

# Electrically Doped Nanoscale Devices: A Comprehensive Survey

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## ABSTRACT

Doping is the key feature in semiconductor device fabrication. Many strategies have been discovered for controlling doping in the area of semiconductor physics during the past few decades. Electrical doping is a promising strategy that is used for effective tuning of the charge populations, electronic properties, and transmission properties. This doping process reduces the risk of high temperature, contamination of foreign particles. Significant experimental and theoretical efforts are demonstrated to study the characteristics of electrical doping during the past few decades. In this article, we first briefly review the historical roadmap of electrical doping. Secondly, we will discuss electrical doping at the molecular level.

**Keywords:** Electrical-doping, DFT, NEGF, First principle, Molecular-modeling

## I. INTRODUCTION

Doping plays a crucial role in determining physical characteristics and their applications of various organic or inorganic materials, especially for semiconductors. This method has been successfully proved for the semiconductor physics industry. A small amount of addition of impurities determines the dopant concentration and electrical conductivities of the materials. It is observed that a good dopant should exhibit an ideal solubility in its host material, and it also exhibits a low defect level. However, some basic problems are related to this type of conventional doping process, for example, doping bottleneck which powerfully affects the device performance. This type of performance degradation has been observed severely for wide bandgap materials. For example, in the case of the minimum of high conduction band device, n-type doping is challenging, whereas for a maximum of the low valence band device is also complicated [1,2]. Therefore, some problems arise for the bipolar doping process in wide band semiconductors. It is observed that either p-type or n-type dopants can be inserted but not together [3]. Therefore, to compensate for this type of problem, a feasible solution has been incorporated into the domain of doping. This type of proposed approach is known as electrical doping, which does not depend on this type of bipolar doping.

On the other hand, it was almost impossible to obtain a p-type GaN semiconductor due to combinations of high n-type background concentration and low p-type doping activity. This problem can be significantly overcome using the electrical doping phenomenon by Rudaz in the year of 1998. During the late 1980s, scientists discovered the importance of growing GaN or AlN buffer layers to demonstrate GaN-based LED at low temperatures. Post-growth thermal annealing process helps to activate the growth of p-type dopants in GaN buffer layers. These advancements accelerated the growth in device development of the III-V nitride semiconductor material system for wide-band optoelectronic devices [4]. GaN substrate and post-growth thermal annealing process also play an important role in this technique [5-7]. This led us to the evolution of nanotechnology, such as

- Various types of radiation may damage the large buildup of positive ions and electrons [8-12].
- The radiation of ultraviolet (UV), vacuum ultraviolet (VUV) ray may also damage nanoscale devices.
- X-ray photons may also cause rupture of nanoscale devices during plasma etching problem [13-21].
- Due to the large buildup due to voltage generation distortion ion trajectories, it also leads to fracture of the gate oxide films.
- In addition to these, UV or VUV photons radiating from the low-density plasma etching technique lead to generate crystal defects.

## **HISTORICAL ROADMAP OF ELECTRICAL DOPING**

Although this study mostly concentrates on electrical doping at the molecular level, it is important to first review the early history of conventional doping. In the year of 1930, it was noticed that the conductivity of semi-conductors was affected due to the presence of a little number of impurities [21,22,23]. In the year 1931, the first quantum-mechanical formalism was used for semiconducting materials. The  $n$ -junction was successfully demonstrated by Davydov in the year of 1938. transistor in the year of 1949. This invention changes the geometry of the semiconductor industry. Though the invention of bipolar junction made a tsunami to the evolution in the semiconductor industry, it had several problems too related to transistors. This is one of the procedures to avoid the ionic bombardment process in the atomic-scale device designing approach. Gao and Kahn have demonstrated this process onto the molecular thin films. These compounds for example poly-carbonate polymer with tris(4-bromophenyl) aminium hexachloroantimonate (TBAHA) 4,4',4''-tris(3-methylphenylphenylamino)-triphenylamine (m-MTDATA) hole transport layer doped with F4-TCNQ are used to successfully fabricate various OLEDs compound device layer. This process has also been used in organic photovoltaic cell (OPVC). This process has also been used for tuning at the molecular level and also for improving the device efficiency enhancement by carrier injection. Molecular film conductivity increases to a large extent for  $n$ - and  $p$ -type doping by using this process. This doping process is extensively used for ohmic contacts on inorganic semiconductors.

## **ELECTRICAL DOPING AT THE MOLECULAR LEVEL**

Recently researchers are interested for controlled doping procedure. Therefore, this electrical doping procedure helps to introduce controlled doping for inorganic semiconductors. Thus, it is also helpful to tune electrical properties of these semiconductors by introducing electrical doping. This doping phenomenon helps to tune optical gap of semiconductors with their chemical variation. This doping procedure is also a low-cost process and useful for flexible substrates.

The electrical doping procedure is the method by which a potential difference has been created between the two ends of the nano device. In this theoretical work we have arranged this by providing different polarity but same-valued voltage at the two ends of the nano device via two-probe electrodes. The schematic diagram for this theoretical process is shown in This theoretical approach is involved to create highly doped positive ( $p^+$ ) and negative ( $n^+$ ) regions, which are important to design an organic semiconductor devices for both Organic and inorganic materials.

Using this procedure charge carrier are to be injected into them molecular interfaces. Electrical doping is a controlled process for organic molecules rather than inorganic thin films. Therefore, conventional  $p$  and  $n$  dopants are not mandatory for insertion. Eventually, electrical doping increases carrier injection and decreases drive voltage which leads to a rise in device efficacy. Thus, electrical doping method solely depends on the injection of either electronic transmission or electron reception to the host molecule.

The hetero junction chain is made with adenine and thymine biomolecules used to sense several gases when the chain passed through the nano pore of a GaAs nano sheet. In that case, also the electrical doping is induced at the two parts of this nano sheet. Due to the effective inductance, this biomolecular chain shows its ability to sense the adsorbed foreign gas molecules. In the case of nano device design is also dealt with adsorption of molecules. For example, adsorption of volatile molecules at 32 °C temperature into ZnO nano wire is investigated Using DFT and NEGF formalisms-based first-principle approach, nano-FET can be designed using various structural modifications. Various properties of these.

### **Molecular Level Research Works Based on Electrical Doping**

Electrical doping at molecular level plays an important role in nano electronics. Researchers are highly interested to introduce this doping procedure at nanoscale device designing procedure. The effect of this doping helps to interface between different molecular level of alignment. This process is not only helpful to study organic hetero-junction molecular level but also acceptable for inorganic materials. This doping helps for the interface formation with the help of dipole and equivalent move in comparative position of molecular interface. Thus, this process of electrical doping is acceptable for molecular interface alignment.

Miniaturization of conventional electronic devices is the most emerging research area nowadays. There are several approaches which lead to motivate researchers to investigate and study the nature of nanoscale devices. One of the most important approaches is to design and simulate analytical nanostructures. Many significant devices can be designed using this simulation procedure and analyze the obtained results. According to the result, the researchers can modify the various simulation parameters as well as the different aspects of the nano scale analytical model. Among these

simulation methods, the first-principle approach is the most effective and popular process. Modernization of electronic devices encourages researchers to innovate conventional devices in a modified version.

## II. CONCLUSION

This report illustrates briefly a comparison between conventional doping and electrical doping process. Therefore, electrical doping is to be implemented in many molecular modeling approaches to bring a new era in nano electronics. This study takes a close look at the electrical doping phenomenon such as why it is important, how it works for the molecular modeling approach, calculation of electrical doping concentration, etc. Hence, we provide a comparative study between electrical doping and conventional doping process for a molecule. To conclude it is emphasized that in future this is one of the approaches which will prove itself in the field of nano device modeling.

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