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Review Article

Design Approaches of Imide Based Organic Solar Cells with Computational Chemistry State-of-the-art Density Functional Theory: A Perspective Review

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Abstract

Imide-based organic solar cells with their theoretical calculations for small molecule based organic solar cells are highly significant for designing and predicting the series of small organic solar cells with non-fullerene acceptors. In this perspective review, we have provided the series of details about the organic and inorganic solar cells and why the organic solar cells are highly significant to avoid the cost issues and large experimental precautions. Secondly, we have also provided the deep guess about the density functional theory and their role in the theoretical prediction of the highly reliable tools for optoelectronic properties. We hope that this perspective report about the organic solar cells with imide central units and details about the density functional theory opens the new ways for thinking and designing the large number of various others optoelectronic materials.

Keywords: Organic solar cells; Density functional theory; Non-fullerene acceptors

Introduction

Due to fast consumption of fossil fuels, generation of viable and most effective viable power becoming important need in future. This is due to increasing the demand of energy sources from the people, which are increasing day by day. Most of energy sources are obtained from the fossil fuels that could be end at one day. Therefore, researchers and scientist working to develop those energy sources that are regenerated also as they are used by the human beings. Demand of energy sources increase rapidly due to the rapid growth of international economy in different region of the world. Different development and funding institutions trying to the change scenario of energy obtained from the fossil fuels to energy obtained from the natural sources that can be regenerated by the natural process as they consumed. These renewable energy systems are low cost as compared to those that are used for the fossil fuels that having a huge cost [1]. Hydel power, wind power, tidal and solar energy are some common examples of renewable energy sources that we can obtained and regenerated from the natural process [2]. Scientist are working on regenerate this energy sources at a rate equal or fast as its rate of consumption by the human being throughout the world [3]. These renewable energy sources are environment friendly and we can be obtained large amount of energy from these natural resources with a little cost [4].

Different technologies and working devices are developed to change the energy obtained from the natural process like turbine engine for hydel power, tidal machine for tidal pools, wind driven turbine and photovoltaic devices for the solar energy [5]. Sun light is great kindness of God for this world. Form sun light, we can be obtained energy at amount equal to amount of its consumption worldwide that is why scientists are working day and night to obtain a more and more benefits on developing low cost, effective, environment friendly photovoltaic devices. Annually, earth receiving the 1.53 TWh amount of energy from the sun light which enhanced the 161,000 TWh amount of power consumption globally [6]. The development of highly efficient, low cost, in-expensive and easily manufactured photovoltaic solar cells devices is important challenge for the scientists [7]. Many techniques are employing to develop this type of solar cells such as roll-to-roll printing etc. Photovoltaic devices show the high efficiencies of power conversions as compared to the perovskites cells which having a short lifetime. Different solar cells devices having a different efficiency like solar cells with fullerene free acceptors reached at 13% efficiency [8] and ternary solar cells at

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12% [9]. Investigation on solar cells have started since 1970 and now a day it become important need for the world power. Because the earth absorbs amount of energy per hour equal to the amount of energy used by the human being per year.

Photovoltaics and solar cells

Photovoltaic is a device that convert the sun light into the electric energy. The word photovoltaic derived from the Greek two words "Photo" means light and "Voltaic" mean electric energy. Photovoltaics contain the large number of solar cells that are made up of semi-conductor type material for the generation of electricity [10]. Similarly, solar cells based on electronic materials that convert the light coming from the sun into the electric energy. Light which coming from the sun when fall on the solar cells produce a current and voltage, which generate the electric current further. Solar cells contain a material that excite the electrons from ground to higher energy states when light fall on it and secondly moved these electrons from solar cells to external circuit. Thirdly, the electrons in the external circuit release own energy and come back in the solar cells [11]. Different types of materials and devices can be used in the photovoltaic and solar cells for the conversion of electricity but the p-n type of semiconductor materials provide efficient results in energy conversion. Photovoltaic and solar cells are most important alternative form of fossil fuels that are environment friendly [12]. Generation of voltage in the exposure of solar cells radiations is called the photovoltaic effect that excite the electrons in the conduction band due to absorption of photon from the sun light.

A. E. Becquerel in 1983 report the photovoltaic effect between the Platinum (Pt) electrode and silver chloride (Ag-Cl) electrolyte in junction and later A. Einstein explained this effect [13]. The devices that produced the photovoltaic effect in the presence of sunlight is called the photovoltaic devices, solar cells and photovoltaic cells. Russel developed the first photovoltaic device by using a p-n junction of silicon based material. Photodetector and solar cells having same working principle. In 1870, R. E. Day and W. G. Adam investigate the photovoltaic effect in the selenium metal with the help of candle light which led to the invention of selenium based solar cells by Burno in 1931. The efficiency of selenium based solar cells were less which increased to 4% by replacing the selenium metal with silicon in 1954 by Calvin [14]. But now a day, the efficiency of silicon based solar cells reached at 15% [15]. In the efficiency of photovoltaics, a lot of development occurs in between the 1957-1960 as its efficiency changed from 8% to 14% [16]. In 1985, South Wales University Australia making silicon based solar cells that having 20% efficiency [17]. A major breakthrough occurs in 1999 when Spectro lab in collaboration with National Renewable Energy Laboratories make solar cells of 33.3 % efficiency and this record are brake down by University of South Wales own hand when it makes solar cells of 34.5% efficiency in 2016 [18]. Photovoltaics play important role in generation of electricity from the sun light with the help of different semi-conductor materials that generate the photovoltaic effect [19].

Organic materials as semi-conductors

Organic materials can be used as semi-conductors that having a capacity to move the electrons in the conduction band [20]. Shirakawa and his colleagues developed a semiconductor material single and double bond of carbon, hydrogen bond with nitrogen, hydrogen bond with sulphur and oxygen [21]. They got the Nobel Prize in 2000 on developing the organic semiconductor materials. Organic semiconductor having strong sp2 hybridization, which enhance the energy difference between the bonding and anti-bonding due to having a strong sigma bond between the two heteroatoms. In organic semiconductors upper energy level are denoted by HOMO, lower energy level by LUMO and gap of energy between the HOMO/LUMO energy orbitals are denoted by band gap of energy and these energy levels play important role in the semiconductor properties of semiconductor materials [22]. Particularly, large size molecules having a wide band of energy therefore their band gap of energy between the HOMO/LUMO energy orbitals are small [23].

Only those semiconductor materials make a better and high efficiency organic solar cells that contain a small energy gaps. Organic materials in the form of semiconductors based upon two main classes like polymers and small oligomers [24]. Geometry and design of organic solar cells are based on the organic semiconductor properties like excitonic properties and it is called excitonic solar cells [25]. The materials that made organic semi-conductors are malleable, ductile, low molecular weight, easily manufactured and having other great properties [26]. Organic materials that showing semiconductor properties showed photo-active layer for organic photovoltaic cells but with the passage of time its demand will be increased due to having other different semi-conducting properties [27] like OFET [28], LASER [29], SENSORS [30] and Solar Cells [31] etc.

Photovoltaic organic materials

Photovoltaic effect is responsible for changing sun light into electric energy from in-organic solar cells with the help of p-n junctions but now a days in-organic solar cells are replaced with the organic solar cells that contain semiconductors of organic materials and it is called organic photovoltaic devices [32]. Organic photovoltaic devices contain the conjugated molecules that showed strong semiconductor properties and this device can be classified into further two types like polymer based and small molecule based organic photovoltaic devices [33]. But polymer based organic photovoltaic device show high power conversion efficiency as compared to the small molecule based organic photovoltaic devices [34]. Whereas, small molecule based organic photovoltaics are preferred due to having better photovoltaic properties like higher electron hole mobilities, improved fill factor, increase V_{oc}, enhance J_{sc}, easy synthesize procedure and also showing a strong absorption band in the visible region [35]. Small molecule based organic photovoltaic cells show high power conversion efficiency with fullerene acceptors [36] as compared to organic solar cells of fullerene free acceptors having power conversion efficiency of < 6% [37] whereas fullerene acceptors having many disadvantages like weakened the absorption band in visible region, increase the cost of synthesis, difficulties in handling the tunable energy levels at large scale and lower the semiconducting properties of organic solar cells.

Factors involving the solar cells designing

Lower energy level of HOMO orbitals, broad absorption band in visible region, high hole mobilities due to low steric hindrance in the structure and low band gap energy between the HOMO/LUMO energy orbitals are important steps in the designing of polymer and small molecule based solar cells [38]. Moreover, replacement of different electron withdrawing groups on the acceptors part of organic solar cells lower the energy level of HOMO orbitals. Moreover, solar

cells efficiency can be enhanced with increasing the molecular weight of structure that constitute the solar cells devices [39].

Classification of organic solar cell's

- Small molecules based organic solar cells
- Polymer based organic solar cells

Small molecules based OSC's

Present research is totally focused on developing the high PCE's of small molecules based OSC's due to having low cost, easy synthesize procedure and tunable absorption properties. But it is big challenge to increase the efficiency of small molecule based organic solar cells as compared to polymer based organic solar cells which still having a high efficiency [40]. In both small and polymer based organic solar cells, gap of energy between the HOMO/LUMO energy orbitals are very important [41]. Polymer based organic solar cells with A-D-A type moiety attain great attention due to their solubility, tunable energy level on large scale and planarity in structure which is called push/pull structure [42]. Push and pull small molecules based organic solar cells develop fastly due to their attractive performance [43].

Small molecules based organic solar cells with A-D-A type moiety contain central donor part of electron and around the donor part of both end it contain a two electron withdrawing groups that showing the properties of electron acceptors which is responsible for the optical and charge transport properties of organic solar cells [44]. Due to their broad absorption band in visible region, excellent charge mobilities of electron/hole and using a conjugate bridge in combination with suitable acceptor-donor-acceptor (A-D-A) pattern, small organic molecules becoming a very important for developing organic solar cells [45]. Phenyl C_{61} Butyric acid Methyl ester used as standard electron acceptor [46] in developing small molecules based organic solar cells that with different and unique materials and showing appropriate frontier molecular orbitals energy levels but high absorption, stability and charge mobilities are still big challenge in making high power conversion efficiency of small molecules based OSC's [47].

Polymer based OSC's

Polymer based organic solar cells made up of different semi-conductor materials that show fundamental properties in other memory devices [48], LEDs photodiodes [49], Diode [50] and field transistor effects [51]. Electronic properties of polymer based organic solar cells depend upon energy of band gap between the HOMO/LUMO energy orbitals. Band gap energy in polymer based solar cells should be narrow which are obtained by designing the central donor part with high HOMO energy values and ending part (acceptor) around donor atom with low LUMO energy values which facilitate the internal charge transfer at the donor/acceptor interface [52]. In polymer based organic solar cells, short exciton diffusion and dissociation occurred due to their strong electron/hole pairs with strong binding energy so the generation of free electron and hole carriers is very difficult to construct a polymer based solar cells. So, structure with Acceptor-Donor-Acceptor (A-D-A) moiety are used for efficient transportation of charge in polymer based solar cells giving upto 60% efficiency [53]. Different electro-chemical process separates the charge that further separate the electron/hole pairs in Acceptor-Donor-Acceptor (A-D-A) type materials [54].

Narrow diffusion length of electron and completely decrease the external quantum efficiency of polymers. Therefore, perception of Bulk hetro-junction is used due to their phase separation that occur at nanoscale which enhanced the transportation rate of electron/holes [31]. So, the bulk hetro-junction will prefer to enhance the working abilities of polymers [55]. Polymer based organic solar cells are much better than small molecules based organic solar cells due to having small gap of energy between the HOMO/LUMO energy orbitals and large power conversion efficiency which are still trying to achieve in small organic solar cells molecules. But low molecular weight that are helpful in their purification, small molecules are largely used to construct active layers in organic solar cells [56]. Polymer based organic solar cells show higher power conversion efficiency due to their large solution processing abilities as compared to silicon based organic solar cells [57]. Naphthalene and Perylene Di-Imide based central donor part are the common examples of polymer based organic solar cells

Imide based polymer solar cells

Strong absorption band and modification in structure could be achieved by making the organic solar cells with imide-based materials. Perylene Di-Imide (PDI) and Naphthalene Di-Imide [58] are two main building block of polymer based solar cells due to having large mobilities of electron/holes and show the well match energy levels with polymer donors which are used as semi-conductor materials [59].

Imide central unit

Small molecules that contain Naphthalene Di-Imide central unit with A-D-A moiety are very important in the construction of small organic solar cells due to their low cost, simple synthesis method, having broad absorption band in visible region, fundamental photovoltaic properties and large solubility power in the organic solvents. Imide based organic solar cells molecules are also important example of n-type acceptors materials that are very helpful in the construction of polymer based organic solar cells [60]. Perylene Di-Imide based fullerene free acceptors are also used in small organic solar cells by restraining their aggregative effect and enhance their miscible properties with polymer donor. Due to their planner and rigid structural unit, Perylene Di-Imide form large sized shining crystals in the solid form that strengthen the morphological properties of bulk hetro-junction [61]. In Perylene Di-Imide, aggregation effect can be control by joining the Perylene Di-Imide units together to form the dimer or multimer by changing the solvent and structural properties which are very helpful in aggregation breakdown [62].

Polymers that are made up of fused Di-Imide rings can also be used as electron acceptors in polymer based organic solar cells. Dimmer or multimer Perylene Di-Imide units show small gap of energy between the HOMO/LUMO energy orbitals due to extended conjugation in their structure and controllable aggregation effect. Polymer solar cells that contain imide based central donor part are important example of n-type acceptors [63]. Naphthalene Di-Imide based fullerene free acceptors show the power conversion efficiency of 3.07% and improve fill factor 0.69 [64]. These fill factor and power conversion efficiency of Naphthalene Di-Imide based solar cells are higher as compared to any previously developed NDI solar cells. The power conversion efficiency of Naphthalene Di-Imide based fullerene

free acceptors can be enlarge by introducing the sulphur in their structure that increase the J_{sc} and V_{oc} [65].

Organic solar cells

Earliest organic solar cells contain single layered electronic material that are sandwiched between two conductors of metallic form in which Indium tin oxide active layer are packed around the magnesium or aluminum layer which was poor in performance [66]. The electronic material that are sandwiched when absorb photon from the sunlight create excited state which are attached to the molecule on polymer chain. These electrostatic interactions are managed by the field produced due to two different layers of metals. Now the electronic material that absorb the photon from the sun light release the electron to acceptor part that produced the electric current [67]. Poor performance of single layered organic solar cells led to the discovery of multi layered organic solar cells which contain two different type of electronic materials that are sandwiched between the two conductive layers. In multi layered organic solar cells, only those electronic material use that have a large ionization energy for the effective collection of charge at acceptors part .

Tang in 1986 [68] report the new organic materials Organic Light Emitting Diodes (OLEDs) that showing strong opto-electronic properties as compared to organic solar cells which are already exist before 1986. Organic solar cells are basically two main types, one is containing donor/acceptor absorption material and second contain the multiple layers of acceptor and donor materials that showing fundamental properties [32]. Small organic molecules that are vacuum deposit and large polymer molecules are used for the construction of organic solar cells [60]. Efficiency of organic solar cells are directly related to the energy of HOMO orbitals because its strongly influence on the V_{oc} of solar cells device. To make the highly efficient organic solar cells device, it should be needed to make its HOMO energy orbitals highly destabilized and band gap of energy between the HOMO/LUMO energy orbitals should be minimum as possible but not less than 0.3 eV for the efficient separation of charge between the donor (HOMO) and acceptor (LUMO) part of organic solar cells [47].

Working principle of organic solar cells

Organic solar cells consist of two main parts, acceptor which is made up of n-type semi-conductor and donor part which is made up of p-type semi-conductor. The mechanism of organic solar cells based on the generation of charge specie with the help of sun-light and divided into four steps; (i) generation of electron/hole pair with the help of light [42b], diffusion of this generated charge, (iii) separation of diffused charge and (iv) movement of charge towards the respective part of solar cells devices like hole move toward the donor fragment and electron move toward the acceptor part. This movement of electron and hole will responsible for the generation of electric current at the donor/acceptor interface [69]. Those molecules that showing low gap of energy between the HOMO/LUMO energy orbitals will be highly efficient and show the large power conversion efficiency [70].

Power conversion efficiency

The term power conversion efficiency are mainly depend upon the band gap of energy between the HOMO/LUMO energy orbitals, Fill Factor (FF), J_{sc}, V_{oc}, absorption trend in visible region and their fundamental properties of electron/hole mobility [24]. Fill factor of OSC's can be enhanced by lowering the energy of its HOMO energy orbitals which could led to the large amount of open circuit voltage occurring at zero current level [71]. Efficiency of OSC's can also be enhanced with increasing diffusion rate of generate charge which than move faster toward their respective poles [72]. But worldwide scientists are working on a single point agenda which is to decrease manufacturing cost of photovoltaic devices that it can come in range of every person. Scientist developed different solar cells devices that showing range of efficiency from moderate to high like dye sensitized small solar cells molecules show < 12% power conversion efficiency normally 11% [73], poly-crystalline solar cells having 12 to 20% efficiency, silicon based solar cells having 20% efficiency and tandem solar cells that having multiple layers of Ga-In-P_2 and Ga-As showing one of highest 30% efficiency in the category of recently developed organic solar cells [74]. Dye sensitized organic solar cells having low manufacturing cost as compared to all others but its power conversion efficiency is less from all others [75].

In-organic & organic solar cells

Electron/hole pairs generation in the presence of sun light is one of main difference between the organic and inorganic solar cells which only happened in organic solar cells [71]. Previously, it was thought that conversion of sunlight into the electric energy is totally based on silicon materials that having strong opto-electronic properties of inorganic semi-conductors. But now a days, scientist developed solar cells that are totally depend on organic semi-conductors materials which replace the inorganic silicon semi-conductors due to their high cost and week electron/hole pairs generating abilities [25]. It's true that efficiency of inorganic solar cells are high but due to high cost and week absorption band in the visible region scientist community are moving toward the organic solar cells which having easy synthetic gateways and strong absorption band in visible range [11].

Computational Chemistry

Chemists playing important role in computational science development. Computational science mainly covers the area of chemical, mathematical, quantum calculations and theoretical calculations of those parameters that we obtained experimentally after paying a huge income and spend lot of our time in lab. Due to development of computational science scientist are no need to go in the experimental labs and work with poisonous chemicals. Now super computers are come on which we do all our theoretical calculations with the help of computational chemistry protocols and commands. In computational chemistry, we find the solutions of problems which the scientist face after performing a lot of chemical reactions and synthesis but they not know that the product which they made or reaction which they run are feasible or not [76]. Computational chemistry is basically the pre-study of any chemistry process and tell us that the work which we want to do are feasible or not. With the help of computation chemistry different quantum calculations are performed that tell us about the rate of reaction, frequency of reacting species, oscillating parameters and much more other factors quickly and fastly. Computational chemistry provides us information about the absorption trend, reaction intermediate stages, symmetry of structures, solubility of products and Eigen strength of our structures.

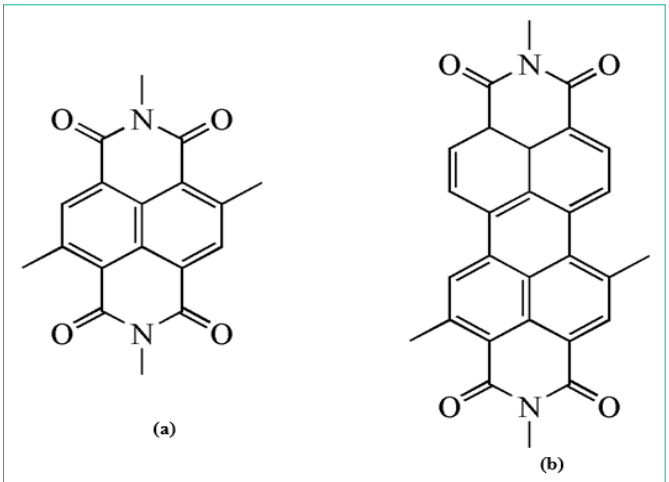

Figure 1: Molecular structure of (a) Naphthalene Di-Imide and (b) Perylene Di-Imide central unit.

Computational chemistry done all the calculation with the help of Gaussian 09 software that contain the different theories, basis sets, functionals and other factors each giving us different results due to their different energy levels [77]. Now the chemistry become so easy with the help of computational science and their quantum calculations. Scientists need to sit in their air conditioner room and work on super computers containing computational software and operating systems like fedora and Linux etc. All the results which we obtained from the simulation analysis of our structure are 100% authentic. We can also perform the aggregation analysis with the help of this computational chemistry tools [78]. Computational chemistry tells bond length, dihedral angle, bond positioning and geometrical optimized structures. In computational chemistry we can also designed large number of new molecules or derivative by taking one experimentally reported molecule reference and matched the opto-electronic properties of newly designed derivatives and molecules which the scientist community are synthesize experimentally later. It solves the 80% problems for the scientist to work experimentally on those molecules on which theoretical study already done by computational chemistry tools and their calculating theories. Computational chemistry also provides us the inner view of our chemical structures and tell us the stability and de-stability of HOMO/LUMO energy levels [79].

In this research work, we designed many new organic solar cells molecules with the help of computational chemistry tools and check their opto-electronic properties, HOMO/LUMO stability, absorption parameters, geometrical states and others influence factors that are matched with reference molecules.

Gaussian 09 package

Computational chemistry based on Gaussian 09 package that provide the authentic, reliable, accurate and faithful results about our chemical structures. Gaussian 09 package is unique from other computational chemistry software's that it can operate in any Microsoft operating systems like 32 and 64-bit operating systems [80]. It contains different functionals, models, basis sets, check point server and other tools which are described in detail as follow:

Functionals and models

Computational chemistry work with different functionals, models and basis sets by involving different orbitals. Each model and basis sets provide us different results which based on their energy levels and basis sets. Some models giving us results in very short time due their calculations occurring immediately but their results are not reliable because the other models whose results are more reliable are exist which provide us results in long time based on their functionals and calculating parameters [81]. So, we say some models best based on results which they produced in a very short time as compared to the others functionals whose calculations are occurring in long time but both types of functionals are working on the principle of computational chemistry operating ways. Three main points kept in mind during the selection of functional and models for your calculations.

- Size of system which you're under consideration
- Time in which you want to complete your calculations
- How many accuracies you want in your results

These three points decided which models and functionals are best for our theoretical calculations. Most reliable results required long time and super computers with multiple processor that reduced the time of our calculations. Some models calculate their jobs in short time but their results are not reliable [82]. Therefore, authentic and reliable results require a time and highly working capacity of super computers with highly advanced processors and their data storage parts which are only possible in latest Linux operating systems [83].

Ab Initio methods

Ab Initio method work without any experimental results and complete their calculations which we demand. This method completes their calculations in long time due to work in the absence of reference compound results. But their results are more authentic and reliable in the field of computational chemistry and scientist trust on this method [84].

Hartree fock method

Hartree Fock method is the main type of Ab Initio method. In this method, we used the central field of approximation for the quantum calculations. This approximation work with average columbic repulsion between the electrons which are responsible for their repulsive interaction. Hartree Fock method work with two different ways depending upon whether our molecules are charged or neutral species [85].

- Un-restricted Hartree Fock method
- Restricted Hartree Fock method

Un-restricted Hartree Fock method performed individual calculations for each electron which is in the paired form. This method is mainly suitable for ions, radicals and excited states calculations of molecules. Restricted Hartree Fock method performed their calculations for the pair of electrons that are in the same pair and having no contamination of spin. This method is best for paired of electrons [86].

Semi Empirical Methods

The working principle of semi empirical method is similar like the

Ab Initio method but semi empirical method requires experimental data of reference molecule for the comparison of results. In every calculation, we are not interested to calculate each parameter again and again. In this method we store our result in the library which are created inside this method that are very helpful in next calculation based on similar parameters. Like in first calculation, we calculate the C = C bond length which is 134 Pico meter which should be same in every structure having same bonding parameter. Semi empirical method performs their calculations in long time but their results are not very accurate and most reliable that's why we need the reference molecule experimental results in this method for the comparison of both theoretical and experimental results and found out their deviation in between both results [87].

ZINDO is sub-class of this method which are large used for computing the transition of electrons in ultra-violet region of solar cells spectrum. Austin model is example of this method which are mostly used for the designing of organic molecules. Zerner-INDO (ZINDO) method is commonly known as S-INDO (spectroscopic-INDO) method because of their largely used for recording the ultra-violet transitions of electrons. To predict the electronic spectra of any structural compound, ZINDO method are commonly used [88]. ZINDO method are used for any types of compound except that having un-paired electron to predict their electronic transition and spectral properties. But ZINDO method don't provide satisfactory results during the ground and excited states of molecules during the geometry optimization stages. To overcome this problem, Austin model are used for the organic molecules geometry optimization steps and further theoretical calculations [89].

Austin model 1 (AM-1)

Austin model 1 are largely used for the computational analysis of organic molecules to predict their formation heat. MNDO method are less accurate as compared to DHF but it also failed to provide accurate results in the case of bromine atom. Austin and Para-meterization model are used for the organic molecules to provide accurate results in semi-empirical method. It also depends upon the system for which we want to use it for the computational analysis of organic structural compounds [90].

Para meterization 3 (PM-3)

Para-meterization method work on similar route like Austin model but it has more reliable parameters that increase the authentication of its results. In comparison of Austin model and Para-meterization method to study the theoretical properties of organic molecules, Para-meterization method provide more authentic results over the Austin model and its reliability are more as compare to the Austin method. Para-meterization method also provide us reliable results in the case of bromine and hydrogen atom which we not obtained with Austin model [91]. But calculation of bond energy will be occurring more accurately in the case of Austin model. So, both Austin model and Para-meterization method having some advantages and disadvantages but overall both these methods provide authentic results as compared to the semi-empirical method because both Austin and Para-meterization methods perform their calculations on logarithm principle [92].

Gaussian theory

Three main types of Gaussian theory like G-1, G-2 and G-3 are very important in the computational chemistry for theoretical calculations of organic molecules electronic properties [93]. These three Gaussian theories were developed due to finding an error in calculating the ground states energy of organic molecules with the help of Ab Initio method. These ground states energy of organic molecules are further confirmed with different equations to make our results authentic and reliable because Ab Initio method missing some calculations during the computational analysis.

Density functional theory

Dirac, Fermi, and Thomas working together on the computational chemistry and developed a theory known as Density Functional Theory which is one of the most authentic and reliable theories in all over the previously existed computational theories. Professor Kohn got the Nobel prize in chemistry in 1998 on giving the idea of Density Functional Theory [93]. This theory explained the electronic properties of the organic and inorganic compounds in the term of density and quantum mechanics. Density Functional Theory are largely used in computational chemistry for theoretical analysis of any compounds and provide most authentic and reliable results from all other theories of computational chemistry [94]. Density Functional Theory become most authentic computational chemistry method for calculating any parameters within shorter time and generate authentic results. Density Functional Theory containing many functionals like LSDA, BPV86, B3LYP, CAM-B3LYP, B3PW91, MPW1PW91, PBEPBE, HSEH1PBE, HCTH, TPSSTPSS and WB97XD [95]. Density Functional Theory results can also make more authentic by involving valence shell electronic orbitals like p, d, and f orbitals with large number of basis sets. Bond length, bond angle, absorption spectra's, stability and destability of any designed compounds, different opto-electronic properties and excited states energy can easily be calculated with the help of this theory [96].

Density Functional Theory are totally based on the density of electrons which provide us the energy of whole systems and electronic density also tell us the number of electrons that exists in whole systems. It was observed that large electronic density is found around the bond and atoms in respective molecules. Density Functional Theory help the Schrodinger wave equation to apply in every type of systems which fall before the discovery of this theory [97]. This theory provides accurate results for those systems which have minimum degree of freedom which can be reduce with the help of Born Oppenhemer rules like the moment of ions and electrons can be compared when their both ionic and electronic force will be in same direction. During the comparison of both electrons and ions, it was observed that ions move with the massive speed as compared to the electrons and their kinetic energy is also small from electrons. When ions are moving electron will respond quickly which is explained by the Born Oppenhemer rules. Electron consider to be in the ground state during the calculation of ions which are helpful in calculating the total energy of system. The Born Oppenhemer rules are applied only when the nucleus considers to be in stationary phase and electrons are in moving phase in any systems [98]. Density Functional Theory reduce the time of theoretical calculations which gives it priority on selecting from other theories for the computational calculations within a shorter time. Hartree Fock method provide us results that are based on the wave functions whereas Density Functional Theory make their whole calculations based on electronic density.

Review of Literature

Demand of solar energy production increase dur to easy availability of sun light, low cost energy conversion systems, no need of its maintenance many time and strong outcome voltage which are used in our daily energy consumption requirements [99]. Solar energy is free from dust and easily obtained from the sun light with the help of different solar cells devices [40]. Researchers developed various alternative energy sources from the fossil fuels but solar energy is best from all other due to its low cost and strong output efficiency. Large number of factors are strongly influenced on our demand of energy [5]. Computational chemistry brings a lot of change in the field of science and are largely used to design new molecules that having better absorption properties in the visible range as compared to already existed molecules. Thermodynamics explain the mathematical term of chemistry and describing the energy, heat of formation, reaction kinetics and entropy parameters in detail of any occurring reactions. Computational chemistry performs whole of their calculation with the help of quantum mechanics that tell us the electronic behavior in mathematical term. Quantum mechanics also explain the different electronic and atomic properties and can also explain the different electronic systems within a short time [100]. Quantum calculations are totally based on the Schrodinger wave equation and Heisenberg uncertainty principle that are important parameters of computational chemistry. Schrodinger wave equation are explained by the following expression:

$$\hat{H}\psi = E\psi$$

In above expression [101], ψ is the same on both side of expression which is called wave function, E is the energy of system and H is known as Hamiltonian operator used for the energy of systems.

Photovoltaic materials from bulk hetero-junction

Electron donor and acceptor part are the main components of thin film bulk hetro-junction solar cells devices. Donor part are made up of conjugated oligomers, polymers and small molecules whereas acceptors part comprising of different electron withdrawing groups. Previously, fullerene derivatives are largely used for electron acceptors in solar cells molecules due to their high efficiency and great light dependent physical properties [102]. But due to their high cost, complex synthesis scheme and absorption properties in the visible range fullerene acceptors are replace with non-fullerene acceptors in the modern bulk hetro-junction organic solar cells devices which consists of thin film active layer that are solution processable and show large area with a little cost [103]. Properties of polymers can easily be controlled by joining different monomers units during the synthesis process which gives us the respective properties of donor and acceptors in solar cells devices. Earlier 2008, conjugated polymers were only synthesized and are used for different semi-conductor's properties such as OLEDs. But now large variety of polymers are synthesized and used for solar cells applications to enhance its power conversion efficiency and provide more output voltages. Polymer based organic solar cells can also be used to control the opto-electronic properties of solar cells devices and can also enhanced the rate of electron and hole mobilities. Synthesis of conjugated polymers are difficult to handle on small scale that require a special reaction blocks. But now a day, its synthesis become easy with the help of Stille poly-condensation reaction, Gilch synthesis route, Suzuki condensation reactions Grignard reagent reactions [104].

Comparison of fullerene and fullerene free acceptors

Fullerene and its derivatives are largely used for acceptors properties in the previous organic solar cells devices. Most commonly used fullerene derivatives are Phenyl C_{61} Butyric acid Methyl easter, Phenyl C_{71} Butyric acid Methyl easter, Indene C_{60} Butyric acid and Indene C_{70} Butyric acid for the high transport rate of electron and hole at nano-scale level in the polymers based organic solar cells [105]. Fullerene derivatives show the excellent properties of electron and hole, high power conversion efficiency and large open circuit voltages but they also show a huge disadvantage like week absorption band in the visible region, complex synthesis procedure, face lot of difficulties during their purification and high cost [106]. That's why scientists are trying to develop the fullerene free acceptors in the organic solar cells devices that overcome this problem which the fullerene acceptors show in the solar cells spectrum and show the satisfactory results [107]. Fullerene free acceptors in the organic solar cells increase the Open Circuit Voltage (V_{oc}) that occurring at the zero-current level, short circuit current density (J_{sc}) occurring between the donor/acceptors terminals, enhance the photovoltaic properties such as mobility of electron and hole, strengthen the absorption band in the visible range of solar cells spectrum and increase the stability of solar cells devices [108]. Perylene Di-Imide, Naphthalene Di-Imide, Benzo-thiazole and Poly-3 hexyl-thiophene based organic solar cells are the important examples of fullerene free acceptors of organic solar cells devices [105].

Fullerene free acceptors in organic solar cells generate a large amount of charge on providing a little energy which is too small that we can also neglect it whereas fullerene acceptors requiring a large amount of energy for the charge generation. This driven energy is required necessarily for the brake down of strongly bonded electron at the donor/acceptors interface and this brake down are responsible for the generation of electric current [109]. Because fullerene acceptors based organic solar cells need large driven energy for charge generation, this driven energy when decreased to minimum point small amount of voltage will be loss that will show the week absorption band in the visible region. Fullerene free acceptors based organic solar cells show the 90% quantum efficiency of internal systems despite having the zero-driven energy because it's require a very small amount of energy for the generation of charged electronic particles which we can be neglected in quantum calculations [110]. That's why fullerene free acceptors show strong V_{oc} and J_{sc} as compared to fullerene derivatives based OSC's. But it is still not clear that generation of charge with small amount of energy are due to the fundamental properties of fullerene free acceptors or due to their associated energy levels that occur between the donor/acceptors interface in fullerene free organic solar cells molecules [111].

Poly 3-hexyl, 2-5 thi-enylene-vinylene polymer showing one of the smallest band gap 1.65 eV between the HOMO/LUMO energy orbitals that are synthesized with the help of diene polymerization reaction and introduced this polymer in thin film active layer of Bulk hetro-junction organic solar cells molecules with respect to the PCBM for improving the electronic properties of polymer based organic solar cells molecules. Polymer blended with PCBM were further analyzed

by different characterization techniques like UV-Vis spectroscopy, atomic emission spectroscopy, atomic force spectroscopy, XRD techniques and thermogravimetric analysis for determine their heat dependent properties. Maximum 60% efficiency of polymer based organic solar cells molecules were recorded by blending the polymer with thin film of PCBM [112]. In this high efficiency polymer based organic solar cells, polymer act as electron donor and PCBM act as electron acceptor that were arranged between the aluminum and indium tin oxide electrode in the form of bilayers. Previously, it was thought that fullerene acceptors show the large open circuit voltage, make the solar cells devices high thermally stable, strong LUMO energy levels, high solution processing abilities and simple synthesis procedure due to their simple configuration at donor/acceptor interface [113]. But with the research on organic solar cells devices, these terms prove wrong which encourage the scientist to develop fullerene free acceptors in the bulk hetro-junction organic solar cells devices. Electrodes of commercially available solar cells devices are designed in such a way that they can tolerate the harmful and severe conditions of environment like air pressure, large moisture contents in environment and temperature variations in those devices that contain reversed structures [114].

Moreover, solar cells devices that based on reversed structures can be changed by rearranging their bilayer arrangements at donor/acceptor interface to enlarge its power conversion efficiency [115]. Perylene Bis-Imide are another important example of fullerene free acceptors that belong to class of n-type semi-conductor. They show the strong pi-conjugated back bone, attractive light dependent physical properties, high thermal stability and strong opto-electronic properties. Perylene Bis-Imide based organic solar cells molecules show the broad absorption band in the visible region that are particularly from 400-650 nm range, low energy levels of LUMO orbitals and show similar properties of small molecule based fullerene free acceptors [116]. Perylene Bis-Imide sometimes show strong aggregation effect due to their planner structure that tend to form the continuous crystallization pattern around which lower the dissociation of electron and device performance [117]. Solubility of Perylene Bis-Imide could be enhanced by the substitution of bulky groups on ortho positions that will create a steric hinderance in their structure. Perylene Bis-Imide based organic solar cells devices provide us large power conversion efficiency due to having strong electron withdrawing groups on the acceptors part. Similarly, thiophene substitution used to create the organic group functionality in the solar cells devices [118].

1,1-Dicyano Methylene 3-Indanone and Indacene based Di-Thiophene are commonly used fullerene free acceptors in organic solar cells that provide efficient results on large scale power conversion. Due to their co-planar and rigid structure, these compounds increase the rate of charge transport between the donor/acceptors moiety, increase the solubility and inter molecular interactions between the target molecules. Due to having strong electron withdrawing groups on the acceptors parts, these molecules show the low HOMO/LUMO energy levels that increase the V_{oc}, J_{sc}, strengthen the absorption band in visible region, increase the electron transport rate and enhanced opto-electronic properties [119]. Small organic molecules containing strong electron withdrawing groups in the form of fullerene free acceptors that are usually joined together with the help of pi-bridges which lower its HOMO/LUMO energy orbitals value that are helpful to enhance the device performance. Bulk hetro-junction organic solar cells device blended with PBDTTT-C-T electron donor provide 3.93% power conversion efficiency which could be enhanced by introducing the ethyl-hexyl based spacer in solar cells structure that will doubled its power conversion efficiency [38]. Similarly, adding the thiophene based PTB-7 ring their structure, power conversion efficiency become 6.3% which are further enhance by replacing the PTB-7 with another PBDTTT-7 fragment that make the 8.4% power conversion efficiency [120].

Central donor part of organic solar cells plays vital role in absorption spectra's, device performance and HOMO/LUMO energy levels. Donor and acceptors part are joined with each other with the help of electron withdrawing pi-bridge which also increase mobility of electrons. In organic solar cells structure, replacement of C - H group with nitrogen increase the affinity of electron that led to increase the device performance. Therefore, thiazole based hetero cyclic compound provide strong electron withdrawing properties due to having C=N units in their structure [121]. But they show the strong acceptors properties and large power conversion efficiency with fullerene acceptors as compared to the fullerene free acceptors due to their low solution processing abilities in Bulk hetro-junction organic solar cells. Many fabrication techniques such as roll to roll printing etc. are largely used to make fullerene free acceptors in organic solar cells but their low efficiency is still a big challenge to gives satisfactory results. But scientists are still working to overcome this problems by introducing thick film in the solar cells structure that having the 100 nm thickness in Bulk hetro-junction devices. But trying to make large area pinhole free organic solar cells with fine reproduceable thin films is very difficult on the large scale. This problem can be overcome to increase the thickness of device around 200 nm that also improve the absorption of light [122]. But here we need to increase the rate of charge transfer for the high mobilities of charge, otherwise recombination will occur between the bi-molecular charge species.

To make high performance thick film organic solar cells, high crystallinity in structure increase the mobilities of charge carrier species that provide more output voltages in Bulk hetro-junction organic solar cells devices. In future, all the fullerene acceptors based solar cells devices will shift to the fullerene free acceptors due to their strong absorption band in visible region, low cost, easy synthesize procedures, excellent photovoltaic properties and great modifications in their structure on large scale [123].

NDI based acceptors for organic solar cells

Naphthalene Di-Imide based electron acceptors are largely used in small organic solar cells molecules due to having strong electron affinity and mobility, strong absorption band and show the similar energy levels of polymer donor [124]. NDI based organic solar cells device show 3.07% power conversion efficiency and 0.69 fill factor which is satisfactory results and encourage the scientist and researcher to develop more NDI based organic solar cells devices [64]. In thin film Bulk hetro-junction solar cells device, efficiency could be increased by decreasing the recombination abilities between the bi-molecular layers, create roughness on their smooth surfaces and lower the orientations on their polymer backbones. Scientist were manufactured the Poly-vinylene and phenylene based donor-acceptors fragments in Bulk hetro-junction solar cells that provide

the satisfactory results. But now the polymer/polymer based solar cells are also used that contain both donor and acceptors of polymer form and provide efficient photovoltaic properties within small amount of sun light [125].

The efficiency of the polymer/polymer based OSC's reached at 8% in the recent years [126]. But this efficiency found to be still lower as compared to fullerene free and fullerene acceptors that showing minimum 12% efficiency in any system of Bulk hetro-junction thick layer. The lower efficiency of polymer/polymer based OSC's is due to their complex structure and strong interaction between their inter molecular fragments [127]. That's why polymer/polymer based Bulk hetro-junction thick layer system show the difficulties in their phase separation process that weekend the charge generation process for the generation of electric output signal. Due to these reasons, it is very difficult to designed high efficiency polymer/polymer based solar cells by controlling the morphology of Bulk hetro-junction layers [128]. Different polymer/polymer based solar cells like small thiophene, medium benzothiophene and large benzothiophene show different power conversion efficiency due to difference in their structural properties [129].

Opto-electronic properties of NDI based solar cells

Organic molecules in conjugated form show the better film forming properties as compared to the oxides of semi-conductor materials. Electrical properties of NDI based organic solar cells devices can also be enhanced by making a modification in their molecular structure on large scale. Due to their planer structure, strong contacts between their inter molecular pathways and large mobilities of electrons. NDI based polymer/polymer solar cells found to be an excellent example of n-type polymer acceptors [130]. Whereas, fullerene free acceptors in polymer/polymer solar cells are not largely used due to their complexed inter molecular layers between the silicon and hybrid organic materials which decreased their efficiency. Silicon in complexed Bulk hetro-junction devices provide large power conversion efficiency due to their highly crystalline structure but cost of silicon is also high which increase the cost of energy conversion that push the scientist to develop low cost organic solar cells based on semi-conductor materials of organic materials. Amorphous silicon solar cells can be manufactured by depositing the layer of silicon on glass/metal substrates in the range of 1μm thickness with the help of vapor deposition method at high temperature. But temperature will lower as 75°C in the case of depositing the silicon layer on plastics [131]. In this form, pi-layers having small sequence in cell structure but this single small pi-payers decreased the 15-35% power output during the generation of electrical output from the sunlight [132].

Decreased in their power output were explained by the two scientist Staebler and Italian scientist named Wronski which is called Staebler-Wronski effect [133]. To overcome this issue, thin films are used across the strength of electric field that will stable the device in the case of harmful temperature conditions. But thin films will show the week absorption band and low efficiency in OSC's which can be improved with increasing the thin layer numbers which are joined together in overlap pattern like the top of one another. Single layer silicon based solar cells show low device performance as compared to the multiple layered organic solar cells that capture the maximum amount of sun light and provide more current density at low voltages. Amorphous single silicon layered show the maximum 7% efficiency whereas the efficiency of crystalline silicon is 18% [134]. OSC's efficiency can be enhanced by introducing crystallinity in solar cells structure that increase the solution processing abilities which are very helpful for further fabrication of Bulk hetro-junction solar cells devices. The 7-10% decrease in the efficiency of amorphous silicon are explained by the Staebler-Wronski effect when placed in sun light for the generation of charge carrier [135]. The only benefit of single layered amorphous silicon based solar cells are they having low cost in comparison with multiple layered tandem type solar cells devices that need special conditions for their synthesis which increase their manufacturing cost.

DFT Study of acceptors molecules

Density Functional Theory are largely used for the optimization of excited and ground states geometries. Fullerene free acceptors show the excellent solution processing properties in the construction of Bulk hetro-junction solar cells devices. Power conversion efficiency of Perylene Di-Imide based organic solar cells are higher as 6% as compared to the Naphthalene Di-Imide based solar cells devices which show 3.07% efficiency and fill factor of 0.69 [64]. Perylene Di-Imide show the strong interactions between their inter molecular orbitals which increase the planarity in structure and phase separation that enhance the rate of electron mobility in solar cells devices [136]. Absence of organic materials that show the excellent properties of semi-conductor is the major hurdle in the way to develop non-fullerene acceptors in organic solar cells devices. Better semi-conductor materials are responsible for the acceptors charge transport properties, solvation ability in organic solvents at suitable energy levels and their morphological characteristics. Naphthalene Di-Imide are also largely used in the form of dye material that change the absorption levels on constructing the device at large scale and can perform the modifications in device structure easily with this material. In the case of Bi-NDI (Bismuth-Naphthalene Di-Imide), methyl group substitution was replaced with large chain of alkyl group and perform their theoretical calculations with the help of DFT by using different functionals and basis sets and then compare all results with the experimentally reported data [137].

In between the Vinyl and Naphthalene Di-Imide groups, torsion angle can be recorded with the help of different states. HOMO/LUMO wave functions were completely delocalized in their structure due to great electronic and semi-conducting properties of Vinyl blended with Naphthalene Di-Imide based solar cells structure [138]. Perylene Di-Imide based fullerene free acceptors are largely reported which contain the n-type acceptors of semi-conductor materials. Perylene Di-Imide based solar cells show the large thermal stabilities, strong electron withdrawing groups at the acceptors part, high power conversion efficiency, excellent absorption properties and great mobilities of electron. Perylene Di-Imide show the better opto-electronic properties as compared to the fullerene acceptors based solar cells devices and their opto-electronic properties are further improved by replacing the imide group with sulphur atom in their structure that provide the more V_{oc} and J_{sc} [139]. But replacing fullerene acceptors with fullerene free acceptors in organic solar cells devices will cause difficulties in frontier molecular orbitals, decrease the absorption in visible range and lower their fabrication process that form crystallization during the synthesis. Whereas fullerene free

acceptors show the absorption band which are tunable at large scale by replacing the acceptors moieties at the end of solar cells structures that increase the extinction co-efficient of electrons for the generation of current [113].

LUMO energy levels also play important role in the electron transfer and open circuit voltage, so its stability is also very important which are achieved by using the polymer donor that reduce the energy loss during the process of electron transfer in the presence of sun light. Bulk hetro-junction solar cells devices are modified with the passage of time from small, electron deficient and planner organic molecules to fullerene acceptors and now with fullerene free acceptors that show the easy synthesis procedure and strong absorption properties in the visible region. Now a day, scientist trying to develop solar cells devices that show the large power conversion efficiency with the help of fullerene free acceptors in their structure [109]. Because fullerene acceptors will become the un-stable in the air pressure, extreme temperature conditions, show the narrow spectral band in visible region and high cost of production [123]. Semi-conductor materials in the form of fused ring like rubrene and pentacene show large mobilities of electron particularly in the range of $20cm^2 V^{-1} s^{-1}$ [140]. LUMO energy levels can be lowered by introducing the amide, imide and cyano groups based electron with-drawing units in the pi-conjugated structure of semi-conductor materials because energy of π^*- level in electron with-drawing groups are closed to LUMO energy level that will stabilize the LUMO orbitals. This strategy changes the donor fragment into electron acceptor units like Rylene to Rylene Di-Imide system. In 2007, Zhan *et.al.* designed the Perylene Di-Imide based polymer acceptor that show the great photovoltaic properties in polymer based solar cells devices [141].

But system based on fused rings show strong aggregation effects due to having highly planner structure that result in formation of crystalline domain which is around 1 μm in range particularly in the case of Rylene Di-Imide [142]. This crystalline domain will reduce the charge separation abilities at acceptor/donor interface, lower the efficiency of polymer based solar cells and enhanced the phase separation in the formation of Bulk hetro-junction solar cells. To overcome this issue, side chains that are rigid and plane are introduced in fused rings which lower the aggregation and planarity effect in their structure. Naphthalene Di-Imide based solar cells are the important example of polymer based solar cells which contain highly electron deficient electron core which require necessarily in the formation of n-type semi-conductor material. Therefore, NDI based polymer show the excellent electron capturing properties when blended it with comonomers and imide group in the structure of NDI can easily be replaced with other substituents for increasing its solubility in the formation of thin film Bulk hetro-junction solar cells [143]. Perylene Di-Imide have small molecular weight as compared to the Naphthalene Di-Imide due to having small conjugated core. Moreover, replacement of imide group with other substituents increase the crystallinity in their structure, improve their morphological properties, phase separation and blending properties of polymer. Purification of NDI based polymer can be controlled during the addition of NDI monomers that facilitate the formation of highly crystalline and planner polymer structure [144].

Based on this principle, large variety of NDI polymers are synthesized that provide satisfactory results and efficient separation of charge at the donor/acceptor interface. Star shaped NDI polymer named NDI-2-OD-2T are also synthesized which are known as N2200 [145]. N2200 show the high mobility of electron and are strongly recommended for the construction of fullerene free acceptors in the polymer based organic solar cells structures. NDI based polymer when blended with P_3HT giving the efficiency of 0.16% [146], with 1/ P_3HT gives 1% efficiency by changing the solvents and solubility conditions and with the mixture of Chloro-Naphthalene and p-xylene gives 1.4% power conversion efficiency [145]. These experiments tell us that NDI based polymer solar cells having different power conversion efficiency under the different conditions by using the different solvents and different reaction conditions. But NDI based polymer blended with BDT system containing the donor/acceptor fragments show the power conversion efficiency of 4-6% in the last two years. It was also observed that power conversion efficiency of polymer based solar cells depend upon the molecular weight of donor part. Larger the molecular weight of donor part, larger will be the crystallinity in their structure and larger will be their intermixing abilities with the acceptors part that harvest the more sunlight and provide the more V_{oc}, large efficiency and their PCE's reached above 5% [147]. So, the efficiency of polymer based solar cells can be enhanced by increasing its molecular weight by joining the large number of monomer units in their structure but it will increase the cost of device which is a major issue in power conversion process of solar cells devices.

Overview of solar cell types and efficiency

Different type of solar cells showing the different power conversion efficiency depending upon their structure and Bulk hetro-junction thin film active layers. Mono-crystalline based silicon solar cells show 22-24% [148] power conversion efficiency whereas poly-crystalline based silicon solar cells show small power conversion efficiency as 18% [149] from their mono-crystalline counterpart. The manufacturing cost of poly-crystalline based silicon solar cells are low as compare to the mono-crystalline silicon solar cells but its power conversion efficiency is low which discourage the scientists which are working on it. Poly-crystalline based silicon solar cells require special reaction conditions for their manufacturing whereas amorphous based silicon solar cells can easily be made by creating its layer on metal or glass substrate with the help of sputtering process which lowered its cost from the commercially manufacturing process [150]. We can also enhance the efficiency of solar cells by making improvements during the designing of organic solar cells structures. PERL solar cells show the 24% power conversion efficiency due to their pyramid structure that increase the area of absorption in the presence of sun light [151].

Solar cells that are manufacture from the same materials contain the same p/n junction. But the solar cells that are manufacture from different materials have large manufacturing cost due to the involvement of different materials and show different absorption properties so the overall absorption band will become week due to counter fight of dissimilar materials. Moreover, to handle different materials in same solar cells devices require special conditions and interrupt the charge separation process at the donor/acceptor interface. Like by making the solar cells with Ga-As layers show different wavelength as compared to those solar cells that are made with Al-Ga-As layers that show the week absorption properties from the first one that contain few different materials in their

composition as compared to the second one that have more different components in their composition [152]. So, high efficiency of solar cells can be achieved only to use minimum different components in their composition and to form strong homo-junction layers that will make the efficient separation of charge at donor/acceptor interface. Passivative layers in their structure remove charge trapping and dangling bonds which increase the gap of energy between the HOMO/LUMO energy orbitals and lower the absorption band in visible range.

Amorphous solar cells based on silicon and germanium materials also have passivative layers of hydrogen atom like Ge-H and Si-H which reduce their charge trapping strength at the acceptors moiety that lower the absorption band and power conversion efficiency of solar cells devices. Solar cells efficiency can be enhanced by connecting large number of the cells in a series to make planner like pattern and add more crystalline units in their structure that enhance its solubility power and crystallinity that are helpful in making thin film Bulk hetro-junction active layer. This type of solar cells is called tandem solar cells. Tandem solar cells form two p/n junction layers in which the first one layer contain high gap of energy between the HOMO/LUMO energy orbitals as compared to the second layer [153]. These two layers are basically made up of two different solar cells that are connected in a series in which first solar cells show week absorption band while the second one generates the strong band of absorption in the visible region. Tandem solar cells show high power conversion efficiency due to containing two different solar cells that absorb the large amount of sun light but their manufacturing cost are also increased due to connecting the two solar cells in series. Tandem solar cells can also be made by using germanium and silicon material with passivative active layer of hydrogen atom [154]. This type of type of tandem solar cells have low manufacturing cost and high-power conversion efficiency.

Cadmium Telluride (Cd-Te) thin film solar cells

Cadmium Telluride (Cd-Te) thin film solar cells is one of the earliest developed photovoltaic technology that having low cost and easy synthesis scheme [155]. Cd-Te based solar cells exhibit the small gap of energy between the HOMO/LUMO energy orbitals which is about 1.5 eV, high opto-electronic properties and large stability in their chemical structure. Due to these benefits, scientist paying a huge attention towards the Cd-Te based solar cells. Due to their small band gap, Cd-Te thin film solar cells lower the hurdles in the way to absorb more sun light and provide strong open circuit voltage. It can be manufacture easily be making the sandwich between the cadmium and sulfide layer which show the diode junction in their circuit potential. Cd-Te based thin film solar cells can be made by creating the layers of poly-crystalline material on metal or glass substrate which are made first from the same poly-crystalline material on which we deposit these layers. As we know Cd-Te based thin film solar cells having 1.5 eV band gap of energy between the HOMO/LUMO energy orbitals and showing $5\times 10^{15}\,cm^{-1}$ molar extension co-efficient [156]. Therefore, its power conversion efficiency found to be 9-11% in range [155a,157]. Cd-Te based solar cells show the malleable, ductile and flexible properties which make its easy deposition on the polymer substrates. But its efficiency can also be affected like other solar cells devices in the harmful conditions of environments. Because the cadmium is heavy metal so it can cause difficulties for the human body, plants and animals on its handling due to their toxic and carcinogenic effects. So, its disposal require special attention and its recycling process is also typical and heavy cost which create difficulties for our society and environmental conditions [158]. Harmful effect of cadmium discourages the scientists and research community to make its usage in the construction of thin film organic solar cells [156,159].

Copper indium gallium selenium thin film solar cells

CIGS thin film solar cells consist of four different components and it is commonly known as quaternary semi-conductor material [158a,160]. CIGS thin film solar cells are directly effect on the gap of energy between their HOMO/LUMO energy orbitals due to having four different components in their composition that are strongly influenced on the absorption band of solar cells spectrum. CIGS thin film solar cells show the 10-12% power conversion efficiency which is little bit higher from the Cd-Te based thin film solar cells. CIGS based thin film solar cells can be manufacture with the help of different techniques like evaporation, electro-chemical coating, sputtering, electronic beam deposition and printing process [161]. Sputtering technique used for the synthesis of CIGS based thin film solar cells can be categorized in to two types; multiple sputtering process which involve the deposition of all the four components first and then mixing it in the sputtering chamber, and the second is single sputtering process in which all the four different components mix immediately after their addition in the sputtering chamber. CIGS materials after sputtering process can be deposited on the glass, steel, polymer and aluminum substrates [155a]. CIGS based thin film solar cells are particularly long life due to their excellent tolerated capacity in the harmful conditions of environment. Moreover, CIGS show the strong solvating properties in different types of solvents that increase its working capacity and power conversion efficiency from other commercially developed thin film solar cells devices [157,162].

Nano crystal based solar cells

Solar cells that are manufacture with the help of nano-crystals commonly known as Quantum Dots that show the excellent properties of semi-conductor materials. Nano-crystals solar cells are made up of transition metals that having the size of nano particles on the basis we say it nano-crystal solar cells. The name Quantum Dots are given to the nano-crystal solar cells due to their small size particularly in the range of few nanometers. Mostly Quantum Dots contain porous TiO_2 and porous silicon based materials in their composition [163]. In modern solar cells devices, Cd-Te, CIGS and silicon based semi-conductor materials are replaced with nano-crystal semi-conductor materials. Nano-crystals thin film solar cells can be made by mixing the nano-crystals in heating bath and then deposit these mixture onto the silicon substrate. Due to centripetal force, these nano-crystals flow and rotate very fastly. In conventional solar cells which are made from normal semi-conductor material, when it absorbs the photon from the sun light the electron will go in the excited states leaving behind the hole which is called hole/electron pair. But in the case of Quantum Dots that consist of special type of semi-conductor materials, when it absorbs the photon from the sun light it will create more than one hole/electron pair particularly two or three and in some case seven hole/electron pair observed [159a,164].

Polymer based solar cells

Solar cells that are based on polymer substrates showed flexible

properties. Tang *et.al.* report the first polymer based organic solar cells [165]. Polymer solar cells are manufactured by connected series of thin layers and coated these layers on ribbon or polymer foil. Polymers solar cells device based on the fullerene acceptors and polymer donor which can be of various types like conducting polymers that show strong absorption properties [166]. In 2000, Shirakawa, Heeger and Mac Diarmid awarded the Nobel prize in chemistry for the discovery of conducting polymers. All solar cells work on same principle whether they based on polymer or organic materials. Polymer and organic solar cells convert the solar radiation into the electric current with the help of photovoltaic effect [167]. Yu *et.al.* synthesize the PPV polymer solar cells that show the large efficiency and their efficiency are further enhanced to 3.0% by the later research work which made improvements in their structures [168]. After the discovery of first polymer solar cells, large number of different polymer materials are used for the conversion of sun light into electricity. Polymer solar cells are largely used to develop sun light converting devices in fabrics and textiles due to their flexible properties [169]. Organic photovoltaics which can be polarized with the help of recycling process increase the working capacity of solar panels, sun light capturing liquid crystals and photovoltaic devices [170].

Perovskite solar cells

Solar cells that are made up of in-organic materials show the large power conversion efficiency as compared to the commercially available solar cells. Inorganic materials based solar cells are generally known as perovskite solar cells. Firstly reported perovskite solar cells are made up of calcium and titanium di-oxide crystals. This perovskite solar cells contain two cations and one anion in their structure that particularly show the geometry of ABX_3 type in which A and B are cations whereas X represented the anion. Large number of in-organic materials based solar cells have been reported which show the large power conversion efficiency like the lead halide based perovskite solar cells but these in-organic materials show two disadvantages like toxic properties and huge cost both these factors show the negative effects on our environment and society [113]. Perovskite solar cells generally show the large power conversion efficiency as 22% from the organic solar cells but its cost is high and show harmful aspects. Perovskite solar cells consists of mesoporous scaffold electron transporting layers which made up of doped fluorine tin oxide particles. Recently developed perovskite and dye sensitized solar cells show the high efficiency from previously developed solar cells devices [171]. Organic solar cells and perovskite solar cells are different from each other due to their different mechanism of charge generation but mechanism of energy conversion is same in both devices. Perovskite solar cells devices show the large stability in the harmful of condition of environment and extreme temperature conditions [172].

Dye sensitized solar cells

Recent researches are totally focused to increase the conversion efficiency of the solar cells by making improvements in their molecular manipulation and use nanotechnology in their light converting process [173]. Michel Gratzel was the first scientist that report the dye sensitized solar cells by adding the dye materials between the more than one different electrodes [158a,161$_b$]. Dye sensitized solar cells contain four main components in their structure like redox mediator, counter electrode, dye sensitizer and semi-conductor electrode [174]. Dye sensitized solar cells can easily be synthesized with different techniques like printing and show the flexible properties that make its structure highly transparent and reduce the manufacturing cost. Their efficiency is greater than 10% due to having the grained nano titanium di-oxide coatings that provide the visible range of absorption [175]. But stability of dye sensitized solar cells is less as compared to the perovskite solar cells due to their complicated dye molecules de-gradation process. Low quality of sensitizer in this device reduce the efficiency whereas the high quality increases the manufacturing cost of dye sensitized solar cells. Infrared and ultraviolet radiations generally de-grade the dye molecules that decreased the stability, lifetime and efficiency of dye sensitized solar cells [155a].

Concentrated solar cells

Concentrated solar cells were largely developed in 1970 [176]. Concentrated solar cells harvest the more sun light with the help of their tiny region on the top of photovoltaic devices. It contains the large number of lens and mirrors that focus the light coming from the sun to the tiny region on the top of their device which provide the large power conversion efficiency. Concentrated solar cells work on the optics principle for focusing the light. Due to large number of mirrors and lens in their arrangements, concentrated solar cells produced more heat on the top of solar cells devices that increased its efficiency from others solar cells devices. Concentrated solar cells show the excellent opto-electronic properties. It can be categorized in to three different types like high, medium and low quality concentrated solar cells depending upon which quality of lens used for focusing the sun light on the top of device. Concentrated solar cells show the large efficiency like > 40% and can be manufacture in the range of different size which control its photovoltaic properties [177].

Bio-hybrid solar cells

Bio hybrid solar cells made by combining the in-organic and organic materials together. Firstly reported bio hybrid solar cells were made from complex photoactive protein that was located on the thylakoid membrane which increase the natural process of photosynthesis that led to more power conversion efficiency. Bio hybrid solar cells belongs to new type of renewable energy sources [178]. Thylakoid membranes absorb the large amount of energy form the sun light and convert it in to the chemical energy that led to the generation of electric current in the bio hybrid solar cells. These solar cells also contain the large amount of other in-organic materials but complex protein layers are introduced in the form of gold layers after some days which become the thin layer that enlarge the PCE's of solar cells device. Bio hybrid solar cells are still not a well-known and scientists are still working on it to improve its properties. After removing the thylakoid membranes from the device, it was observed that density of electric current increase 1000 times more as compared to the those which contain the thylakoid membranes in their structures. Photovoltaic properties of bio hybrid solar cells can also be modified by arranging their organic and in-organic layers [179].

Buried contact solar cells

BCSCs can be made with the help of metals buried in grooves that are formed in the inner side of laser. The efficiency of BCSCs are 25% which is higher from the commercially developed screen printed solar cells [180]. Metal buried in the BCSCs provide the large height to width ratio. This will provide the large contact of metal with

finger that will increase the power conversion efficiency from 2-3% from the printed screen solar cells in which 10-15% efficiency loss occur. So, small amount of sun light is reflected in the BCSCs which increased its J_{sc} and V_{oc}. But BCSCs provide less resistance against the parasite attacks due to having the large ratio of metals contact with the finger. Emitter resistance can be reduced in the BCSCs by lowering the space between the finger and their metal contact. Large metal volume particularly the cooper in laser grooves decrease the resistance against current density and lower the grid resistance in their device performance. BCSCs provide the low contact resistance as compared to their screen printed counter parts due to having the large amount of nickel silicide in their metal and semi-conductor interface. Low resistivity's of BCSCs provide us large fill factor that increase the device performance and efficiency [181].

Black silicon solar cells

Black and crystalline silicon solar cells are similar with each other in their photovoltaic properties. Silicon is common material used to manufacture the both types of solar cells. In black silicon solar cells, silicon absorbs the large amount of energy from the sun light and provide more output voltages. Black silicon solar cells are mostly suitable for those areas that having few sun light sources because it requires small amount of solar radiations and provide more efficiency due to their black colour on top of solar panel [182]. Black silicon solar cells can be made by adding thick nano scales like needles on the top of silicon materials. It also shows the small reflective properties against the sun light that increase its power conversion efficiency. Moreover, black silicon having low cost as compared to their white silicon counter parts and not require any anti-reflection coatings on the top of solar panels for harvesting the more sun light. But black silicon fails to provide satisfactory results in the re-combinations of charge carrier that are generated after capturing the sun light. Silicon material absorbs the photon from the sun light that will excite the electron from ground to excited states and leaving behind the hole that will responsible for the generation of electric current.

Shape of laser pulse can be changed with the help of pulse laser shape equipment in the laser formation process of black silicon [183]. Changing shape will damaged the less crystals during the interaction of laser and silicon which lower the loss of re-combinations on surface. Structuring of laser produced the texture and emitter on front side that enable the silicon to absorb infra-red region of solar cells radiations. After structuring the laser, evaporated fronts are contact with each other which facilitate the rear printed contact on the screen. Here the no need for the isolation of edge because only emitter formed on front side. This process generates the pulsed laser in the range of few femto-second that displayed on the top of black silicon solar cells. As the emitter and texture formed on the front side they will reduce the cost of production and numbers of un-necessary steps. Black silicon solar cells provide large amount of current density particularly in the range of 38 $mAcm^{-2}$ to 42 $mAcm^{-2}$ due to absorbing the infra-red region of solar cells radiations. Without applying any passivative layers, black silicon solar cells provide 4.5% efficiency [167].

Plastic solar cells

PSCs are manufactured with the help of fullerene and conjugated polymers by using the thin film casting technology. To improve the photovoltaic properties of PSCs, it is very necessary to lower their gap of energy between the HOMO/LUMO energy orbitals. PSCs excite the electrons after capturing the sun light which also stable the generated hole/electron pairs destabilize their HOMO energy orbitals that transfer own electron to the acceptor part of device [185]. Electron will move from ground to excited states leaving behind the hole in the ground states and this charge transfer process complete in 50 femto-seconds. Previously developed PSCs gives 2.5% PCE which are enhanced by making improvements in their structural properties. In PSCs, conductivity of hole will be increased by employing the annealing process at high temperature. Mobility of charge increased by applying external potential difference in light dependent medium. Same temperature effect also observed in OLEDs. The 2.5% efficiency of PSCs enhanced by increasing the temperature and provide 2.7 V external voltage in combination with the brightness of white light that increase the power conversion efficiency of PSCs from 2.5% to 3.5% [185].

Summary

Computational chemistry becoming the important research tool in modern age to design, theoretical studies and computing the absorption properties of compounds in research field. DFT is more reliable theory of computational chemistry that provide us authentic results which based on electrons density in given systems. In theoretical designing research work, we can use DFT with a series of functionals and basis sets for ground state and excited state optoelectronic calculations. For excited state properties, we can calculate the absorption properties, electron/holes mobility, solubility strength, molecular orbitals stability, band gap calculations, open circuit voltages, oscillating strength and electrons transport contributions between the HOMO/LUMO energy orbitals of reference molecule and newly designed organic solar cells molecules. This mode of research analysis provides us a lot of benefit as (i) no need to spend a lot of time in experimental labs for checking the series of research ideas because due to this way of theoretical research, we can firstly predict the theoretical results and idealize that the design molecules will be suitable for experimental study or it should be wastage of time in experimental labs with huge cost. Nowadays, the density functional theory has been modified with many revisions and its latest version as Gaussian 16 are also available for more reliable calculations with low cost. Secondly, as we discussed the NDI based organic solar cells which are also the prime importance materials now due to their excellent photogeneration and photoexcitation properties. Their power conversion efficiency is still lower but scientists communities are continuously working for their enhancement and improvement in their charge loss and charge recombination properties to develop better and high performance organic solar cells with non-fullerene acceptors.

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References

1. Banos R, Manzano-Agugliaro F, Montoya F, Gil C, Alcayde A, Gómez J. Renewable and Sustainable Energy Reviews. 2011; 15: 1753-1766.

2. Farret FA, Simoes MG, Integration of alternative sources of energy. John-

Wiley & Sons. 2006.

3. Al-Sehemi AG, Irfan A, Asiri AM, Ammar YA. Bulletin of the Chemical Society of Ethiopia. 2015; 29: 137-148.

4. Ali U, Tariq A, Kiran A, Abbas F, Khalil MT. Tuning the absorption and optoelectronic properties of naphthalene diimide based solar cells with non-fullerene acceptors. Chemical Papers. 2021; 75: 4327-4336.

5. Chinnammai S. A study on energy crisis and social benefit of solar energy. International Journal of Environmental Science and Development. 2014; 5: 404.

6. Randhir K. Porous reactive structures for thermochemical processes. University of Florida. 2016.

7. Hussain Z, Shoaib M, Ali U, Ramzan H, Ali M, Tariq A. Theoretical study of Isoxazoles and their derivatives for evaluating its pharmaceutical properties with density functional theory. 2020.

8. Zhao W, Li S, Yao H, Zhang S, Zhang Y, Yang B. Molecular Optimization Enables over 13% Efficiency in Organic Solar Cells. Journal of the American Chemical Society. 2017; 139: 7148-7151.

9. Lu L, Xu T, Chen W, Landry ES, Yu L. Ternary blend polymer solar cells with enhanced power conversion efficiency. Nature Photonics. 2014; 8; 716.

10. Mah O. National Solar Power Research Institute; 1998: 1-10.

11. Bagher AM. Comparison of Organic Solar Cells and Inorganic Solar Cells. International Journal of Renewable and Sustainable Energy. 2014; 3: 53-58.

12. Grätzel M, Perspectives for dye-sensitized nanocrystalline solar cells. Progress in photovoltaics: research and applications. 2000; 8: 171-185.

13. Glass A, Linde DVD, Negran T. High-voltage bulk photovoltaic effect and the photorefractive process in LiNbO3.World Scientific. 1995; 371-373.

14. Chandrasekaran J, Nithyaprakash D, Ajjan K, Maruthamuthu S, Manoharan D, Kumar D. Hybrid solar cell based on blending of organic and inorganic materials—An overview. Renewable and Sustainable Energy Reviews. 2011; 15: 1228-1238.

15. Tull B, Columbia University 2011; 20.

16. Chamberlain G. Organic solar cells: A review. Solar cells. 1983; 8: 47-83.

17. Green MA. High efficiency silicon solar cells. Seventh EC Photovoltaic Solar Energy Conference. 1987; 681-687.

18. Green MA, Hishikawa Y, Warta W, Dunlop ED, Levi DH, Hohl-Ebinger J. Solar cell efficiency tables (version 50). Progress in Photovoltaics: Research and Applications. 2017; 25; 668-676.

19. Buyukozkan G, Güleryüz S. An integrated DEMATEL-ANP approach for renewable energy resources selection in Turkey. International Journal of Production Economics 2016; 182: 435-448.

20. Fine GF, Cavanagh LM, Afonja A, Binions R. Metal Oxide Semi-Conductor Gas Sensors in Environmental Monitoring. Sensors. 2010; 10: 5469-5502.

21. Iftikhar T, Ali U, Shoaib M. Theoretical study of α, β unsaturated carbonyl thiophene derivatives to investigate optoelectronic properties toward organic photovoltaics. Journal of Molecular Modeling 2020; 26: 342.

22. Cui C, Min J, Ho CL, Ameri T, Yang P and Zhao J, et al. Synthesis and photovoltaic properties of alternative copolymers of benzo[1,2-b:4,5-b′] dithiophene and thiophene. Chemical Communications 2013; 49: 4409-4411.

23. Min J, Peng B, He Y, Zhang M, Zhang ZG and Zhang J, et al. Polymer bulletin. 2012; 68: 2107-2119.

24. Coropceanu V, Cornil J, da Silva Filho DA, Olivier Y, Silbey R, Brédas JL. Erratum: Charge transport in organic semiconductors. Chemical reviews 2007; 107; 926-952.

25. Brédas JL, Norton JE, Cornil J, Coropceanu V. Accounts of chemical research 2009; 42: 1691-1699.

26. Forrest SR. Organic Thin Film Transistors Based on Distyryl-Oligothiophenes: Role of AFM Images in Analyses of Charge Transport Properties. Nature. 2004; 428: 911.

27. Kim JY, Lee K, Coates NE, Moses D, Nguyen TQ, Dante M, et al. Efficient Tandem Polymer Solar Cells Fabricated by All-Solution Processing. Science. 2007; 31: 222-225.

28. Garnier F, Hajlaoui R, Yassar A, Srivastava P. Science. All-Polymer Field-Effect Transistor Realized by Printing Techniques. 1994; 265: 1684-1686.

29. Pisignano D, Anni M, Gigli G, Cingolani R, Zavelani-Rossi M, Lanzani G, et al. Monolithic polymer microcavity lasers with on-top evaporated dielectric mirrors. Applied Physics Letters. 2002; 81: 3534-3536.

30. Roncali J. Electrogenerated functional conjugated polymers as advanced electrode materials. Journal of Materials Chemistry. 1999; 9: 1875-1893.

31. Halls J, Walsh C, Greenham NC, Marseglia E, Friend RH, Moratti S, et al. Efficient photodiodes from interpenetrating polymer networks. Nature 1995; 376: 498.

32. Xu T, Yu T. How to design low bandgap polymers for highly efficient organic solar cells. Materials today. 2014; 17: 11-15.

33. Mishra A, Bäuerle P. Small molecule organic semiconductors on the move: promises for future solar energy technology. AngewandteChemie International Edition. 2012; 51: 2020-2067.

34. Kyaw AKK, Wang DH, Gupta V, Zhang J, Chand S, Bazan GC, et al. Barium: An Efficient Cathode Layer for Bulk-heterojunction Solar Cells. Advanced Materials. 2013; 25: 2397-2402.

34a. Walker B, Kim C, Nguyen TQ. Small Molecule Solution-Processed Bulk Heterojunction Solar Cells. Chemistry of Materials. 2010; 23: 470-482.

34b. Welch GC, Perez LA, Hoven CV, Zhang Y, Dang XD, Sharenko A, et al. Enhanced Performance of Fluorinated Quinoxaline-Containing Polymers by Replacing Carbon with Silicon Bridging Atoms on Dithiophene Donor Skeleton . Journal of Materials Chemistry. 2011; 21: 12700-12709.

35. Liao SH, Jhuo HJ, Cheng YS, Chen SA. Fullerene Derivative-Doped Zinc Oxide Nanofilm as the Cathode of Inverted Polymer Solar Cells with Low-Bandgap Polymer (PTB7-Th) for High Performance. Advanced materials 2013; 25: 4766-4771.

36. Jiang W, Ye L, Li X, Xiao C, Tan F, Zhao W, et al. Bay-linked perylenebisimides as promising non-fullerene acceptors for organic solar cells. Chemical Communications. 2014; 50: 1024-1026.

37. Lin Y, Zhan X. Nonfullerene n-Type Organic Semiconductors for Perovskite Solar Cells. Advanced Energy Materials. 2015; 5.

38. Peet J, Kim JY, Coates NE, Ma WL, Moses D, Heeger AJ, et al. Efficiency enhancement in low-bandgap polymer solar cells by processing with alkane dithiols. Nature materials 2007; 6: 497.

39. Sahu D, Tsai CH, Wei HY, Ho KC, Chang FC, Chu CW. Solution-processed benzotrithiophene-based donor molecules for efficient bulk heterojunction solar cells. Journal of Materials Chemistry. 2012; 22: 7945-7953.

39a. Chen LM, Hong Z, Li G, Yang Y. Recent progress in polymer solar cells: manipulation of polymer: fullerene morphology and the formation of efficient inverted polymer solar cells. Advanced Materials 2009; 21: 1434-1449.

39b. Heeger AJ. Semiconducting polymers: the third generation. Chemical Society Reviews. 2010; 39: 2354-2371.

39c. Arias AC, MacKenzie JD, McCulloch I, Rivnay J, Salleo A. Materials and Applications for Large Area Electronics: Solution-Based Approaches. Chemical reviews. 2010; 110: 3-24.

40. Duan C, Huang F, Cao Y. Recent development of push–pull conjugated polymers for bulk-heterojunction photovoltaics: rational design and fine tailoring of molecular structures. Journal of Materials Chemistry. 2012; 22: 10416-10434.

41. Dou L, You J, Hong Z, Xu Z, Li G, Street RA, et al. 25th anniversary article: A decade of organic/polymeric photovoltaic research. Advanced materials. 2013; 25: 6642-6671.

42. Stuart AC, Tumbleston JR, Zhou H, Li W, Liu S, Ade H, et al. Monodisperse Au Nanoparticles for Selective Electrocatalytic Reduction of CO2 to CO.

Journal of the American Chemical Society. 2013; 135: 1806-1815.

43. Tamayo AB, Dang XD, Walker B, Seo J, Kent T, Nguyen TQ. A low band gap, solution processableoligothiophene with a dialkylateddiketopyrrolopyrrole chromophore for use in bulk heterojunction solar cells. Applied Physics Letters. 2009; 94: 73.

44. Chen Y, Wan X, Long G. High Performance Photovoltaic Applications Using Solution-Processed Small Molecules. Accounts of chemical research. 2013; 46: 2645-2655.

45. Shen S, Jiang P, He C, Zhang J, Shen P, Zhang Y, et al. Solution-Processable Organic Molecule Photovoltaic Materials with Bithienyl-benzodithiophene Central Unit and Indenedione End Groups. Chemistry of Materials. 2013; 25: 2274-2281.

45a. Xue L, He X, Gu X, Yang Z, Xu B, Tian W. Simple Method of Preparing Graphene Flakes by an Arc-Discharge Method. The Journal of Physical Chemistry C. 2009; 113: 12911-12917.

45b. Yang Y, Zhang J, Zhou Y, Zhao G, He C, Li Y, et al. Chemical Reduction of Graphene Oxideto Graphene by Sulfur-Containing Compounds . The Journal of Physical Chemistry C. 2010; 114: 3701-3706.

45c. Li Z, Dong Q, Li Y, Xu B, Deng M, Pei J, et al. Design and synthesis of solution processable small molecules towards high photovoltaic performance. Journal of Materials Chemistry. 2011; 21: 2159-2168.

46. He C, He Q, Yang X, Wu G, Yang C, Bai F, et al. Synthesis and Photovoltaic Properties of a Solution-Processable Organic Molecule Containing Triphenylamine and DCM Moieties. The Journal of Physical Chemistry C. 2007; 111: 8661-8666.

47. Scharber MC, Mühlbacher D, Koppe M, Denk P, Waldauf C, Heeger AJ, et al. Design Rules for Donors in Bulk-Heterojunction Solar Cells—Towards 10 % Energy-Conversion Efficiency. Advanced materials. 2006; 18: 789-794.

48. Yang Y, Ouyang J, Ma L, Tseng RH, Chu CW. Electrical Switching and Bistability in Organic/Polymeric Thin Films and Memory Devices. Advanced Functional Materials. 2006; 16: 1001-1014.

49. Gustafsson G, Cao Y, Treacy G, Klavetter F, Colaneri N, Heeger A. Flexible light-emitting diodes made from soluble conducting polymers. Nature. 1992; 357: 477.

50. Tomozawa H, Braun D, Phillips S, Heeger A, Kroemer H, Metal-polymer schottky barriers on cast films of soluble poly(3-alkylthiophenes). Synthetic metals. 1987; 22: 63-69.

51. Torsi L, Dodabalapur A, Rothberg L, Fung A, Katz H. Intrinsic transport properties and performance limits of organic field-effect transistors. Science. 1996; 272: 1462-1464.

52. Kimura M, Hamakawa T, Hanabusa K, Shirai H, Kobayashi N. Synthesis of Multicomponent Systems Composed of One Phthalocyanine and Four Terpyridine Ligands. Inorganic chemistry. 2001; 40: 4775-4779.

53. Li G, Shrotriya V, Huang J, Yao Y, Moriarty T, Emery K, et al. Introduction to Organic Solar Cells. Nature materials. 2005; 4: 864.

54. Abbas M, Ali U, Faizan M, Siddique MBA. Spirofluorene based small molecules as an alternative to traditional non-fullerene acceptors for organic solar cells. Optical and Quantum Electronics. 2021; 53: 246.

55. Shrotriya V, Li G, Yao Y, Moriarty T, Emery K, Yang Y. Accurate measurement and characterization of organic solar cells. Advanced Functional Materials. 2006; 16: 2016-2023.

55a. Mikroyannidis JA, Sharma S, VijayY, Sharma G.ACS Applied Materials & Interfaces. 2 Triphenylamine−Thienylenevinylene Hybrid Systems with Internal Charge Transfer as Donor Materials for Heterojunction Solar Cells. 009; 2: 270-278.

55b. Walker, Tamayo AB, Dang XD, Zalar P, Seo JH, Garcia A, et al. Nguyen, Advanced Functional Materials. Nanoscale phase separation and high photovoltaic efficiency in solution-processed, small-molecule bulk heterojunction solar cells. 2009; 19: 3063-3069;

55c.Loser S, Bruns CJ, Miyauchi H, Ortiz RP, Facchetti A, Stupp SI, et al. Journal of the American Chemical Society. A naphthodithiophene-diketopyrrolopyrrole donor molecule for efficient solution-processed solar cells. 2011; 133: 8142-8145.

56. Youn H, Park HJ, Guo LJ. Small. Organic Photovoltaic Cells: From Performance Improvement to Manufacturing Processes. 2015; 11: 2228-2246.

57. Yella A, Lee HW, Tsao HN, Yi C, Chandiran AK, Nazeeruddin MK, et al. science. Porphyrin-sensitized solar cells with cobalt (II/III)-based redox electrolyte exceed 12 percent efficiency. 2011; 334: 629-634.

58. Jones BA, Facchetti A, Wasielewski MR, Marks TJ. Tuning Orbital Energetics in AryleneDiimide Semiconductors. Materials Design for Ambient Stability of n-Type Charge Transport. Journal of the American chemical society. 2007; 129: 15259-15278.

59. Gunes S, Neugebauer H, Sariciftci NS. Conjugated Polymer-Based Organic Solar Cells. Chemical reviews.2007; 107: 1324-1338.

60. Iwan A, Chuchmała A. Progress in Polymer Science. Perspectives of applied graphene: Polymer solar cells. 2012; 37: 1805-1828.

61. Ali U, Javed A, Ramzan H, Shoaib M, Raza A, Khalil MT, et al. SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy. Molecular designing of naphthalene diimide based fullerene-free small organic solar cell - Acceptors with high photovoltaic performance by density functional theory. 2020; 228: 117685.

62. Wang M, Wang H, Yokoyama T, Liu X, Huang, Y Zhang y, et al. High Open Circuit Voltage in Regioregular Narrow Band Gap Polymer Solar Cells. Journal of the American Chemical Society. 2014; 136: 12576-12579.

63. Sung MJ, Huang M, Moon SH, Lee TH, Park SY, Kim JY, et al. Solar Energy. 2017; 150: 90-95.

64. Sun D, Meng D, Cai Y, Fan B, Li Y, Jiang W, et al. Non-Fullerene-Acceptor-Based Bulk-Heterojunction Organic Solar Cells with Efficiency over 7%. Journal of the American Chemical Society. 2015; 137: 11156-11162.

65. Shirota Y. Journal of Materials Chemistr. 2000; 10: 1-25.

66. Kiran A, Ali U, Hussain A, Ahmad HMR, Abbas F, Memon TA, et al. Chemical Papers. 2021.

67. Tang CW. Applied Physics Letters. Two-layer organic photovoltaic cell. 1986; 48: 183-185.

68. Cheng YJ, Yang SH, Hsu CS. Synthesis of Conjugated Polymers for Organic Solar Cell Applications. Chemical reviews.2009; 109: 5868-5923.

69. Abbas F, Ali U, Ahmad HMR, Tallat A, Shehzad A and Zeb Z, et al. ournal Pre-proofs Role of Iodo-Substituted Subphthalocyanine (Subpcs) π-conjugated aromatic N-fused di-Iminoisonidole units on the performance of non-fullerene small or- ganic solar cells Role of Iodo-Substituted Subphthalocyanine (Subpcs) π-conjugated aromatic N-fused di- Iminoisonidole units on the performance of non-fullerene small organic solar cells. Computational and Theoretical Chemistry. 2022; 1207: 113508.

70. Riede M, Mueller T, Tress W, Schueppel R, Leo K. Small-molecule solar cells-status and perspectives.Nanotechnology. 2008; 19: 424001.

71. Brabec CJ, Sariciftci NS, Hummelen JC. Plastic Solar Cells. Advanced functional materials. 2001; 11: 15-26.

72. Deb SK. World Renewable Energy Congress VI. 2000; 2658-2663.

73. Tanabe K, Morral AFI, Atwater HA, Aiken DJ, Wanlass MW. Applied physics letters. 2006; 89: 102106.

74. Ali U, Javed A, Tallat A, Iqbal J, Raza A. Molecular designing of four high performance pyrazine-based non-fullerene acceptor materials with naphthalene diimide-based small organic solar cells. Journal of Molecular Modeling. 2019; 25: 50.

75. Bahmanyar S, Houk K. Journal of Molecular Modeling. Transition States of Amine-Catalyzed Aldol Reactions Involving Enamine Intermediates: Theoretical Studies of Mechanism, Reactivity, and Stereoselectivity. Journal of Molecular Modeling.2001; 123: 11273-11283.

76. DiLabio GA, Johnson ER, Roza AODL. PPerformance of conventional

and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. hysical Chemistry Chemical Physics. 2013; 15: 12821-12828.

77. Neumann S, Bocker S. Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules.Analytical and bioanalytical chemistry.2010; 398: 2779-2788.

78. Zhan CG, Nichols JA, Dixon DA. Open3DQSAR: a new open-source software aimed at high-throughput chemometric analysis of molecular interaction fields.The Journal of Physical Chemistry A.2003; 107: 4184-4195.

79. Tosco P, Balle T. Open3DQSAR: a new open-source software aimed at high-throughput chemometric analysis of molecular interaction fields.Journal of molecular modeling. 2011; 17: 201-208.

80. Grimme S, Antony J, Ehrlich S, Krieg H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu.The Journal of chemical physics. 2010; 132: 154104.

81. Cohen AJ, Sanchez PM, Yang W. Challenges for Density Functional Theory. Chemical Reviews.2011; 112: 289-320.

82. Tetko IV, Gasteiger J, Todeschini R, Mauri A, Livingstone D, Ertl P, et al. Virtual computational chemistry laboratory--design and description.Journal of computer-aided molecular design. 2005; 19: 453-463.

83. Stephens P, Devlin F, Chabalowski C, Frisch MJ. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields.The Journal of Physical Chemistry. 1994; 98: 11623-11627.

84. Dewar MJ, Hashmall JA, Venier CG. Journal of the American Chemical Society. 1968; 90: 1953-1957.

85. Levine IN, Busch DH, Shull H. Quantum chemistry, Prentice Hall Upper Saddle River. NJ. 2000.

86. Schleyer PVR, Allinger NL, Clark T, Gasteiger J, Kollman P, Schaefer HF, et al. Encyclopedia of computational chemistry, Wiley Chichester. 1998.

87. Berova N, Bari LD, Pescitelli G. Application of electronic circular dichroism in configurational and conformational analysis of organic compounds. Chemical Society Reviews. 2007; 36: 914-931.

88. Fogarasi G, Zhou X, Taylor PW, Pulay P. The calculation of ab initio molecular geometries: efficient optimization by natural internal coordinates and empirical correction by offset forces. Journal of the American Chemical Society. 1992; 114: 8191-8201.

89. Willoughby PH, Jansma MJ, Hoye TR. A guide to small-molecule structure assignment through computation of (^{1}H and ^{13}C) NMR chemical shifts. Nature protocols. 2014; 9: 643.

90. Chamberlin AC, Cramer CJ, DG Truhlar. B. Extension of a Temperature-Dependent Aqueous Solvation Model to Compounds Containing Nitrogen, Fluorine, Chlorine, Bromine, and Sulfur. The Journal of Physical Chemistry. 2008; 112: 3024-3039.

91. Sin LT, Rahman W, Rahmat A, Samad A. Polymer. 2010; 51: 1206-1211.

92. Curtiss LA, Raghavachari K, Redfern PC, Rassolov V, Pople JA. Gaussian-3 (G3) theory for molecules containing first and second-row atoms. The Journal of chemical physics. 1998; 109: 7764-7776.

93. Adamo C, Barone V. Synthesis and Evaluation of Corrosion Inhibiting Activity of New Molecular Hybrids Containing the Morpholine, 1,4-Naphthoquinone, 7-Chloroquinoline and 1,3,5-Triazine Cores.The Journal of chemical physics.1999; 110: 6158-6170.

94. Yanai T, Tew DP, Handy NC. A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP).Chemical Physics Letters. 2004; 393: 51-57.

95. Grimme S, Ehrlich S, Goerigk L. Effect of the damping function in dispersion corrected density functional theory.Journal of computational chemistry. 2011; 32: 1456-1465.

96. Kohn W. Landau Theory of Fermi Liquid in a Relativistic Nonlinear (σ, ω) Model at Finite Temperature . Reviews of Modern Physics.1999; 71: 1253-1266.

97. May V. Charge and energy transfer dynamics in molecular systems, John Wiley & Sons. 2008.

98. Rachchh R, Kumar M, Tripathi B. Solar photovoltaic system design optimization by shading analysis to maximize energy generation from limited urban area.Energy Conversion and Management. 2016; 115: 244-252.

99. Gross EK, Dreizler RM. Density functional theory, Springer Science & Business Media. 2013.

100. Durr D, Goldstein S, Zanghi N. arXiv preprint quant-ph/9512031. Bohmian Mechanics and the Meaning of the Wave Function. 1995.

101. Wong WW, Banal JL, Geraghty PB, Hong Q, Zhang B, Holmes AB, et al. Organic Photovoltaic Materials—Design, Synthesis and Scale-Up. The Chemical Record. 2015; 15: 1006-1020.

102. Guo H, Weng C, Wang G, Zhao B, Tan S. Dyes and Pigments. 2016; 133: 16-24.

103. Glaser JB, Wong D, Maroun R. Jama. 2015; 313: 2494-2495.

104. Cheng P , Zhao X, Zhou W, Hou J, Li Y, X. Zhan. Polymer/Polymer Blend Solar Cells Improved by Using High-Molecular-Weight Fluorene-Based Copolymer as Electron Acceptor. Organic Electronics. 2014; 15: 2270-2276.

105. Ajmal M, Ali U, Javed A, Tariq A, Arif Z and Iqbal J, et al. Designingindacenothiophene-based three new molecules containing non-fullerene acceptors as strong electron withdrawing groups with DFT approaches. Journal of Molecular Modeling. 2019; 25: 311.

106. Dai S, Lin Y, Cheng P, Wang Y, Zhao X and Ling Q, et al. Perylenediimide–thienylenevinylene-based small molecule and polymer acceptors for solution-processed fullerene-free organic solar cells. Pigments. 2015; 114: 283-289.

107. Ali U, Ahmad HMR, Faizan M, Kiran A, Khalil MT. Optical and Quantum Electronics. 2021; 53: 541.

108. Ala'a FE, Sun JP, Hill IG, Welch GC. Recent advances of non-fullerene, small molecular acceptors for solution processed bulk heterojunction solar cells. Journal of Materials Chemistry A. 2014; 2: 1201-1213.

109. Li Y, Liu X, Wu FP, Zhou Y, Jiang ZQ and Song B, et al. Non-fullerene acceptor with low energy loss and high external quantum efficiency: towards high performance polymer solar cells. Journal of Materials Chemistry A. 2016; 4:5890-5897.

110. Ali U, Javed A, Amanullah, Shoaib M, Kashif M and Raza A, et al. Optical and Quantum Electronics. 2019; 51: 332.

111. Kim YJ, Qin Y, Stevens Dm, Ugurlu O, Kalihari V and Hillmyer MA, et al. Low Band Gap Poly(thienylenevinylene)/Fullerene Bulk Heterojunction Photovoltaic Cells.The Journal of PhysicalChemistry C.2009; 113: 10790-10797.

112. Ganesamoorthy R, Sathiyan G, Sakthivel P. Review: Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications. Solar Energy Materials and Solar Cells. 2017; 161: 102-148.

113. Omer AM. Energy Analysis and Proposals for Sustainability from the Energy Transition.Renewable and sustainable energy reviews. 2008; 12: 2265-2300.

114. Nho S, Baek G, Park S, Lee BR, Cha MJ and Lim DC, et al. Energy & Environmental Science. 2016; 9: 240-246.

115. Wicklein A, Ghosh S, Sommer M, Wuurthner F, Thelakkat M, ACS nano. Self-Assembly of Semiconductor Organogelator Nanowires for Photoinduced Charge Separation. 2009; 3: 1107-1114.

116. Amanullah, Ali U, Ans M, Iqbal J, Iqbal MA, Shoaib M. Benchmark study of benzamide derivatives and four novel theoretically designed (L1, L2, L3, and L4) ligands and evaluation of their biological properties by DFT approaches. Journal of Molecular Modeling. 2019; 25: 223.

117. Tamayo AB, Walker B, Nguyen TQ. Design, Synthesis, and Self-assembly

of Oligothiophene Derivatives with a Diketopyrrolopyrrole Core. The Journal of Physical Chemistry C. 2008; 112: 11545-11551.

118. Patil H, Zu WX, Gupta A, Chellappan V, Bilic A and Sonar P, et al. A non-fullerene electron acceptor based on fluorene and diketopyrrolopyrrole building blocks for solution-processable organic solar cells with an impressive open-circuit voltage. Physical Chemistry Chemical Physics. 2014; 16: 23837-23842.

119. Nielsen CB, Holliday S, Chen HY, Cryer SJ, McCulloch I. Accounts of chemical research. Non-Fullerene Electron Acceptors for Use in Organic Solar Cells.2015; 48:2803-2812.

120. Katritzky AR, Ramsden CA, Joule JA, Zhdankin VV. Handbook of heterocyclic chemistry, Elsevier. 2010.

121. Meng D, Sun D, Zhong C, Liu T, Fan B and Huo L, et al. High-Performance Solution-Processed Non-Fullerene Organic Solar Cells Based on Selenophene-Containing PeryleneBisimide Acceptor. Journal of the American Chemical Society. 2015; 138: 375-380.

122. Duan C, Gao K, FranekerJJv, Liu F, Wienk MM, Janssen RA, et al. Soc. 2016; 38: 10782-10785.

123. Srivani D, Gupta A, Raynor AM, Bilic A, Li J, Bhosale SV, et al. RSC advances. 2016; 6: 38703-38708.

124. Gao L, Zhang ZG, Xue L, Min J, Zhang J and Wei Z, et al. Advanced materials. All-Polymer Solar Cells Based on Absorption-Complementary Polymer Donor and Acceptor with High Power Conversion Efficiency of 8.27%. 2016; 28: 1884-1890.

125. Raynor AM, Gupta A, Patil H, Ma D, Bilic A and Rook TJ, et al. RSC advances. A non-fullerene electron acceptor based on central carbazole and terminal diketopyrrolopyrrole functionalities for efficient, reproducible and solution-processable bulk-heterojunction devices.2016; 6: 28103-28109.

126. Abbas F, Ali U, Ahmad HMR, Tallat A, Shehzad A and Zeb Z, et al. Optical and Quantum Electronics. NDI-Based Small Molecule as Promising Nonfullerene Acceptor for Solution-Processed Organic Photovoltaics. 2021; 54: 21.

127. Liu Y, Zhang L, Lee H, Wang HW, Santala A and Liu F, eta al. Advanced Energy Materials. 2015; 5.

128. Earmme T, Hwang YJ, Murari NM, Subramaniyan S, Jenekhe SA. All-Polymer Solar Cells with 3.3% Efficiency Based on Naphthalene Diimide-Selenophene Copolymer Acceptor. Journal of the American Chemical Society. 2013; 135: 14960-14963.

129. Sazonov A, Striakhilev D, Natha A. Low-temperature amorphous, nanocrystalline silicon materials, and thin-film transistors. Springer. 2009; 53-73.

130. Takeuchi Y, Murata M, Takano A, Nishimiya T, Morita S, Aoi T, et al. Amorphous silicon solar cell. Google Patents. 2001.

131. Kołodziej A. Opto-electronics review. Staebler-Wronski effect in amorphous silicon and its alloys. 2004; 12: 21-32.

132. Galloni R. Amorphous silicon solar cells. Renewable Energy. 1996; 8: 400-404.

133. Erdogan G. Low temperature photoconductivity of hydrogenated amorphous silicon (a-Si: H) thin flims, İzmir Institute of Technology. 2003.

134. Wu Z, Sun C, Dong S, Jiang XF, Wu S and Wu H, et al. n-Type Water/Alcohol-Soluble Naphthalene Diimide-Based Conjugated Polymers for High-Performance Polymer Solar Cells. Soc. 2016; 138: 2004-2013.

135. Guo X, Watson MD. Conjugated polymers from naphthalene bisimide. Organic letters. 2008; 10: 5333-5336.

136. Zhan X, Facchetti A, Barlow S, Marks TJ, Ratner MJ and Wasielewski MR, et al. Rylene and Related Diimides for Organic Electronics. Advanced Materials 2011; 23: 268-284.

137. Yan Q, Zhou Y, Zheng YQ, Pei J, Zhao D. Towards rational design of organic electron acceptors for photovoltaics: a study based on perylenediimide derivatives. Chemical Science. 2013; 4: 4389-4394.

138. Wang C, Dong H, Hu W, Liu Y, Zhu D. Semiconducting π-conjugated systems in field-effect transistors: a material odyssey of organic electronics. Chemical Reviews. 2011; 112: 2208-2267.

139. Yuan Z, Li J, Xiao Y, Li Z, Qian X. Core-PerfluoroalkylatedPeryleneDiimides and Naphthalene Diimides: Versatile Synthesis, Solubility, Electrochemistry, and Optical Properties. The Journal of organic chemistry. 2010; 75: 3007-3016.

140. Miasojedovas A, Kazlauskas K, Armonaite G, Sivamurugan V, Valiyaveettil S and Grazulevicius J, et al. Concentration effects on emission of bay-substituted perylenediimide derivatives in a polymer matrix. Dyes and Pigments. 2012; 92: 1285-1291.

141. Fazzi D, Caironi M, Castiglioni C.Quantum-Chemical Insights into the Prediction of Charge Transport Parameters for a Naphthalenetetra. Journal of the American Chemical Society. 2011; 133: 19056-19059.

142. Kim R, Amegadze PS, Kang I, Yun HJ, Noh YY and Kwon SK, et al. Advanced Functional Materials 2013; 23: 5719-5727.

143. Guo X, Tu D, Liu X. Recent advances in rylenediimide polymer acceptors for all-polymer solar cells. Journal of energy chemistry. 2015; 24: 675-685.

144. Fabiano S, Chen Z, Vahedi S, Facchetti A, Pignataro B, Loi M. Role of photoactive layer morphology in high fill factor all-polymer bulk heterojunction solar cells. Journal of Materials Chemistry. 2011; 21:5891-5896.

145. Kang H, Uddin MA, Lee C, Kim KH, Nguyen TL and Lee W, et al. Determining the Role of Polymer Molecular Weight for High-Performance All-Polymer Solar Cells: Its Effect on Polymer Aggregation and Phase Separation. Journal of the American Chemical Society. 2015; 137: 2359-2365.

146. Zhao J, Wang A, Green MA, Ferrazza F. 19.8% efficient “honeycomb” textured multicrystalline and 24.4% monocrystalline silicon solar cells. Applied Physics Letters. 1998; 73: 1991-1993.

147. Green MA, Emery K, King DL, Hishikawa Y, Warta W. Progress in Photovoltaics: Research and Applications. 2007; 15: 35-40.

148. Shah A, Meier J, Buechel A, Kroll U, Steinhauser J and Meillaud F, et al. 24·5% Efficiency silicon PERT cells on MCZ substrates and 24·7% efficiency PERL cells on FZ substrates. Thin solid films. 2006; 502: 292-299.

149. Zhao J, Wang A, Green MA. Progress in photovoltaics: research and applications. 1999; 7: 471-474.

150. Hou Y, Huang T, Wen Z, Mao S, Cui S, Chen J. Metal−Organic Framework-Derived Nitrogen-Doped Core-Shell-Structured Porous Fe/Fe3C@C Nanoboxes Supported on Graphene Sheets for Efficient Oxygen Reduction Reactions .Advanced Energy Materials. 2014; 4.

151. Conibeer G, Green M, Cho EC, Konig D, Cho YH and Fangsuwannarak T, et al. Silicon quantum dot nanostructures for tandem photovoltaic cells. Thin Solid Films. 2008; 516: 6748-6756.

152. Shah A, Meier J, Sauvain EV, Droz C, Kroll U and N. Wyrsch, et al. Microcrystalline silicon and ‘micromorph’ tandem solar cells.Thin Solid Films. 2002; 403: 179-187.

152a. Bertolli M. Course: Solar Cells: In Research and Applications—A Review. Department of Physics, University of Tennessee, Knoxville. 2008.

152b. Kreith F, Goswami DY. Handbook of energy efficiency and renewable energy, Crc Press.2007.

152c. Luque A, Hegedus S. Handbook of photovoltaic science and engineering, John Wiley & Sons. 2011.

153. Elsabawy k, El-Hawary W, Refat M. International Journal of Chemical Sciences. 2012; 10: 1869-1879.

154. Badawy WA. A review on solar cells from Si-single crystals to porous materials and quantum dots. Journal of advanced research. 2015; 6: 123-132.

154a. Bagher AM, Vahid MMA, Mohsen M. Comparative Analysis between Single Diode and Double Diode Model of PV Cell: Concentrate Different Parameters Effect on Its Efficiency. American Journal of optics and Photonics .2015; 3: 94-113.

154b. Maehlum M. Last updated 2015; 6.

155. Goswami DY, Kreith F. Energy conversion, CRC press. International journal of chemical engineering and applications. 2007.

156. Sethi V, Pandey M, Shukla MP. Solar Cells: In Research and Applications—A Review.2011; 2: 77-80.

157. Andorka F. Solar Cells: In Research and Applications—A Review. Solar Power World. 2014.

158. Razykov TM, Ferekides CS, Morel D, Stefanakos E, Ullal HS, Upadhyaya HM. Solar photovoltaic electricity: Current status and future prospects. Solar Energy. 2011; 85: 1580-1608.

159. Srinivas B, Balaji S, NagendraBabu M, Reddy Y. Solar Cells: In Research and Applications—A Review. International Journal of Engineering Research-Online .2015; 3: 178-182.

160. Imamzai M, Aghaei M, Hanum Y, Thayoob MD, Forouzanfar M. Solar Cells: In Research and Applications—A Review.Proceedings of National Graduate Conference. 2012; 1-5.

161. Fritz KP, Guenes S, Luther J, Kumar S, Sariciftci NS, Scholes GD. IV-VI Nanocrystal-polymer solar cells.Journal of Photochemistry and Photobiology A: Chemistry. 2008; 195: 39-46.

162. Choubey P, Oudhia A, Dewangan R. A review: Solar cell current scenario and future trends. Recent Research in Science and Technology. 2012; 4.

163. Wang X, Koleilat GI, Tang J, Liu H, Kramer IJ and Debnath R, etal.Tandem colloidal quantum dot solar cells employing a graded recombination layer. Nature Photonics. 2011; 5: 480-484.

164. Ganesh B, Supriya YV, Vaddeswaram G. International Journal of Electronics and Computer Science Engineering. 2013; 2: 565-573.

165. Sharma S, Jain KK, Sharma A. Solar Cells: In Research and Applications—A Review.Materials Sciences and Applications. 2015; 6: 1145-1155.

166. Brabec CJ, Shaheen SE, Winder C, Sariciftci NS, Denk P. Equivalent Circuit Modification for Organic Solar Cells.Applied physics letters. 2002; 80: 1288-1290.

167. Li G, Zhu R, Yang Y. Polymer solar cells.Nature photonics. 2012; 6: 153-161.

168. Zhu R, Kumar A, Yang Y. Polarizing Organic Photovoltaics. Advanced Materials. 2011; 23: 4193-4198.

169. Baena JPC, Abate A, Saliba M, Tress W, Jacobsson TS, Gratzel M, et al. The rapid evolution of highly efficient perovskite solar cells.Energy & Environmental Science .2017; 10: 710-727.

170. Marinova N, Valero S, Delgado JL. Organic and perovskite solar cells: Working principles, materials and interfaces Journal of colloid and interface science. 2017; 488: 373-389.

171. Li B, Wang L, Kang B, Wang P, Qiu Y. Solar Cells: In Research and Applications—A Review .Solar Energy Materials and Solar Cells 2006; 90: 549-573.

172. Nozik AJ. Nanoscience and Nanostructures for Photovoltaics and Solar Fuels. Nano letters 2010; 10: 2735-2741.

173. Suhaimi S, Shahimin MM, Alahmed Z, Chysky J, Reshak A. Materials for Enhanced Dye-sensitized Solar Cell Performance: Electrochemical Application. International Journal of Electrochemical Science. 2015; 10: 2859-2871.

174. Graetzel M, Janssen RA, Mitzi DB, Sargent EH.Materials interface engineering for solution-processed photovoltaics. Nature. 2012; 16: 488-304.

175. Liang M, Xu W, Cai F, Chen P, Peng B, Chen J. Solar Cells: In Research and Applications—A Review. Journal of Physical Chemistry C. 2007; 111: 4465-4472.

176. Philipps SP, Bett AW, Horowitz K and Kurtz S. Current status of concentrator photovoltaic (CPV) technology, NREL (National Renewable Energy Laboratory (NREL), Golden, CO (United States)). 2015.

177. Guter W, Schone J, Philipps SP, Steiner M, Siefer G and Wekkeli A, et al. Current-matched triple-junction solar cell reaching 41.1% conversion efficiency under concentrated sunlight.Applied Physics Letters. 2009; 94: 223504.

178. McEvoy AJ, Castaner L, Markvart T. Solar cells: materials, manufacture and operation, Academic Press. 2012.

179. Fahrenbruch A, Bube R, Google Scholar.

180. Green MA, Emery K, Hishikawa Y, Warta W. Solar cell efficiency tables. Progress in photovoltaics: research and applications. 2010; 18: 346-352.

181. Ghozati S, Ebong A, Honsberg C, Wenham S. Improved fill-factor for the double-sided buried-contact bifacial silicon solar cell. Solar Energy Materials and Solar Cells. 1998; 51: 121-128.

182. Han SE, Chen G. Toward the Lambertian Limit of Light Trapping in Thin Nanostructured Silicon Solar Cells. Nano letters. 2010; 10: 4692-4696.

183. Nayak BK, Iyengar VV, Gupta MC. Efficient light trapping in silicon solar cells by ultrafast-laser-induced self-assembled micro/nano structures. Progress in Photovoltaics: Research and Applications. 2011; 19: 631-639.

184. Brabec CJ, Cravino A, Meissner D, Sariciftci NS, Fromher T and Rispens MT, et al. Advanced Functional Materials. 2001; 1: 374-380.

185. Padinger F, Rittberger RS, Sariciftci NS. Effects of Postproduction Treatment on Plastic Solar Cells. Advanced Functional Materials. 2003; 13: 85-88.