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# Enrichment of Photoluminescence Quantum Efficiency in Semiconductor Based on the Einstein Mass Energy Relation

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**ABSTRACT:** Quantum mechanical existences of hole in semiconductor are longevity for existence of modern semiconducting technological devices in addition to the existence of electron. Existences of hole and variation of its properties causes greatly influences the changes in physical properties of semiconductor and these properties predominately influences at reduced dimensionalities also. In detail quantum mechanical knowledge of physics parameters and fundamental nature of semiconductor is of great interest in order to evaluate their potential use in a wide class of optoelectronics devices such as laser diodes, photo luminescent diodes and light emitting diodes.

Theoretically, realization and characterization of hole and its parameters is great challenge under the different cases which in turn influences devices performance. Along with stabilization of energy gap is one of the most important achievements in semi conducting materials with respect change in quantum vacancy (hole) properties. Meanwhile the energy gap is important to determine the region of the light spectrum where the semiconductor can be applied like photonic device. Detail theoretical analysis on hole and its properties useful in understating of semiconducting properties such as recombination process, life time of charge carriers. All the theoretical work has been considered to understand the complete behavior of the semiconducting materials in order to suit them effectively for technological applications.

**KEYWORDS:** Luminescence, energy gap, lifetime of charge carriers

## I. INTRODUCTION

The last few decades have seen the birth of a great diversity of products and services associated with electrical and electronic equipment, which are subject to constant change with advancement of quantum mechanics [1,2]. During the last few years, since semiconductor manufacturing processes have gradually diminished in size, the number of transistors that can be fabricated on a sole silicon wafer can amount to a billion units. In order to account for the dynamic evolution of production and distribution and changes caused by technological advances, due to rapid changes in the demands in field of science and technology need to be flexible and to be able to adapt quickly to a constantly changing environment through fundamental enrichment of science [3-5].

The knowledge of physics parameters of semiconductor compounds is of great interest in order to evaluate their potential use in a wide class of optoelectronics devices. These parameters have been investigated not only experimentally, but also theoretically. From the standpoint of the latter, crystal lattice energies are important in considering the stability of new materials and reflect the natural tendency towards the organization of matter, meanwhile the energy gap is important to determine the region of the light spectrum where the semiconductor can be applied like photonic device [6]. Realization and stabilization of hole and its properties is great challenge under the different cases which in turn inflecting devices performance. Along with stabilization of energy gap is one of the most important achievements in semi conducting materials with respect internal factors as well as external factors [7]. The present work, more attention is given to understand the formation of holes and its properties are studied with help of Einstein mass energy relation in semiconductors. In order to understand the semiconducting properties such as

recombination process, life time of charge carriers to meet continuously changing demand in semiconducting technology [8].

## II. EXPLANATION

Theoretical validation of the existence of fictitious holes and its properties are gained much significance in understanding of amplification, rectification, sensing properties and recombination process are discussed below.

Valence shell electrons of pure semiconductor like Ge and Si are bonded covalently with neighborhood atoms in the crystal and consequently they are not available for electrical conduction at room temperature. With increase of temperature causes the thermal vibration may break some of the covalent bonds which yield free electrons that can participate in current conduction. Once an electron moves away from a covalent bond, there is an electron vacancy associated with that bond. This vacancy may be filled by a neighboring electron, which results in a shift of the vacancy location from one crystal site to another. This vacancy may be regarded as a fictitious particle called as a hole. Both charge carriers electrons and the holes move through the crystal and conduct the electric current, but motion of electron and holes are in opposite direction. In case of pure semiconductor, there exist an equal number of free electrons and holes with different mobility [9,10]. Even though, both electrons and holes existed as a charge carrier with equal magnitude of charge with opposite charge. Fundamental point of view, electron regarded as elementary particle and it possess mass, charge, spin. But existence of the hole regarded as quasi particle with positive charge and mass alone. The existing properties of the electron and hole are get differed which in turn effect the semiconducting properties such as amplification, rectification, sensing properties and recombination process. Recombination process may be between electron and hole when the momentum of the both charge carriers must be equal [11]. To Balance moment between element particle and virtual particle with different properties need to consider much attention on microscopic mechanism of the virtual particle hole then the elementary particle with help of quantum mechanics are discussed below.

Hole in condensed matter physics name is given to a missing electron in certain solids especially semiconductors. Holes and its properties affect the electrical, optical and thermal properties of the semiconducting substance which in turn influences the efficiency of the electronic devices. As described that above, when electron get excited cause it leaves quantum vacancy behind it. Creation of the quantum vacancies and its mass in semiconductor in place of electrons are get influenced by Lattice energy and Phonon energy ( $E_1$ ), Nature of chemical bonding and bond strength ( $E_2$ ), External factors causes energies ( $E_3$ ) and Others form of energies ( $E_4$ ). And all these energies are constituted to form hole and its mass based on the Einstein mass energy relation.

### Lattice Energy and Phonon energy ( $E_1$ ):

Lattice energy is the Measure of the energy contained in the crystal lattice of a crystal equal to the energy that would be released if the component ions were brought together from infinity. Lattice Energy is a type of potential energy that may be defined as the lattice energy is the energy required to break apart an ionic solid and convert its component atoms into gaseous ions. In this case, the value of the lattice energy is always positive because it will always be an endothermic reaction. The other definition says that lattice energy is the reverse process, meaning it is the energy released when gaseous ions bind to form an ionic solid. As implied in the definition, this process will always be exothermic, and thus the value for lattice energy will be negative. Lattice Energy is used to explain the stability of ionic solids. Some might expect such an ordered structure to be less stable because the entropy of the system would be low. However, the crystalline structure allows each ion to interact with multiple oppositely charge ions, which causes a highly favorable change in the enthalpy of the system. A lot of energy is released as the oppositely charged ions interact. It is this that causes ionic solids to have such high melting and boiling points. Some require such high temperatures that they decompose before they can reach a melting and boiling point [12-14]. Lattice energy is a critical parameter used to the measure the powers that bind between ions in a crystal. However, the lattice power for these compounds has received little attention to know the connection between creations of hole in semiconductor.

The subject of lattice energy and its lattice dynamics is the study of the vibrations of the atoms in a crystal. We intuitively understand that, atoms must be vibrating within crystals it is the natural interpretation of temperature traditional crystallography often leads to the image of atoms being held in static positions through stiff chemical bonds. Yet crystallographic measurements tell us that atoms can be vibrating with amplitude that can be of order of 10% of an



inter-atomic distance [15, 16]. Thus we need to understand lattice dynamics in order to have a complete picture of crystalline materials. Understanding lattice dynamics is important for a number of key applications. Especially in case of semiconducting substances lattice energy and dynamics place an important role in formation of electron hole. As per lattice dynamics, lattice energy of binary compounds is given by

$$U = 381.9 + 24.3 (\hbar \omega_p)$$

Where U- lattice energy and  $\hbar \omega_p$  phase change energy

A quantum theory of lattice vibrations or elastic waves leads to quantization of energies. The quantization of the energies found to be similar to that of the energies of a harmonic oscillator having three normal modes of vibration. We need to understand that the energy of a harmonic oscillation is quantized in units of  $\hbar\omega$ . However, this quantization applies to all harmonic vibrations and a single wave of atomic oscillations is similarly quantized thus the quantum in this case is called a phonon. The energy of a single oscillation that is quantized can be written as:

$$E_n = (n + \frac{1}{2}) \hbar \omega$$

The additional constant value of  $\hbar/2$  is called the zero point energy and reflects the fact that in quantum mechanics a harmonic oscillator can never be at rest. Then with help of Energy of the crystal in terms of the normal mode coordinates is given by

$$E = \sum \omega_{k\lambda}^2 |Q(k, \lambda)|^2 = \sum (n_{k\lambda} + \frac{1}{2}) \hbar \omega_{k\lambda}$$

In practice it is not the instantaneous value of  $n_{k\lambda}$  that we need, but its average value at a particular temperature. It turns out that the average value of  $n_{k\lambda}$ , only depends on  $k$  and through the dependence on  $\omega_{k\lambda}$ . Expectation value of  $n_{k\lambda}$  is given by  $= 1 / \exp(\hbar\omega_{k\lambda}/K_B T) - 1$ . This is known as the Bose-Einstein equation. Given that the average number of excited phonons depends only on the frequency and that in a harmonic system its excited waves are independent of each other [17,18].

### Nature of bonding and bond strength ( $E_2$ ):

Si, Ge, and GaAs are the semiconductors of choice for the electronics industry requires some understanding of the atomic structure of each and how the atoms are bound together to form a crystalline structure. A chemical bond is formed between two atoms by the complete transfer of one or more electrons from one atom to the other as a result of which the atoms attain their nearest inert gas configuration. Chemical bonds are the attractive forces that hold atoms together in the form of compounds. They are formed when electrons are shared between two atoms. There are 3 types of bonds: covalent bonds, polar covalent bonds and ionic bonds.

**Ionic bonds:** There are primarily three ways in which two atoms combine to lose energy and to become stable. One of the ways is by donating or accepting electrons to complete their octet configuration. The bond formed by this kind of combination is known as an ionic bond or electrovalent bond. This kind of bond is formed when one atom gains electrons while the other atom loses electrons from its outermost level or orbit [19-21].

If the normal valence of an atom is not satisfied by sharing a single electron pair between atoms, the atoms may share more than one electron pair between them. Some of the properties of covalent bonds are: Covalent bonding does not result in the formation of new electrons. The bond only pairs them. They are very powerful chemical bonds that exist between atoms. A covalent bond normally contains the energy of about ~80 kilocalories per mole (kcal/mol). Covalent bonds rarely break spontaneously after it is formed. Covalent bonds are directional where the atoms that are bonded showcase specific orientations relative to one another. Most compounds having covalent bonds exhibit relatively low melting points and boiling points. Compounds with covalent bonds usually have lower enthalpies of vaporization and fusion. Compounds formed by covalent bonding don't conduct electricity due to the lack of free electrons. A covalent bond is formed by equal sharing of electrons from both the participating atoms. The pair of electrons participating in this type of bonding is called shared pair or bonding pair. The covalent bonds are also termed as molecular bonds. Sharing of bonding pairs will ensure that the atoms achieve stability in their outer shell which is similar to the noble gases. In generally, Covalent Solids Covalent solids are composed of atoms which are not electropositive enough for metallic bonding but are too polarizable for ionic bonding. Their compositions typically include groups III, IV, V and VI atoms. The distinguishing property of the covalent bond is its directionality.



**External factors ( $E_3$ ):**

External factors such as increasing the temperature, applying the electric field, magnetic field and application of electromagnetic waves greatly influence the semiconducting properties with great extent. All above external factors, causes the changing the mass of the hole and its energies with great extent but not on the mass of the electron and influences energy and moment of the electron. Due to these external energy factor causes can be possible to tune and enhance the efficiency of the semiconductor based devices[22].

**Others of form of energies ( $E_4$ ):**

During the formation of the semiconducting crystal in crystallization process, naturally some imperfections may occur. Such as existing of the impurities, dislocation of the atoms in lattice site, different types of defects ... etc which in turn effect the lattice energy in case of ionic crystals and also phonon energy in case of covalent crystals.

**Einstein mass energy Relation- formation of hole:**

Electron excitation is the transfer of a bound electron to a more energetic but still bound state. This can be done by photo excitation, where the electron absorbs a photon and gains all its energy or by electrical excitation where the electron receives energy from another, energetic electron. Within a semiconductor crystal lattice, thermal excitation is a process where lattice vibrations provide enough energy to transfer electrons to a higher energy band such as a more energetic sublevel energy level. When an excited electron falls back to a state of lower energy, it undergoes electron relaxation. This is accompanied by the emission of a photon or by a transfer of energy to another particle [23, 24]. The energy released is equal to the difference in energy levels between the electron energy states. In general, the excitation of electrons in atoms strongly varies from excitation in solids which is due to the different nature of the electronic levels. The electronic excitation can take place by different processes. During the excitation of electrons into the conduction band it leaves quantum hole behind electron realized based on the Einstein mass energy relation as follows:

As discussed above the different form of energies exist in semiconducting crystals in form of pure elemental, binary or ternary semiconducting compounds. Any atom in semiconducting crystals holed by these energies naturally and when ever semiconductor exposed to the external energies electron get relived from the these kind of energies by the electron, during this process bonded and other energies could be balanced by crating the virtual mass or quantum vacancy called hole[25].

German-born physicist Albert Einstein's theory of special relativity that expresses the fact that mass and energy are the same physical entity and can be changed into each other by equation  $E = mc^2$ . Whenever the electron becomes free electron, in order to balance existing above energies need to equalize with virtual particle based on energy to mass conversion. Einstein mass energy relation is applied to convert energy equivalent mass as follows

$$(E_1+E_2+E_3+E_4)= mC^2$$

$$m = (E_1+E_2+E_3+E_4)/ C^2$$

Where m- mass is equal to the hole mass and C- is the velocity of light and which is constant and doesn't make to alter the mass of the hole. Major contribution of formation of the mass of the hole are considered due to the  $E_1, E_2, E_3$  and  $E_4$  energies. Due to variation in these energies in the crystal causes change in the mass of the hole semiconductor to semiconductor. To evaluate the mass of the hole need to apply the quantum mechanics. By applying the Schrödinger wave equation to the equivalent virtual particle for each energy ( $E_1, E_2, E_3 \& E_4$ ) then solutions for the equation used to give the Eigen values equal to the mass of the hole [26].

In addition to creation of mass hole, charge of the electron and hole are get balanced with based on the conservation of charges by have equal and opposite charges. Addition properties of the electron such as spin(half integral spin) multiples and its moment could be balanced with hole spin exists as 3/2 multiples. Mass of the hole is much greater than electron and but moment of the electron greater than the hole those changes could be balanced with same momentum microscopically [27]. This leads to the recombination of electron hole pair in semiconductor in addition to the continuous variation of holes mass due to above factors causes moment could changed which cases life time of electron can be controlled effectively under stable conditions. Based on these energies mass of the hole calculated for silicon and germanium crystals. Due to variation of mass of the hole in semiconductor that in term influences the recombination and other processes causes controllability over photoluminescence Quantum Efficiency.



### III. CONCLUSIONS

Physical concept based understanding the concepts of semiconducting materials are studied in detail to under the properties at microscopic level in order to apply for suitable electronic devices applications. Especially, more importance is given in studying formation of hole and its properties consequences in understanding the different properties of semiconductor have been studied theoretically. Electron excitation nothing but transfer of a bound electron to a more energetic state and this can be done by photo excitation, where the electron absorbs a photon and gains all its energy or by electrical excitation where the electron receives energy from another, energetic electron. Within a semiconductor crystal lattice, thermal excitation is a process where lattice vibrations provide enough energy to transfer electrons to a higher energy band such as a more energetic sublevel energy level. In general, the excitation of electrons in atoms strongly varies from excitation in solids which is due to the different nature of the electronic levels. During excitation of the electron it leaves the quantum vacancy behind it is realized with help Einstein mass energy. Major contribution of formation of the virtual particle mass of the hole are considered due to the  $E_1, E_2, E_3$  and  $E_4$  energies. Mathematical form of mass equivalent energies based on the mass energy relation  $m = (E_1 + E_2 + E_3 + E_4) / c^2$

In addition to creation of mass hole, charge of the electron and hole are get balanced with based on the conservation of charges by have equal and opposite charges. Due to variation in these energies in the crystal causes change in the mass of the hole in terms greatly influences physical propertice of the semiconductor such as recombination process and life time. Yet crystallographic measurements tell us that atoms can be vibrating with amplitude that can be of order of 10% of an interatomic distance. Intrinsic spin of the electron exists as half integrals where as in case of the hole spin exists as 3/2 multiples. Reviewed that, two same kind of semiconducting crystal existed the created fictitious mass of hole may not be same. And mass of the hole is much greater then electron and but moment of the electron greater than the hole those changes could be balanced with same momentum. This leads to the recombination of electron hole pair in semiconductor in addition to the continuous variation of holes mass due to above factors causes moment can be changed which cases life time of electron can be controlled effectively under ambit conditions. Due to variation of mass of the hole in semiconductor that in term influences the recombination causes controllability over photoluminescence and electronic devices.

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