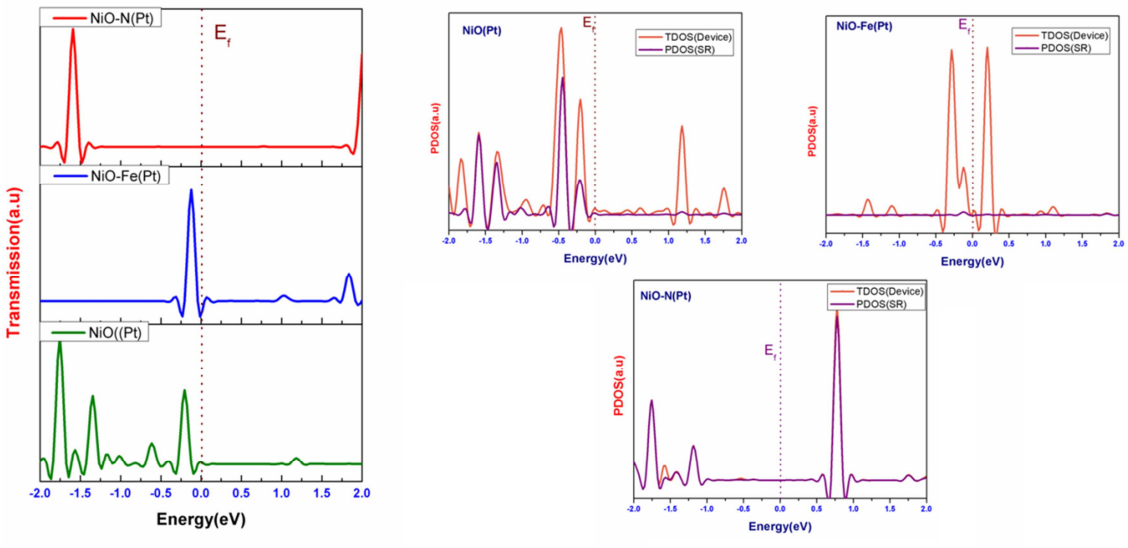

Fig.4 Zero bias transmission and PDOS spectra of NiO nano device with platinum electrode

The platinum electrode attached NiO nano device zero bias transmission and PDOS spectra are shown in figure 4. For the NiO device, the transmission spectrum shows many peaks in the valance band (below Fermi level) side. The corresponding PDOS spectrum shows the combined density of states is produced by the electrode and the device. However, some quasi bound states are produced in the conduction band side(above Fermi level), which are due to the gold electrode atoms. A strong transmission peak is observed for Fe doped NiO nano device indicates easy flow of charge carriers enabled at zero bias. The corresponding PDOS spectrum of the Fe doped NiO nano device shows that electrode plays a vital role in this transmission. In the case of N doped NiO nano device, strong peaks are observed on both sides of the Fermi level indicates smooth transmission is enabled. In the corresponding PDOS many number of bound states are formed which is mainly influenced by device region rather than the electrode region that are observed in other two devices.

Transport properties of NiO nanowire with Au and Pt electrodes

The transport properties of the NiO nano devices with Fe and N dopants attached with gold and platinum electrodes are studied by varying the applied bias voltage between 0V to 1V. Figure 5 shows the transmission and PDOS spectrum of the NiO nano devices attached with gold electrodes.

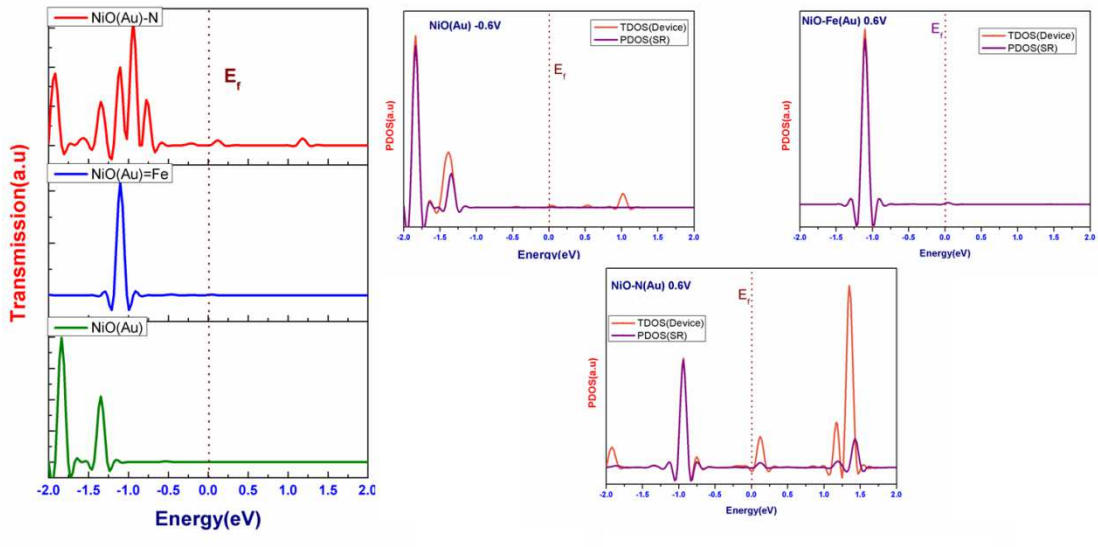

Fig. 5. Transmission and PDOS spectra of NiO nano device with gold electrodes at 0.6V

From the figure it is seen that for the NiO device at bias voltage 0.6, strong transmission peaks are observed below the Fermi level. This indicates possibility of small current through the device. The corresponding PDOS spectrum shows same trend which denotes more states are formed due to the device and electrode atoms. Near the Fermi level a small hump shows the easy flow of the current through the device. In the case of Fe doped NiO nano device attached with the gold electrodes, show a strong transmission peak below the Fermi level which is shifted towards the Fermi level compared to the NiO nano device. This indicates the incorporation of the Fe atom in the device. N doped NiO nano device shows more number of peaks below the Fermi level enables the current flow through the device. A small hump is identified above the Fermi level indicates the incorporation of the nitrogen in the device. The PDOS spectrum of the N doped NiO nano device shows high number of density of states on both sides of the Fermi level. However, it is identified that below the Fermi level, the device region and the electrode generates high number of states due to Ni and Au atoms. Above the Fermi level, the states are formed due to only the electrode Au atoms. From this, it is clear that the gold electrode attached with Fe doped NiO nano device will give a clear transmission and enable the current flow since it has near Fermi level density of states. Which indicates a strong coupling between the electrode and the molecular device is established at higher bias voltages.

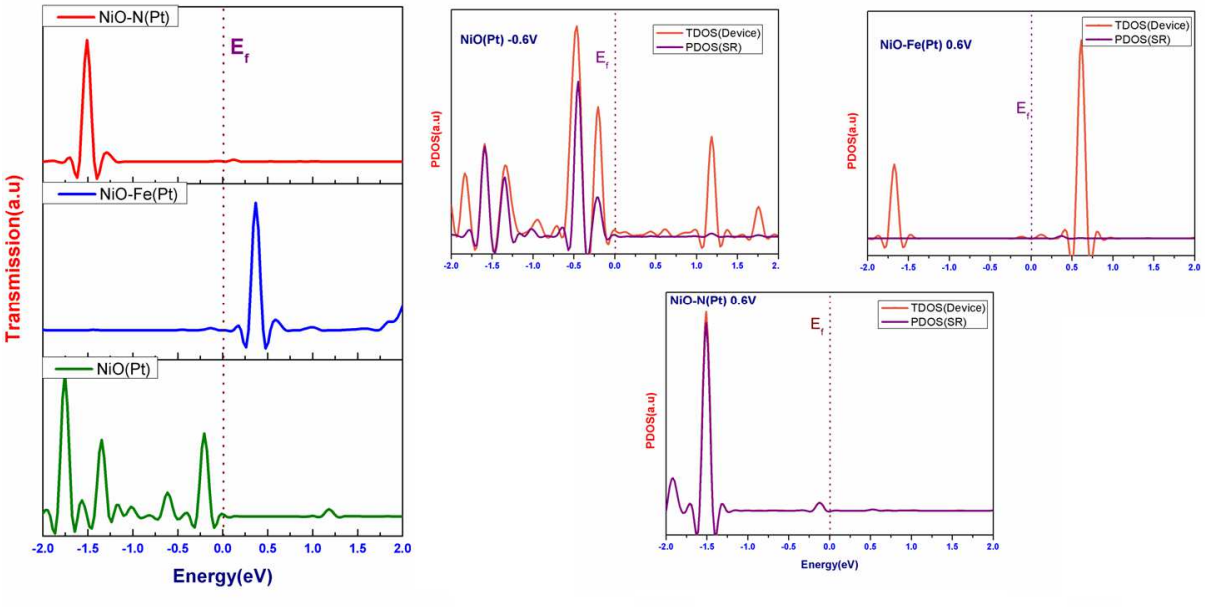

Fig. 6. Transmission and PDOS spectra of NiO nano device with platinum electrodes at 0.6V

Transmission and PDOS spectra of NiO nano devices with platinum electrodes are shown in the Figure 6 for the bias voltage 0.6V. For the NiO nano device, the transmission spectrum shows many peaks below and near the Fermi level. The corresponding PDOS spectra reveal that the transmission peaks corresponding to the device and electrode Ni and Pt atoms. A small peak is observed above the Fermi level is due to the electrode Pt atoms. The Fe doped NiO nano device transmission spectrum shows a sharp peak above the Fermi level and enables the transmission on that energy level. From the PDOS spectrum of the Fe doped NiO nano device, two peaks are observed on both sides of the Fermi level are due to the electrode Pt atoms at this bias voltage. Only small amount of contribution is due to the device atoms in this device. In the case of N doped NiO nano device, strong peak below the Fermi level indicates a good coupling between the electrode and the device is established in this energy level. The PDOS spectrum shows the same trend and indicates that these states are formed due to both electrode and device atoms. Near the Fermi level a small peak is observed which enables the current flow through the device. From the above it is observed that compared to NiO nano device and N doped NiO nano device, Fe doped NiO nano device is having better transmission since it exhibits a strong peak the near Fermi level when attached with the Pt electrode.

V-I characteristics of NiO nano devices

V-I characteristics of NiO nano devices with gold and platinum electrodes are studied by the two probe system. The V-I characteristics of the devices with different electrodes are shown in Figure 7 and figure 8. From the V-I characteristics spectrum in figure 7, it is shown that the current value increases with increase in bias voltage for NiO nano device with gold electrodes. However, there is no appreciable increase in the current when Fe doped with NiO nano device. In the case of N doped NiO nano device with gold electrodes, the current increases drastically when the bias voltage increases above 0.7 V. This is confirmed with its corresponding transmission and PDOS spectrum. The order of the current for the NiO nano devices with gold electrodes is in the order of 10^{-10} amperes. In the case of platinum electrode attached a NiO nano device which is shown in the figure 8, NiO and N doped NiO nano devices

did not show any appreciable variation in the current. They simply resemble ohmic behaviour when the bias voltage is increased. In the case of Fe doped NiO nano device the current drastically increased when the bias voltage is increased above 0.6V. This indicates that this device has more preferable than the other two NiO devices attached with the platinum electrode. The current along the NiO nano devices is in the order of 10^{-12} amperes with the platinum electrodes.

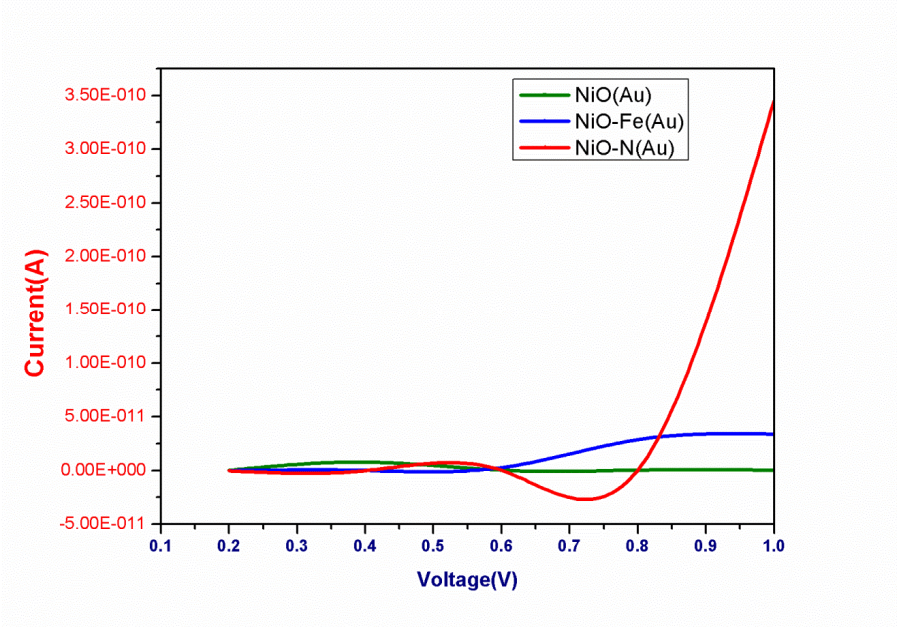

Fig. 8. V-I characteristics of NiO nano device with golden electrodes

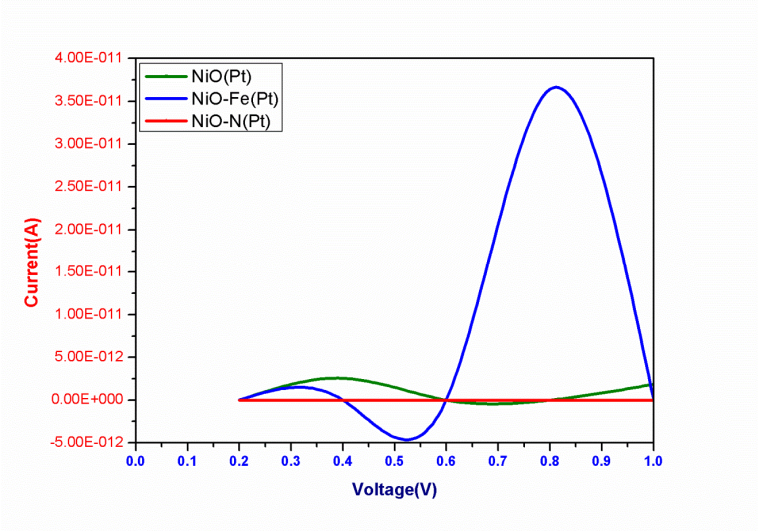

Fig. 9. V-I characteristics of NiO nano device with platinum electrodes

CONCLUSION

NiO nano wire devices are constructed with gold and platinum electrodes. The effect of the electrodes in the transport properties has been studied. Apart from the pristine NiO nano device, Fe and N atoms are substituted in the device and their effects are also studied. From the obtained results, gold electrode devices are having better performance than the platinum electrode devices. The transmission and PDOS spectra of the gold electrode NiO nano devices shows that N doped NiO nano device is performed well than the other two NiO nano devices with gold electrodes. In the case of platinum electrode NiO nano devices, the Fe doped NiO nano device shows better performance than the other two devices. The V-I characteristics of the NiO nano devices with gold atoms give the current in the order of 10^{-10} amperes whereas the platinum NiO nano devices show the current in the order of 10^{-12} amperes. Overall the golden electrode NiO nano devices show better performance than that of platinum electrode NiO nano device.

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