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Enhancing Optical and Electrical Properties of Layered Transition Metal-Doped Semiconductors

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Abstract: This study delves into the enhancement of optical and electrical properties in layered transition metal- doped semiconductors, examining the transformative effects of doping on their performance. Transition metal doping leads to notable improvements in band gap modification, luminescence, conductivity, and charge carrier concentration, crucial for applications in optoelectronics and renewable energy technologies. The research investigates hole transport in MEH-PPV and P3HT diodes through various diode configurations, revealing the significant impact of non-zero Schottky barriers. J-V characteristics measured at different temperatures and thicknesses were compared with theoretical models, validating both conventional and modified theories. These findings underscore the potential of transition metal- doped semiconductors for advanced technological applications and highlight the importance of optimizing both optical and electrical properties to meet the increasing demands of modern technology.

keywords: Transition metal doping, Layered semiconductors, Optical properties, Electrical properties, MEH- PPV

I. INTRODUCTION

Transition metal-doped semiconductors have garnered significant interest in recent years due to their unique optical and electrical properties, offering promising applications in various fields such as optoelectronics, catalysis, and sensing. The incorporation of transition metal dopants into semiconductor matrices introduces new energy levels and alters the electronic band structure, leading to tailored optical and electrical behaviours. This manipulation of material properties opens up avenues for developing novel materials with enhanced functionalities and performance [1]. Layered transition metal-doped semiconductors have received a lot of interest in recent years because of its potential to revolutionise several technical disciplines, such as optoelectronics, photonics, and electronics. The integration of transition metals into semiconductor matrices may result in unique optical and electrical features that are not possible with conventional semiconductor materials. The goal of this research is to investigate the optimisation of synthesis processes as well as the detailed characterisation of these unique materials in order to fully understand and exploit their characteristics [2]. Layered transition metal-doped semiconductors represent a subclass of these materials, characterized by their layered crystal structure and the presence of transition metal ions within the semiconductor lattice.

1.1 Overview of Semiconductors

Semiconductors are crucial in building a future marked by environmental sustainability and more automation in the constantly changing field of technological innovation. In light of the pressing need to decrease carbon footprints and improve efficiency, semiconductors are becoming essential components for the advancement of environmentally friendly and highly automated technology. Semiconductors are materials with electrical conductivity between that of conductors (metals) and insulators (ceramics). This distinguishing feature enables them to regulate electrical current, making them indispensable in contemporary electronics [4].The research and use of semiconductors started in the early twentieth century, with important milestones such as the discovery of the transistor in 1947 and the integrated circuit in 1958, both of which revolutionised technology and industry. Silicon has long been the most popular semiconductor material owing to its abundance and favourable electrical characteristics. Semiconductors are used to make a wide variety of electronic devices, including diodes, transistors, and photovoltaic cells, all of which are vital components in computers, cellphones, and solar panels. Their capacity to effectively control electrical signals and energy has accelerated technological growth, allowing for the creation of more powerful, compact, and energy-efficient gadgets. As the need for high- performance and adaptable electronic devices continues to expand, continued research in semiconductor materials and technology remains vital, opening the way for advances in diverse industries including as telecommunications, computers, and renewable energy[4].

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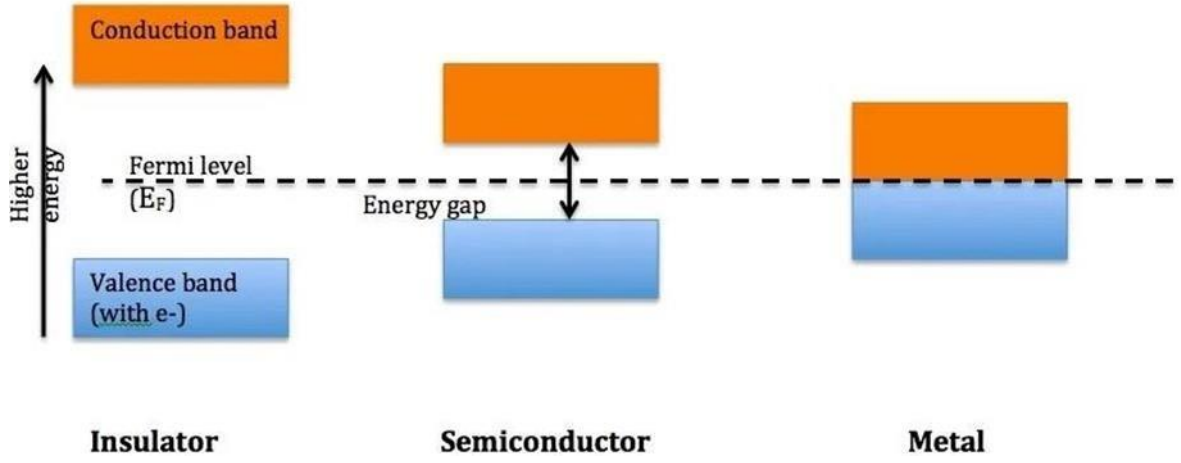

Fig 1: An overview of semiconductors

(source: https://www.eeweb.com/an-overview-of-semiconductors/)

1.1.1 Classification of Semiconductors

I. Intrinsic semiconductor: There are two ways to define an intrinsic semiconductor. In simple words, an intrinsic semiconductor is one which is made up of a very pure semiconductor material. In more technical terminology it can stated that an intrinsic semiconductor is one where the number of holes is equal to the number of electrons in the conduction band. The forbidden energy gap in case of such semiconductors is very minute and even the energy available at room temperature is sufficient for the valence electrons to jump across to the conduction band. Another characteristic feature of an intrinsic semiconductor is that the Fermi level of such materials lies somewhere in between the valence band and the conduction band[6]. This can be proved mathematically which is beyond the scope of discussion in this article. In case you are not familiar with the term Fermi level, it refers to that level of energy where the probability of finding an electron is 0.5 or half (remember probability is measured on a scale of 0 to 1). If a potential difference is applied across an intrinsic semiconductor, electrons will move towards positive terminal while holes will drift towards negative terminal.

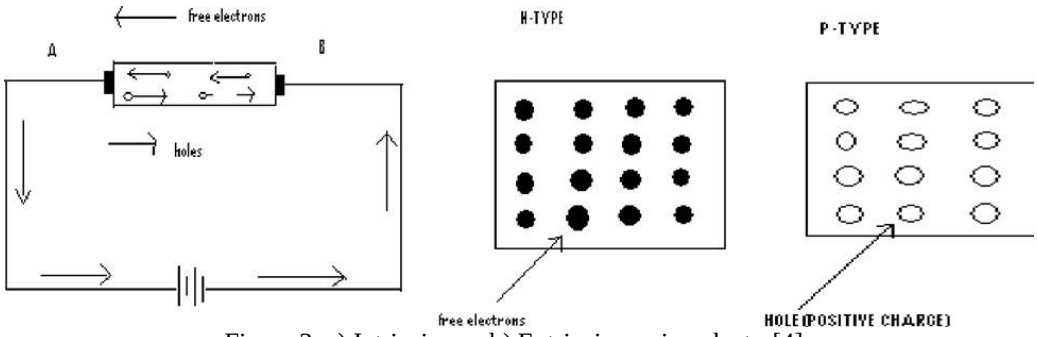

Figure 2. a) Intrinsic b) Extrinsic semiconductor[4]

EXTRINSIC SEMICONDUCTOR: These are semiconductors in which the pure state of the semiconductor material is deliberately diluted by adding very minute quantities of impurities. To be more specific, the impurities are known as dopants or doping agents. It must be kept in mind that the addition of such impurities is really very minuscule and a typical dopant could have a concentration of the order of 1 part in a hundred million parts or it is equivalent to 0.01 ppm. The materials chosen for doping are deliberately chosen in such a manner that either they have 5 electrons in their valence band, or they have just 3 electrons in their valence band. Accordingly such dopants are known as pentavalent or trivalent dopants respectively. The type of dopant also gives rise to two types of extrinsic semiconductors namely P- type and N-type semiconductors.

1.2 Semiconductor Materials

Materials with semiconductor properties may control electric current flow, serve as insulators and conductors simultaneously, and are capable of conducting electric current. Since their creation, semiconductors have been valuable in the electronics area because to their properties.

Typical environmental factors that affect a semiconductor's conductivity include temperature, light, magnetic field, and even trace amounts of impurity atoms.

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Because of its very high conductivity sensitivity, semiconductors are among the most significant materials used in electronics[7].

Fig 1.3: Global Semiconductor Materials [8].

Semiconductors are fundamental materials in modern electronics, categorized by their composition, structure, and electrical properties. Intrinsic semiconductors such as silicon and germanium are pure materials that can conduct electricity under specific conditions due to their balanced number of electrons and holes. Intentionally introducing impurities transforms these into extrinsic semiconductors. N-type semiconductors are doped with elements like phosphorus to increase electron concentration, while p-type semiconductors incorporate acceptors like boron to generate holes as the predominant charge carriers.

1.2.1 Semiconductor Nanoparticles

Semiconductor nanocrystals (NCs) are made from a variety of different compounds. They are referred to as II-VI, III-V or IV-VI semiconductor nanocrystals, based on the periodic table groups into which these elements are formed. For example, silicon and germanium are group IV, GaN, GaP, GaAs, InP and InAs are III-V, while those of ZnO, ZnS, CdS, CdSe and CdTe are II-VI semiconductors[9].

1.2.2 Classifications of Semiconductor Nanostructures

In nanocrystalline materials, the electrons are confined to regions having one, two or three dimensions (Figure) when the relative dimension is comparable with the de Broglie wavelength. For a semiconductor like CdSe, the de Broglie wavelength of free electron is around 10 nm. The nanostructures of semiconductor crystals having the z direction below this critical value (thin film, layer structure, quantum well) are defined as 2D nanostructures. When the dimension both in the x and z direction is below this critical value (linear chain structure, quantum wire) the nanostructures are defined as 1D and when the y direction is also below this threshold (cluster, colloid, nanocrystal, quantum dot) it is referred to as 0D[10].

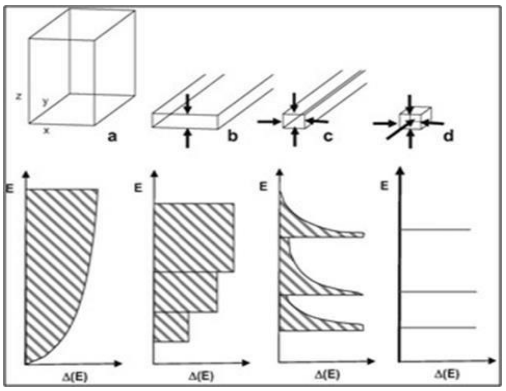

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Figure 4: Schematic drawing to show the concept of system dimensionality: (a) bulk semiconductors (3D); (b) thin film, layer structure, quantum well (2D); (c) linear chain structure, quantum wire (1D); (d) cluster, colloid, nanocrystal, quantum dot (0D). In the bottom, the corresponding density of states[Δ(E)] versus energy (E) diagram (for ideal cases) [11]

1.2.2 1 Zero Dimensional (0D) Nanostructures

In the early stages of research on nano-building block synthesis, zero dimensional shapes were regarded as the most basic and symmetric, including spheres and cubes. Several semiconductor nanocrystals have been grown from the ageing processes of ionic precursors inside organic micelles. However, nanocrystals obtained by this method have relatively poor crystallinity or polydispersity in their size. As an alternative way to solve these problems, a thermal decomposition method of organometallic precursors under hot organic solution was adopted. L. Brus et al (1986) [12] synthesized various II–VI semiconductor nanospheres with high colloidal stability, using coordinating solvents (e.g., 4- Ethylpyridine), but the size tunability and monodispersity of the nanocrystals obtained, were still poor. Murray et al (1993) successfully developed a more advanced methodology to prepare CdSe nanocrystals of varied sizes via the method of injecting a precursor solution containing dimethylcadmium and trioctylphosphine selenide into a hot trioctylphosphine oxide (TOPO) solution. The size of nanocrystals varied from 1.2 to 12 nm with high monodispersity and crystallinity; the nanocrystals obtained were highly soluble in various organic solvents. Optical spectra clearly exhibited size dependent quantum confinement effects, indicating the high monodispersity and high crystallinity of nanocrystals[13]. 1.2.2.2 Quasi One Dimensional (1D) Nanostructures.

1.2.2 2 Two Dimensional (2D) Nanostructures

The family of 2D nanosystems encompasses all those systems that exhibit two dimensions exceeding the third one. However, the number and variety of inorganic nano objects belonging to this family is far lower. with respect to 0D and 1D nanosystems. Indeed, nature tends to organize materials in a three dimensional way. 2D assemblies usually do not grow except under special and controlled experimental conditions. The main synthesis methodologies of 2D nanostructures can be summarized as follows: (i) anisotropic crystal growth, (ii) surfactant-assisted synthesis and (iii) the assembly of simpler 0D or 1D nanosystems. All 2D flat nanocrystals possess an overall size in the order of 10 nm. Such a size limitation is pursued, in order to prevent the growth along only one specific direction, leading to a 1D system. The synthesis of two dimensional nanocrystals is achieved by the self-assembly of solutions and the constituting elements of these systems are usually metals. Discoidal nanocrystals are typical flat building blocks. They are typically obtained by surfactant assisted synthesis, or anisotropic crystal growth passing through colloidal systems. 2D prismatic shapes can be prepared by photoinduced shape changes.

1.2.2 3 Three Dimensional (3D) Nanosystems

Objects having either an overall size in the non-nanometric range (mainly in micrometer or millimeter range), but displaying Nano metric features (such as nanosized confinement spaces) or resulting from the periodic arrangement and assembly of nanosized building blocks, can be classified as _3D nanosystems‘. They exhibit different molecular and bulk properties. In particular, 3D Nano crystals superstructures are prepared by assembling basic nanosized building blocks such as; 0D spheres 1D rods and 2D plates, to have bigger sized structures of innovative shapes. On the contrary, nanoporous materials are made with a _complementary‘ approach, since a system of Nano sized void pores is obtained within a continuous bulk material. Simpler nanosystems can otherwise be used as _artificial atoms‘ to build three-dimensional superstructures, such as super lattices in which a given nanoparticle is in a predictable and periodic lattice point. For this purpose, 0D nanosystems (and mainly nanoparticles) are the best choice, since they can easily lead to the highly ordered 3D closely packed patterns, kept together by chemical interparticle interactions. Super
lattices of CdSe nanocrystals can be obtained, using a selective evaporation technique from a solution of octane & octanol containing spherical CdSe nanocrystals. Such superstructures display a face centered cubic packing of CdSe nanocrystals. They exhibit novel optical properties which are different from those of diluted CdSe nanospheres in solution.

1.3 Transition Metal Doping

Transition metal doping refers to the process of introducing transition metal atoms into a host material, typically a semiconductor, to modify and enhance its properties. Transition metals, which are elements found in the d-block of the periodic table (such as iron, cobalt, nickel, and copper), possess unique electronic configurations that allow them to impart significant changes to the electronic, optical, magnetic, and structural characteristics of the host material[18].

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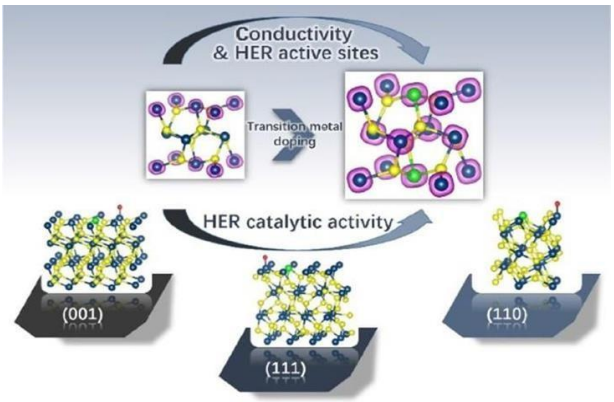


Figure 5: Transition-metal-doped NiSe2 [19]

The above Figure illustrates the impact of transition metal doping on the conductivity and hydrogen evolution reaction (HER) catalytic activity of semiconductors. The top section shows that incorporating transition metal atoms into the semiconductor matrix introduces new electronic states, enhancing conductivity and providing active HER sites. The bottom section compares different crystallographic orientations—(001), (110), and (111) planes—demonstrating that these planes influence HER catalytic efficiency due to variations in atomic arrangement and active site density. The arrows indicate the relationship between doping, increased conductivity, and improved HER activity, highlighting the importance of crystallographic orientation in optimizing semiconductor performance for catalytic applications.

1.3.1 Potential of Transition Metal-Doped Semiconductors

Transition metal-doped semiconductors have garnered significant interest due to their unique electronic, optical, and magnetic properties. By integrating transition metals into semiconductor matrices, researchers have created materials with versatile applications across various fields. In spintronics, these materials are particularly promising because the inclusion of transition metals can induce ferromagnetic ordering at room temperature, a key requirement for developing spintronic devices such as spin transistors and magnetic memory. This could lead to advancements in data storage and processing technologies by leveraging the intrinsic spin of electrons in addition to their charge[21].

Optoelectronics is another area where transition metal-doped semiconductors show great potential. The doping process can significantly alter the optical properties of the semiconductor, including its absorption, emission, and luminescence characteristics. This makes these materials suitable for use in devices like light-emitting diodes (LEDs), laser diodes, and photodetectors. For instance, manganese-doped zinc sulfide (ZnS) exhibits enhanced luminescence, making it a strong candidate for LED applications. Additionally, the ability to tune the band gap of semiconductors through doping enables the creation of materials that can absorb or emit light at specific wavelengths, which is crucial for the development of efficient solar cells and photodetectors. In the realm of catalysis, transition metal-doped semiconductors have shown promising results due to their ability to enhance photocatalytic activity. These materials can be used to catalyze chemical reactions under light irradiation, offering applications in environmental remediation, such as the degradation of pollutants, and in energy production through water splitting and hydrogen generation. The unique combination of semiconductor and transition metal properties enables efficient charge separation and transfer, which is essential for catalytic processes[21].

1.4 Optical and Electrical properties in Layered Metal-Doped Semiconductor

In the synthesis of layered metal-doped semiconductors, the resulting materials exhibit unique optical and electrical properties due to their composition and structure. The optical and electrical properties of layered metal-doped semiconductor materials play a crucial role in determining their suitability for various applications. In terms of optical properties, these materials exhibit tunable absorption spectra and photoluminescence characteristics due to the presence of transition metal dopants and the unique band structures of the semiconductor host. The absorption spectra can be tailored through bandgap engineering techniques, allowing for efficient light absorption across a wide range of wavelengths[22].

Here are some key optical and electrical properties observed in such materials:

Optical Properties:

Band Gap Modification: The incorporation of transition metal dopants can modify the band gap of the semiconductor, leading to changes in its optical properties. This can result in a shift in the absorption edge and changes in the material's color.

Absorption and Reflection: Metal-doped semiconductors may exhibit different absorption and reflection properties compared to the pure semiconductor, affecting their light absorption and reflection characteristics.

Luminescence: Some metal-doped semiconductors exhibit luminescence properties, emitting light when excited by an external energy source. This property is valuable for applications such as LEDs and displays.
Optical Transparency: Depending on the dopant concentration and type, metal-doped semiconductors can vary in their optical transparency, influencing their suitability for transparent electronic applications[22].

Electrical Properties:
Conductivity: Transition metal dopants can alter the electrical conductivity of semiconductors, leading to changes in their overall electrical behavior. This can include changes in resistivity and carrier mobility.
Charge Carrier Concentration: Doping can introduce additional charge carriers into the semiconductor, affecting its overall charge carrier concentration and conductivity.
Fermi Level Position: The position of the Fermi level, which determines the energy level at which electrons are most likely to be found, can be influenced by transition metal doping, affecting the semiconductor's electronic properties.
Semiconducting Behavior: Metal-doped semiconductors may exhibit typical semiconducting behavior, including the ability to conduct electricity under certain conditions while acting as an insulator under others[22].

1.5 Need for Enhanced Optical and Electrical Performance in Semiconductor Devices

The desire for improved optical and electrical performance in semiconductor devices is driven by the growing need for more efficient and adaptable technology in a variety of industries. Optically, advancements are critical for obtaining improved efficiency in light emission and absorption, which is required for applications ranging from lighting and displays to telecommunications and sensors. Improved optical properties allow devices to emit, detect, and control light more effectively, resulting in higher energy efficiency and performance. Electrically, enhancing conductivity, carrier mobility, and dielectric properties is critical for creating speedier and more reliable electronic devices. These innovations enable faster data transfer, lower power consumption, and improved device dependability. Improved electrical properties benefit many applications, including integrated circuits, sensors, and power electronics, allowing for smaller and more powerful devices.

II. LITERATURE SURVAY\

This literature review explores the foundational principles of semiconductors and delves into the transformative effects of transition metal doping. By examining the applications and effects of these dopants on semiconductor erformance, this study aims to elucidate how such modifications enhance functionality, paving the way for innovative applications in fields ranging from optoelectronics to renewable energy technologies.

2.1 Overview of Semiconductors

Md. Atikur Rahman et.al (2021), discusses the history and classification of semiconductor materials and explores the impact of temperature on their properties, including MOSFET energy band gap, carrier density, mobility, diffusion, velocity saturation, current density, threshold voltage, leakage current, and interconnect resistance. Semiconductors have revolutionized the world, transforming communication and data processing. Essential to electronics and computing, they enable the creation of small, lightweight, high-speed, and low-power devices Additionally, it highlights the diverse applications of semiconductors in modern electronics and communications, such as optoelectronics and solar systems.

Gourav Nama et.al (2018), discuss in their paper how semiconductors have revolutionized the world beyond previous imaginations. Essential for communication and data processing, semiconductors have significantly reduced the time required for these tasks compared to the era of vacuum tubes. As the foundational elements of the electronics and computing sectors, semiconductor materials are indispensable for creating compact, lightweight, high-speed, and low-energy devices, particularly through integrated circuits (chips). The paper delves into the history, classification, and impact of semiconductors, with a focus on the effects of temperature on various properties such as the MOSFET band gap, carrier density, mobility, carrier diffusion, velocity saturation, current density, threshold voltage, leakage current, and interconnect resistance.

Man Hoi Wong et.al (2021), explore the renaissance of ultrawide-bandgap (UWBG) semiconductor technology, emphasizing advances in material understanding, novel device concepts, and applications. This focus issue presents a comprehensive overview of UWBG materials and applications, featuring experimental results and theoretical developments.

Andrew Mills et.al (2002), explores the prominent commercial applications of semiconductor photochemistry worldwide, focusing on its utilization in various sectors such as photo-mineralization of organics, photo- sterilization, and photo-demisting. It discusses the underlying principles behind these applications and highlights companies and their products that employ semiconductor photochemistry. Emphasis is placed on the geographical distribution of commercial activities, noting Japan's strong presence in this field. The analysis also covers the patent landscape, noting trends in the number and distribution of patents, particularly between the United States and Japan over the past six years.

Overall, while commercial activities in semiconductor photochemistry are expanding globally, Japan emerges as a dominant force in driving innovation and applications in this specialized area[26].

2.2 Overview of the importance of transition metal doping in semiconductors.

Shanshan Gao et.al (2021), investigates the impact of transition metal (TM) doping (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn) on the stability, electronic structure, and optical properties of β-Ga2O3 using density functional theory (DFT) with generalized gradient approximation (GGA) and GGA + U methods. The research focuses on how the introduction of TM elements modifies the crystal structure and affects electronic transitions within β- Ga2O3. Results indicate that the inclusion of a suitable Hubbard U parameter (U) corrects strong d-orbital interactions, influencing the positioning and density of impurity energy levels. This adjustment shifts the conduction band to higher energies and diminishes the influence of Ga-3p orbitals in the valence band. Among the TM-doped systems, Ti-doped β-Ga2O3 demonstrates the highest stability, followed by V, Cr, Sc, Fe, Mn, Co, Ni, Cu, and Zn doping. Moreover, all doping scenarios induce a red shift in β-Ga2O3's optical absorption spectrum, with Cu-doped β-Ga2O3 showing significantly enhanced absorption in the visible light range. This property suggests Cu as a promising dopant for improving the semiconductor's performance in visible light applications. In conclusion, this research provides insights into how TM doping alters β-Ga2O3's properties, paving the way for tailored applications in optoelectronics and semiconductor technologies[21].

Anielle C.A. Silva et.al (2021), explores TM-doped nanocrystals (NCs), focusing on how doping levels and concentrations influence their applications and biocompatibility. TM-doped NCs exhibit strong sp-d exchange interactions between their charge carriers and TM's unpaired electrons, leading to the emergence of unique properties. These NCs can be synthesized as nanopowders or embedded within glass matrices, depending on specific application requirements. The study reviews synthesis methodologies, characterization techniques, and applications of iron or copper-doped ZnO nanopowders, chromium-doped Bi2S3, nickel-doped ZnTe, and manganese- doped CdTe quantum dots in glass matrices. It highlights how incorporating TM alters the physical, chemical, and biological properties of these nanocrystals. Interestingly, iron-doped ZnO NCs showed comparable efficiency to pristine ZnO NCs in malachite green degradation, while copper-doping enhanced biocompatibility. Furthermore, TM doping in semiconductors induces magneto-optical properties, exemplified by manganese, chromium, or nickel-doped NCs, whose manipulation depends on doping concentration and thermal treatments in glass matrices[1].

2.3.1 Applications of Transition Metal-Doped Semiconductors

Pushpendra Singh et.al (2019), focuses on the effects of transition metal (TM) doping on the physical properties of zinc oxide (ZnO) nanoparticles and their applications. ZnO nanoparticles have garnered significant research interest due to their versatility in doping with various TMs, offering a wide range of applications. The diverse morphological structures, high electron mobility, and n-type carrier defects of ZnO make it suitable for use in memory devices, spintronics, optoelectronic devices, solar cells, and sensors. The review discusses theoretical models commonly used to explain variations in physical properties due to TM doping. Furthermore, it provides insights into sensing, photocatalytic, and optoelectronic processes in different classes of devices. Comparative studies of these devices are also presented to facilitate a better understanding of the impact of TM doping on the performance of ZnO nanoparticles in various applications[27].

Eryk Fernandes et.al (2022), compares the application forms and doping benefits of semiconductors, specifically TiO2, WO3, and g-C3N4, for wastewater treatment, focusing on the removal of contaminants of emerging concern (CECs) and micropollutants. While TiO2 is a well-optimized material, its reliance on ultraviolet radiation limits its efficiency. Alternative visible light driven (VLD) materials like WO3 and g-C3N4 have gained attention for their ability to harness natural light sources, reducing costs. The review discusses recent developments in CEC degradation using TiO2 as a reference catalyst, alongside WO3 and g-C3N4. Techniques to enhance catalyst photo-activity, such as doping with multiple elements and forming composite materials, are explored. Additionally, the combination of photocatalysis and ozonation is discussed as a route to enhance efficiency. Overall, semiconductors show potential for efficient water treatment, with the addition of ozone further improving the process. Further studies are needed to fully understand and optimize the use of these materials in wastewater treatment[28].

Mengqi Fang et.al (2023), examine the remarkable properties of transition metal dichalcogenides (TMDs), this review explores dopant-induced modifications as a strategy to tailor these materials. Two-dimensional (2D) TMDs offer unique electrical, optical, and chemical characteristics, making them promising for various applications. The review focuses on chemical vapor deposition (CVD) methods to introduce dopants into TMD monolayers

Effects of Transition Metal Doping on Semiconductors

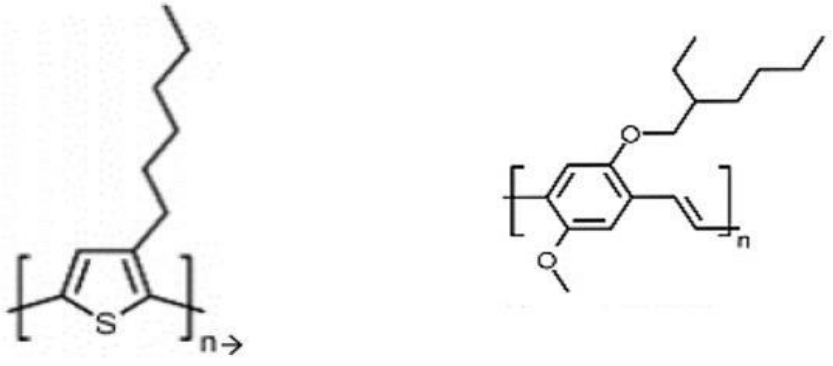
Zhongqiang Suo et.al (2020), investigates the impact of transition metal (TM) doping (Sc, Ti, V, Cr, and Mn) at various distances on the stability, electronic structure, conductivity, and optical properties of CdS using VASP code. Results indicate that Cr-doped CdS is the most readily formed, followed by V, Ti, Sc, and Mn. The next nearest-neighbor doping is the most stable in each TM-doped system. Band gaps decrease with Sc, Ti, V, Cr, Mn doping, leading to a degenerate semiconductor state.

Doping enhances conductivity and photocatalytic performance, particularly noticeable in Mn-doped CdS. Absorption intensity in the visible light range is higher in single-doping compared to dual-doping systems, with Mn and Cr showing the most significant effects. Overall, Mn proves to be the most beneficial dopant for improving CdS conductivity and light absorption. The study provides insights into optimizing CdS for optoelectronic applications[31].

Mengqi Fang et.al (2023), reviews the use of chemical vapor deposition (CVD) methods to introduce dopants into TMD monolayers, discussing their impacts on structural, electrical, optical, and magnetic properties. Dopants alter carrier density and type, influencing optical and magnetic properties. Challenges include controlling synthesis for uniformity and large-area coverage, and low Curie temperatures in magnetic TMDs. Co-doping shows potential for enhancing properties, suppressing recombination, and inducing ferromagnetic ordering. Electronic interactions between dopants further modify band structures and energy levels. The review highlights the potential applications of doped TMDs in spintronics, optoelectronics, and magnetic memory devices, emphasizing the need for further research to overcome synthesis challenges and optimize magnetic properties[29].

Raksan Ko,Dong Hyun Lee et.al (2023), investigates the impact of annealing and chemical doping on the properties of transition metal dichalcogenides (TMDCs), focusing on crystal quality, defect density, carrier mobility, electronic properties, and energy levels within the bandgap. Annealing improves crystal quality and carrier mobility, while doping modifies conductivity and introduces energy levels in the bandgap. Various doping types, annealing conditions, and ambient atmospheres are considered. Technological barriers, including temperature control and dopant uniformity, must be addressed for industrializing TMDC processing. Despite these challenges, continuous research advancements are expanding TMDC applications in photodetectors, sensors, and logic circuits. Innovative approaches, such as advanced annealing and doping methods, show promise for TMDC- based field-effect transist. Transition metal doping in semiconductors like MEH-PPV and P3HT.

Kanupriya Sharma et.al (2020), In the present work, the optical properties of transition metal (Mn, Fe, Cu and Ag) doped ZnS nanoparticles in PVK polymer composites have been studied. The pure and transition metal (TM) doped ZnS nanoparticles were prepared by co-precipitation method and PVK/ZnS(TM) nanocomposites were synthesized by spin coating technique. The nanocomposites were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), optical absorption, energy and time-resolved photoluminescence spectroscopic techniques. The XRD patterns suggest the formation of the cubic phase of ZnS nanoparticles while FTIR spectroscopy reveals the incorporation of transition metal dopants in ZnS nanoparticles. The wide variation in surface morphology for differently doped nanoparticles in PVK based composites has been observed from FESEM technique. The optical gap has been found to increase with nanoparticle incorporation while the increased luminescence quenching is observed for PVK/ZnS:Mn nanocomposites .



(a) (P3HT) n (b) (MEH-PPV) n

Figure 6 : Basic structures of (a) P3HT and (b) MEH-PPV polymers. [37]

III METHODOLOGY

In this study, we investigated the effect of a non-zero Schottky barrier on hole transport in MEH-PPV and P3HT using ITO/PEDOT, /MEH-PPV/Au and ITO/PEDOT,/P3HT/Au diode configurations. The J-V characteristics were measured at various temperatures for different sample thicknesses. For MEH-PPV, we examined two samples with thicknesses of 120 nm and 65 nm, correcting the applied voltage for the ITO series resistance. The experimental data were compared with Ohm‘s law at low voltages and then with space charge limited current (SCLC) theories.

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We validated our theory by measuring J-V characteristics at different temperatures and thicknesses, showing agreement with both conventional and modified theories.

For P3HT, we measured J-V characteristics at 310, 248, and 210 K, comparing the data with the conventional power law and our modified theory. The parameters for each sample were meticulously recorded and analyzed to ensure the reliability and accuracy of our findings across different conditions.

IV RESULT AND DISCUSSION

In this study, we analyzed hole transport in MEH-PPV and P3HT diodes by measuring J-V characteristics at various temperatures and thicknesses. For MEH-PPV, we tested samples with 120 nm and 65 nm thicknesses. Our corrected J-V data for ITO series resistance showed Ohmic behavior at low voltages, transitioning to space charge limited current (SCLC). Both conventional power law and our modified theory were validated. For P3HT, J-V characteristics at 310, 248, and 210 K initially agreed with the conventional power law but deviated at higher voltages. These results demonstrate the significant impact of the Schottky barrier on hole transport and confirm the reliability of our theoretical model across different conditions.

4.1 Impact of non-zero Schottky barriers on hole transport in MEH-PPV.

In this section, examine the impact of a non-zero Schottky barrier on hole transport in MEH-PPV diodes. Utilizing ITO/PEDOT /MEH-PPV/Au diodes, we measured the J-V characteristics across various temperatures. Our goal was to understand the underlying transport mechanisms and how they deviate from ideal behavior due to the Schottky barrier. By comparing the experimental data with theoretical models, we aim to shed light on the role of the Schottky barrier and the integration constant in influencing hole transport. This analysis provides valuable insights into optimizing the performance of organic semiconductor devices.

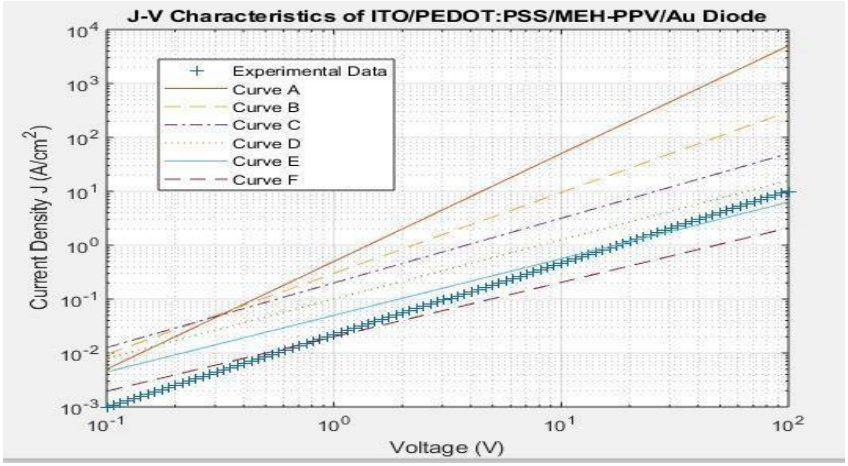

Figure 7: J-V characteristics of ITO/PEDOT:PSS/MEH-PPV/Au diode at 240 K. Symbols represent the experimental data

The above figure illustrates the J-V characteristics of the ITO/PEDOT /MEH-PPV/Au diode measured at 240 K. The experimental data is depicted by the '+' symbols. At low voltages, the current density follows Ohm's law (dash-dot curve), indicating Ohmic behavior due to background doping or thermally generated carriers up to point
B. As the voltage increases, the diode transitions to a space charge limited current (SCLC) regime, following an exponential trap distribution (dotted curve ADF). Beyond point D, the experimental data aligns with both the conventional theory (dashed line ADC) and our modified theory up to point E. However, at higher voltages, the modified theory (solid curve) deviates from the conventional theory, emphasizing the role of the integration constant C in describing the transport behavior more accurately. This comprehensive analysis highlights the complex nature of hole transport in MEH-PPV diodes.

4.2 Validation of theories under various temperatures and thicknesses

In this section, aim to validate our theoretical model across different temperatures and thicknesses of the MEH- PPV layer in diodes. To achieve this, we prepared another ITO/PEDOT /MEH-PPV/Au diode with an MEH-PPV thickness of approximately 65 nm. We measured the J-V characteristics of this diode at 300 K, 243 K, and 210 K. Our goal was to verify that our model, which incorporates the integration constant C, accurately describes the hole transport behavior across varying conditions.
The consistency of the experimental data with the theoretical predictions across different temperatures and thicknesses confirms the robustness and applicability of our model.

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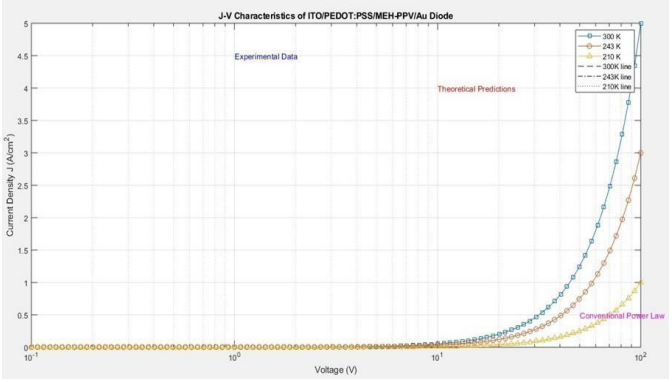

Figure 8: Calculated and experimental J-V characteristics of ITO/PEDOT:PSS/MEH-PPV/Au diode at different temperatures with an MEHPPV thickness of 65 nm.

The above figure illustrates the J-V characteristics of ITO/PEDOT,/MEH-PPV/Au diodes with a 65 nm thick MEH- PPV layer, measured at 300 K (squares), 243 K (circles), and 210 K (triangles). The experimental data are indicated by symbols, while the solid lines represent theoretical predictions incorporating the integration constant C. The dash-dot lines depict the conventional power law, aligning with the experimental data at intermediate voltages. However, at higher voltages, the experimental data diverge from this conventional law. The theoretical model, which includes the effect of the integration constant, fits the experimental data well across the entire voltage and temperature range. This demonstrates that the proposed theory effectively accounts for the transport behavior and the deviations observed at higher voltages.

4.3 Effects of a non-zero Schottky barrier on hole transport in P3HT.

The effect of a non-zero Schottky barrier on hole transport in P3HT (Poly(3-hexylthiophene)) is examined in this section. In devices configured with ITO/PEDOT /P3HT/Au, the Schottky barrier height influences current-voltage characteristics, notably affecting charge carrier transport. Experimental data compared against theoretical models illustrate deviations at higher voltages, highlighting the barrier's impact on conductivity. This study utilizes parameters such as carrier density, temperature, and mobility to analyze how variations in the Schottky barrier height (fB) alter the transport properties of P3HT, crucial for optimizing device performance in organic electronics.

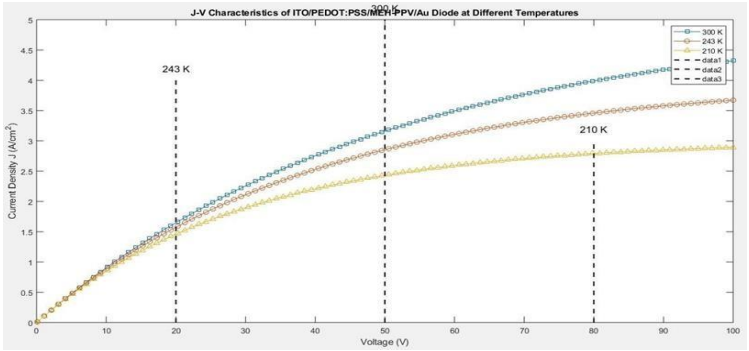

Figure 9: Calculated and experimental J-V characteristics of ITO/PEDOT:PSS/P3HT/Au diode at different temperatures. Symbols represent the experimental data.

The above figure depicts the calculated and experimental current-voltage (J-V) characteristics of an ITO/PEDOT /P3HT/Au diode at varying temperatures (310 K, 248 K, and 210 K). Experimental data points, shown with symbols, illustrate the measured behavior, while dashed lines represent the conventional power law model. Solid curves correspond to at the respective temperatures. At intermediate voltages, the experimental data align closely with the power law model. However, at higher voltages, deviations occur, bending the curves downward. The agreement between experimental data and the model is particularly strong for a Schottky barrier height (fB) of 0.2 eV, consistent with previous determinations based on material properties.

V. CONCLUSION

The study on enhancing the optical and electrical properties of layered transition metal-doped semiconductors has provided valuable insights into how transition metal doping can significantly improve semiconductor performance. The optical properties such as band gap modification, absorption, reflection, luminescence, and optical transparency are vital for applications requiring efficient light manipulation. Enhanced electrical properties, including conductivity, charge carrier concentration, and Fermi level position, are crucial for developing faster and more reliable electronic devices. The investigation of hole transport in MEH-PPV

and P3HT diodes under varying temperatures and thicknesses confirmed the significant impact of non-zero Schottky barriers on device performance. The validation of the theoretical models across different conditions demonstrated their robustness and applicability, providing a deeper understanding of the transport mechanisms in these materials. These findings underscore the importance of ongoing research to optimize both optical and electrical properties, aiming to meet the increasing demands of modern technology and pave the way for future advancements in semiconductor device.

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