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Improvement in the Capacity of K-Ion Battery to Supply V-I Capacity in Renewable Technology

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Abstract *- The increase in power consumption has increase the power generation technologies in sustainable manners which leads the renewable energy sources to generate power, but the main issue is to store that generated energy for the future use, this opens the research doors in batteries design for the best performance and long life. From last decays the most research work is going on the K-Ion batteries (PIBs) because of the K-Ion size (1.38Å) which is large than Li-ion (0.76 Å) in radius the carbon-based materials are under consideration for the design of electrode anode. In this work we will observe the properties of K-ion anode based on some modified 1D CNTs materials. With the help of doping electrochemical properties of Carbon based anode can be improved, which enhance the capacity of k ion battery, deliver more energy when connected with load and improves its stability. The discovery of new 1D materials could lead to a better energy storage device, which could help to overcome the limitations of non-conventional energy sources like solar and wind. This piece of work focuses on the main issue of energy storage. The choice of a potassium ion battery is significant due to its numerous advantages over other types of batteries.*

Keywords — *K-ion Batteries; Doping; CNTs 1D materials;*

I. INTRODUCTION

The power generation by consumption of fossil fuels increases the energy crisis worldwide and also increase the environmental pollution that leads the increase demand in sustainable clean energy. For that sustainable energies sources such as Li, Na, K batteries are being used to store energy which is generated by sustainable energy sources, the Na and K are the other alkali metals have the alike chemical and physical properties. So, the same as a Li+ battery is based on the working theory of the "rocking-chair" battery (example: take a K-ion battery: during the charging time of a battery K^+ is produced at the positive electrode and via the electrolyte submerge in negative electrode and during same time period all other remaining negative charges reach on the negative outer-circuit electrode. The phase becomes reversed during battery discharge as shown in Figure1. Sodium ion and potassium ion batteries are the most promising Li-ion battery alternatives [1]. A Sodium ion battery or a Potassium battery has a similar basic energy / energy density value to the lithium ion battery stated by eftekhari, or has numerous benefits for unique energy compared to the Na-ion battery. [2].New Potassium ion batteries (PIBs) have also gained considerable attention because of the large reservoirs available on Earth and are cost-effective as opposed to Li ion batteries. The K^+ batteries are supposed to offer excessive-voltage operation than Na^+ batteries and even Li^+ batteries. Before the Li-ion the less standard potential of electrode for K-ion battery proven in carbonate ester electrolyte solution [3].Accepted with the measured potential of standard electrodes reported in earlier literature [4]. High-power densities in K-ion batteries can be realized based on K^+ ions' rapid diffusion rate, which has poor Columbic interactions. K^+ ions have these special advantages which makes potassium batteries an alternative to Lithium-ion batteries that's why they have taken much attention. In 2015 after the experimental demonstration in graphene of low potassium ion K^+ potential &electrochemical K-intercalation [5].

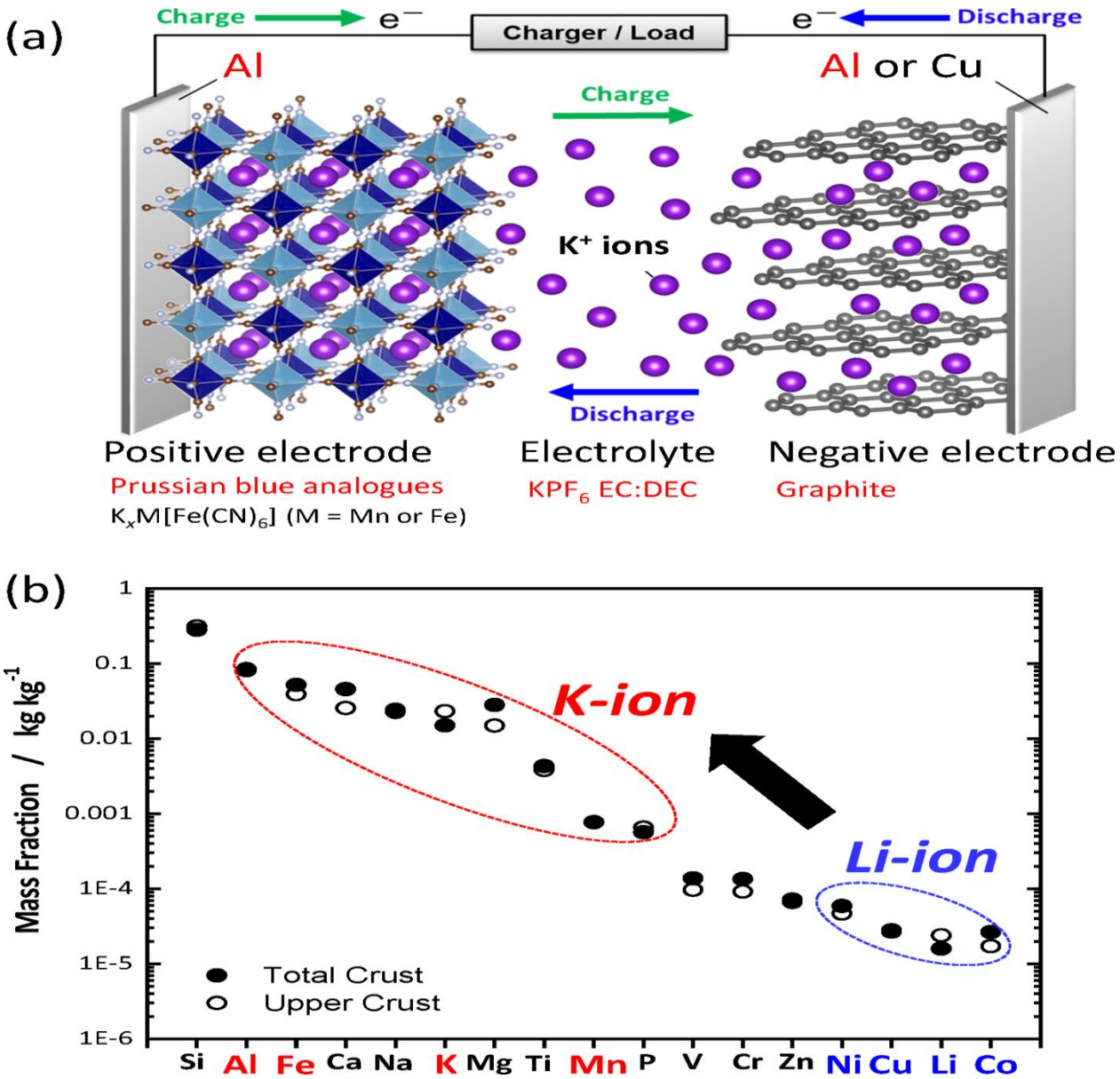


Fig 01: a) An overview diagram showing a schematic illustration of k-ion battery "rocking chair". b) Elements abundance in earth's crust.

That's why high ionic conductivity and better mobility is displayed by a solvation K-ion [7].When comparing the entire battery mass K atomic mass is heavier, Alkaline metal ions have a very small proportion. Some analysis is being carried out on complete potassium batteries [7] gives Na+/Na greater potential for future practical application of potassium ion batteries (2.71 V versus NHE) than the K-ion (2.93 V, versus NHE), Especially when it comes to large-scale energy storage with references, Which makes the potassium ion battery more competitive in terms of performance, potential and in power than the Na ion battery [8]. Potassium ion batteries have more advantages As regards the carbon anode content than Na-ion batteries which have the same intercalation reaction in graphite as Li ion. The first phase intercalation of graphite compounds KC8 is created in the potassium ion battery and attain the theoretical potential (279 mA h g1) is due to the sink of full K^+in the Anode of Graphite as shown in Fig 02. The embedded graphite K-ion has Potential 0.23 Volt that is greater, that of potassium deposition and the Lithium ion battery has the potential of only 0.1 volt. For this purpose, potassium dendrites are less likely to form in the K-ion battery, rendering the K-ion charging-discharge phase safe. However, for carbon content K-ion has a higher reaction rate than Na + for intercalation process, which means that potassium batteries are more effective. There are also several problems due to the greater radius of K-ion, like the deformation of the graphite arrangement, which results in a rapid decay of power [8].In lithium batteries still difficult problem is lithium dendrites. Much weaker are the mechanical properties of dendrites in K due to low boiling point, by controlling the temperature formation of K dendrites can be reduced, at room temperature the mixture of Na and K become liquid. The high potential (579 mA h

g1)is delivered by the alloy of (Na-K) if used in anode .There is also no dendrite formation for the K-ion battery on the Na-K alloy anode, since the metal deposited will become liquid during charging. More importantly, because aluminum and potassium do not form alloys, the liquid metal anode is created from the immiscibility of Na-K alloy with organic electrolyte without any solid electrolyte, allowing the battery to function with Na-K alloy anode at ambient temperature. As an anode, you can utilize less expensive aluminum [9].

Figure 2Calculations DFT. (A) Demonstrating intercalation From K ions to graphite for various blue line Setting up scenarios (Theory (a)) The stage of intercalation refers to: KC24 (Stage III)/KC16 (Step II)/KC8 (Step I);)))). Green dotted line (theory (b)) Corresponds to staging values that have already been recorded: KC24 (Stage II) / KC8 (Stage I). The red dotted line refers to the average experimental data moved by 26mAh g1 to correct the SEI efficiency contribution. [10]. (B) Diagram of K-intercalated graphite phases, with K in blue and C in yellow [10]. (C) Semi-hollow carbon micro-battery rods TEM pictures and high-resolution TEM image [11], (d) complete battery diagram of K-ion. For Columbic, cyclic performance and associated efficacy [11]. Reproduced from reference 10, With the American Chemical Society's permission. Reproduced with the permission of The Royal Society of Chemistry from ref. 11

II. COMPUTATIONAL DETAILS AND GEOMETRY MODELS

The investigation is carried out utilising the First Principles System DFT (FPS-DFT) computing approach in conjunction with the generalised gradient approximation (GGA) and the VASP software package, which is an accurate and efficient computational tool [12,13]. Computations for 1D AIN with 15 vacuum thickness in the Z-direction are done using a plane-wave basis set in conjunction with ultra-soft psuedopotentials [12,14] and a 450 eV cut-off energy on a 4x3 super cell configuration [14,15]. Vacuum thickness is increased to eliminate interaction between neighbouring layers. The influence of doping on the electrical and structural characteristics of 1D CNTs is studied using various configurations of K doped, Ti doped, and K adsorption. After optimization of K and Ti doped and K adsorbed materials such as AlN systems, the Hellmann-Feynman force parameter gained 0.02 eV/ value and the total energy value exceeded the 0-45 eV limit. Different. The Gaussian smearing approach is used to address the partial occupancy problem.

Our study on electric parameters focuses on manipulating and improving the aforementioned characteristics of 1D CNTs in the low electron energy range, i.e., 0–45 eV. The main goal of this research is to tailor and improve the energy storage capability of K-ions by doping K and Ti into a 1D AlN system to form an

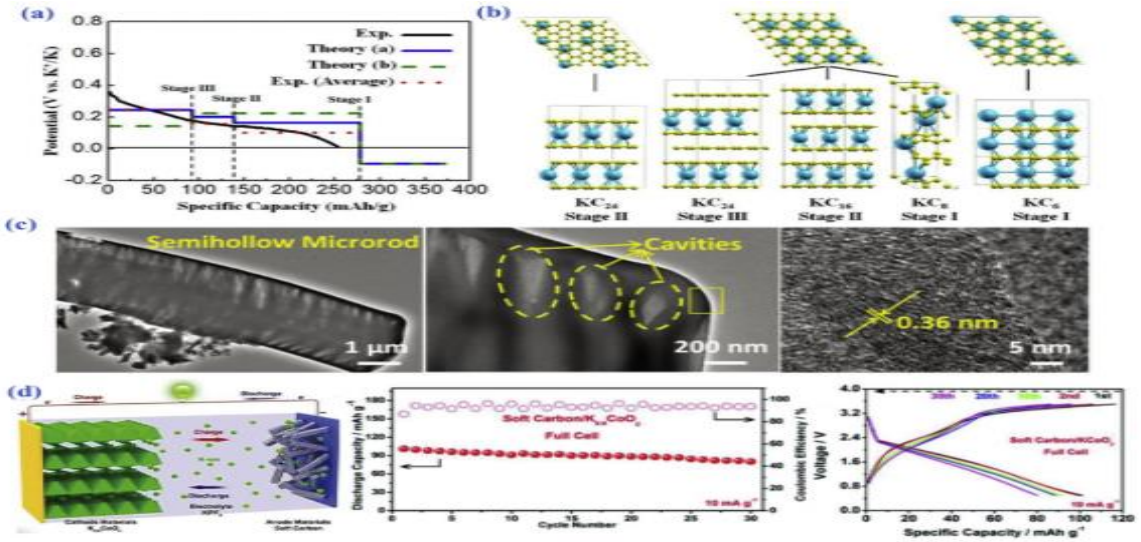


Figure 2Calculations DFT. (a) Demonstrating intercalation From K ions to graphite for various blue line setting up scenarios. (b) Diagram of graphite phases K-intercalated, K in blue and C in yellow. (c) TEM images and high-resolution TEM image of semi-hollow carbon micro-battery rods. (d) Complete battery diagram of K-ion. For Columbic, cyclic performance and associated efficacy.

This paper work is regarding electrical parameters of 1D CNTs layer in low electron energy range i.e., 0–12 eV energy to improve the performance and efficiency of a PIB. Ti and K doped in carbon nanotubes to improve K ion capturing capability of 1D CNTs anodes used in PIBs, making it a suitable material for storage applications.

anode/cathode material. K/Ti atoms increased the electronic band gap and decreased conduction, allowing charge to be stored instead of electron flow on the surface.

III.RESULTS AND DISCUSSION

To manage electrical and electronic properties of carbon nano tubes in a 1D AlN system, first-gauges estimations based on thickness utilitarian speculation system are utilized. For all computations, Materials Studio and Vienna Ab initio re-enactment pack (VASP) with

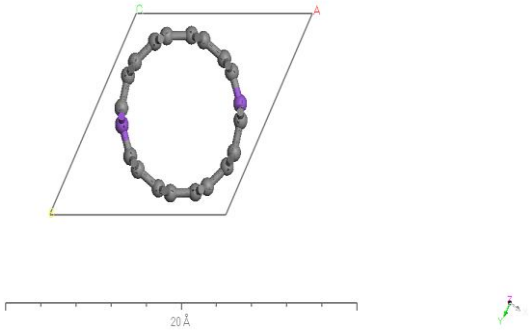
plane wave premise set were utilized. Geometry optimization is also done using the Materials studio 7.1 programming package. Both programming groups utilize the same utilitarian speculation scheme.

The assessment organization is looking for new approaches to create capable K-Ion batteries that can satisfy the growing demands of the twenty-first century, according to a recently mentioned research institution and study. In any event, there has been no or inadequate compositional work on carbon and carbon-like 1D structures for application in the PIB sector. Because K-molecule batteries are such an essential part of our daily lives, finding innovative methods to make them more lucrative and efficient is critical. This study can offer a new avenue in the field of PIB by arranging K and Ti doped intercalated carbon layered 1D systems to be considered as anode/cathode materials.

The major findings of this study, as well as related analysis and discussion, are listed below:

A. Structure diagrams of K and Ti doped monolayer K-Ion Anode.

The FPS-DFP approach is used to study structures and certain essential electrical characteristics for various combinations and compare them to one another. Figure shows the structural diagrams of various combinations of K-Ti doped 1D CNTs Figure03 (a)-(d).



0Fig 03 (a) Ring structural diagram of 1D K doped carbon nanotube.

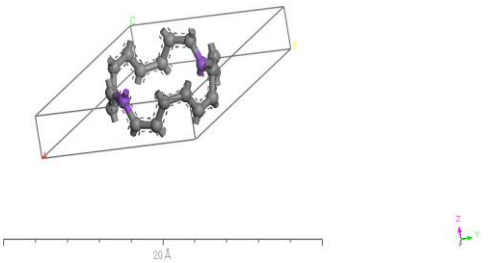


Fig 03 (b) structural diagram (side view) of K doped 1D carbon nanotube.

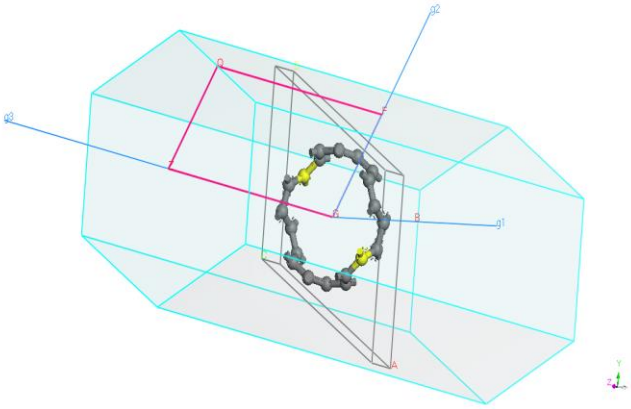


Fig 03 (c) Ring structural diagram (typical view) of Ti doped 1D carbon nanotube.

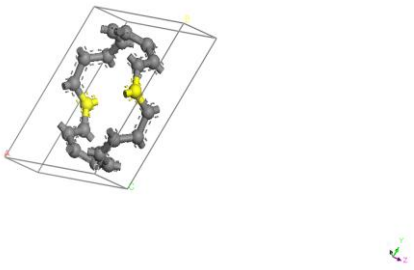


Fig 03 (d) structural diagram (side view) of Ti doped 1D carbon nanotube.

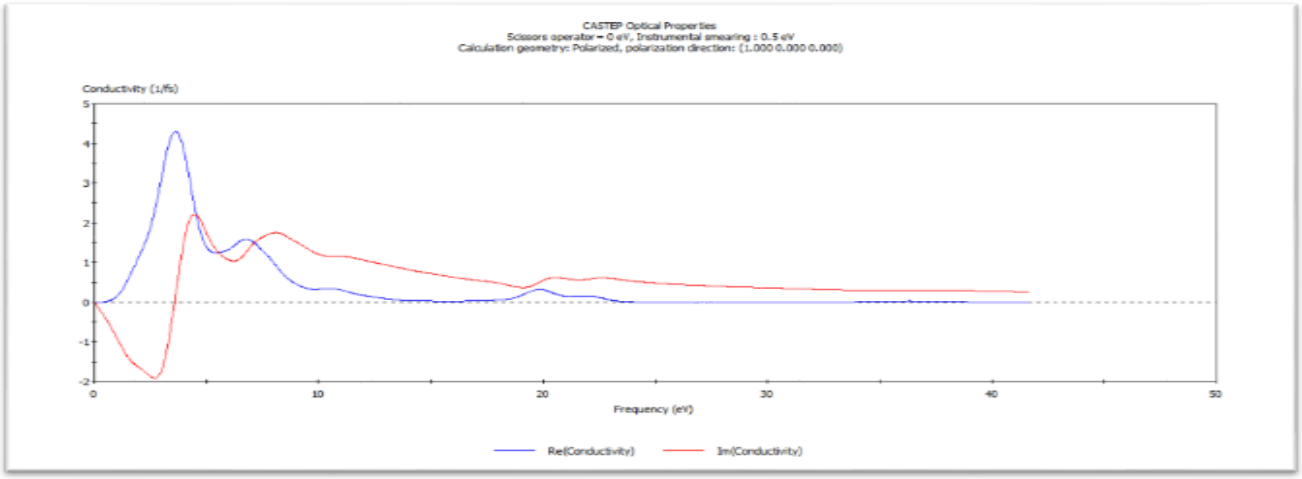


Figure 04 shows the Real and Imaginary conductivity of K doped material

The doping of K and Ti in carbon nanotubes disrupts the original layer's bonding. This implies that the addition of both elements increased the anode's binding structure, therefore allowing for more energy storage.

B. Conductivity and Density of State of K doped 1D carbon nanotubes.

Here we analysis the real and imaginary conductivity of K doped 1D CNT. The figure04 shown above indicates Real & Imaginary Conductivity of the material is indicated at different energy levels specified wrt frequency, the real value attains positive peak at about 4eV and red attains negative peak just before 4eV whereas it attains positive peak at 4.5eV among the range 0-50eV. From figure 04 it's cleared that after few periods of frequency in the terms of eV both conductivities become stable and become positive. The real conductivity attains stability faster than the imaginary one and it became stable.

Density of state:

Density of state of material shows the Ability of material to lose the number of electrons per eV energy. The figure 05 given below shows the density of state for K doped carbon nanotube. In which the highest peak point at about -17 eV with different levels in between -20eV to 0eV. The given figure also shows that second maximum peak achieved near to 7eV, so that above two points provide maximum number of electrons which can be beneficial for the battery storage capacity. The figure also shows that after -20eV to -31eV no electron is achieved same at 0eV we have No any free electron.

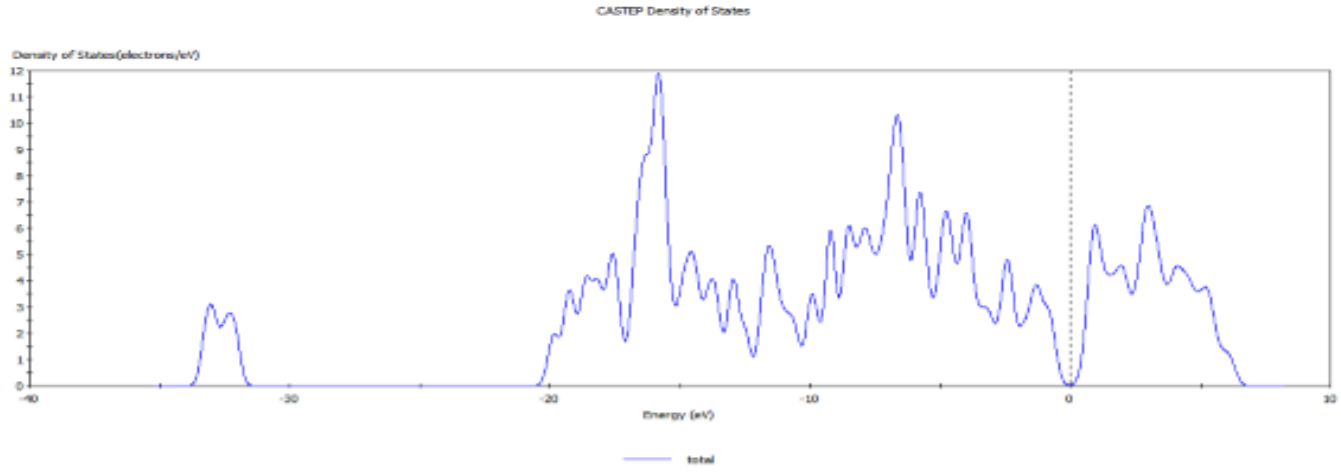


Figure 05 shows the density of state (electrons/eV) of K doped carbon nanotube.

C. Conductivity and Density of state of Ti doped 1D carbon nanotube.

Real and Imaginary conductivities of Ti doped Carbon nanotube shown in below figure4.13 in which real conductivity attains positive maximum peak at 3.7eV and imaginary negative peak occur at 2eV and after 4eV it becomes positive and decreases with increasing energy level and it became negative after 30eV. After some frequency the real conductivity become zero after 20eV to 32eV, after that both real and imaginary conductivities with respect to frequency (eV) become smooth and tends to zero.

Density of State:

Density of states (electrons/eV) at different energy levels of the indicated material are shown in figure07 illustrates the highest peak point at about -32 eV with different levels in between -20eV to -55eV.From -20eV to 6ev energy levels continues varies and the desired energy can be used to produce the required amount of electrons. The maximum number of electrons can be achieved at -32eV. Because at the energy level material attains maximum peak.

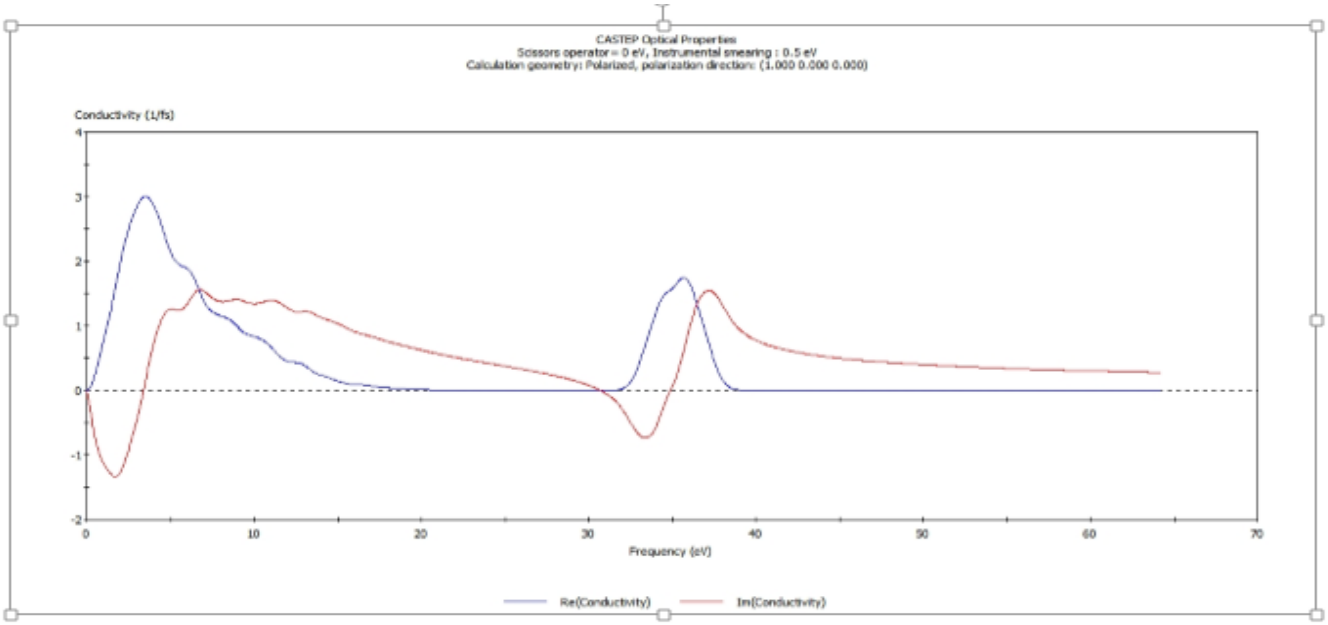


Figure 06 shows the Real and Imaginary conductivity of Ti doped Carbon nanotube.

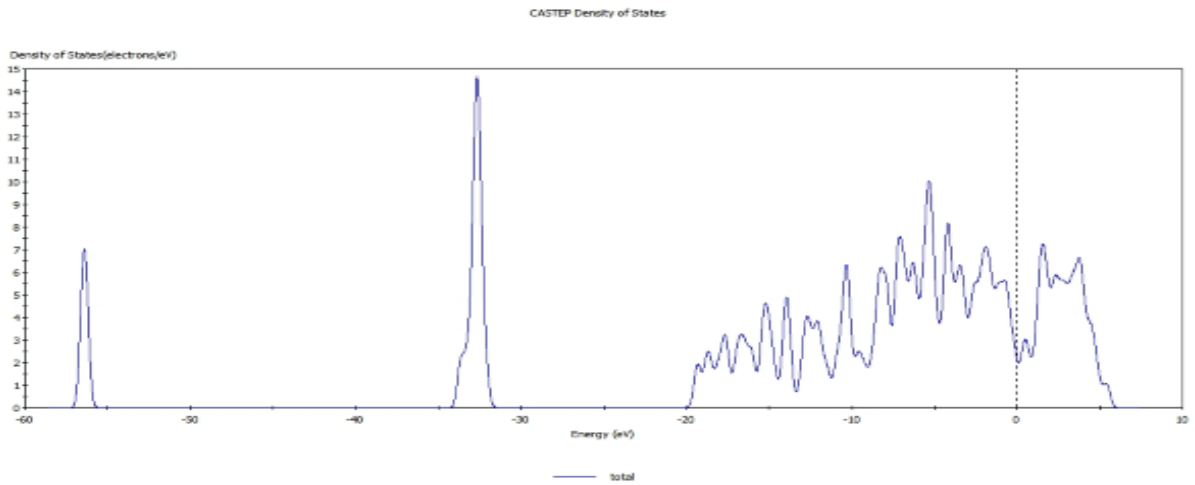


Figure 07 shows the Density of State (Electrons/eV) of Ti doped carbon nanotube.

D. Conductivity and Density of state of K adsorbed 1D carbon nanotube.

Real & Imaginary Conductivity of the material is indicated at different energy levels specified wrt frequency, and shown in given figure4.19. The real value attains positive peak at about 3eV and red attains negative peak at -1eV whereas it attains positive peak at 2.5eV among the range 0-3eV. The conductivities of K adsorbed carbon nanotubes shown in above figure indicates that the its real conductivity achieved peak value near to starting point it means that it is more conductive with the absorption ok K ions on carbon nanotubes conductivity increased.

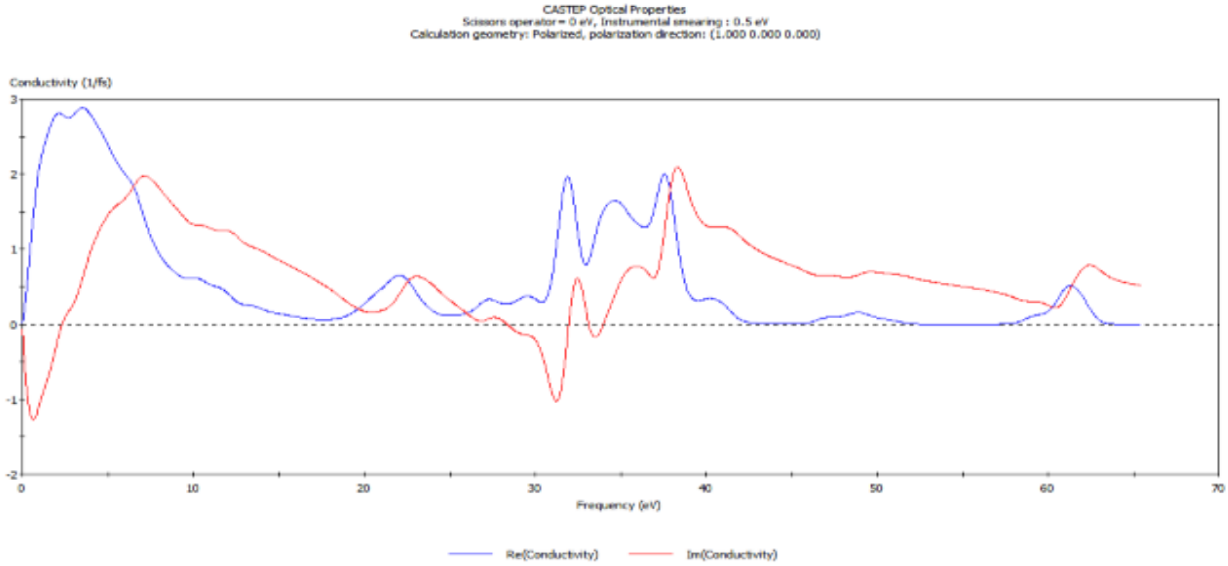


Figure 08 shows the Real and Imaginary conductivities of K adsorbed 1D carbon nano tube.

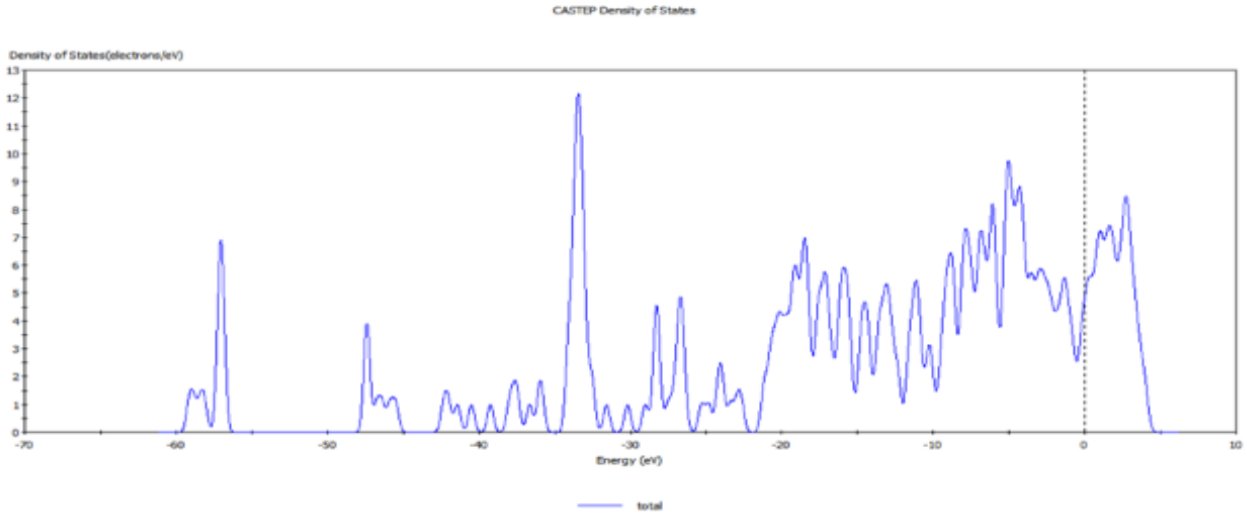


Figure 09 shows the Density of State of K adsorbed carbon nanotube.

Density of State:

Density of states (electrons/eV) at different energy levels of the indicated material are shown, figure4.20 illustrates the highest peak point at about -25 eV with different levels in between -60eV to 5eV. Also it can be shown that the density of state most of the time remain non zero at different energy levels which increases the number of electrons obtained from the material which causes increment in the capacity of battery. The above figure shows that maximum peak achieved at -5eV and from -22eV to 5eV has no any non-zero value which means increases the number of electrons obtained and as much maximum electrons obtained much better will be the capacity of battery.

IV. DISCUSSION

Here we have investigated the geometrical diagrams, band structure, conductivity and density of state of different combinations of potassium (K), Titanium (Ti) and carbon nanotubes. Our main objective of work is to

enhance the capacity of K ion battery, and develop a suitable anode material which can be used in applications of PIB. In our work we have investigated the optical parameters of K doped carbon nanotube, Ti doped carbon nanotube and K adsorption on carbon nanotubes. All the parameters were examined by performing ab initio method. We have doped K and Ti with carbon nanotubes and observed the real and imaginary conductivities and also the density of state of materials after the chemical doping. And also we have investigated another process for the comparison which is the absorption of K on carbon nanotubes in which we have examined the same parameters as in doping process but this process shows good conductivity and more number of electrons obtained in this process because of the density of state of material which remain non zero.

The plane wave premise package was used to do all calculations using Materials Studio and the Vienna Ab initio re-enactment tool (VASP). The Materials studio 7.1 programming package is also mostly used to enhance geometry. The utilitarian thickness assumption technique is used in both programming classes. The organization of the assessment seeks for altered ways to manufacture capable K-Ion batteries that can satisfy the rising demands of centuries of back and forth movement, according to a recently stated research establishment and analysis. In any case, no incomplete composition work on carbon nanotube and carbon composites-like 1D structures to be employed in the field of PIB is being done. Because K-molecule batteries are such an essential component of our ongoing electrical power consumption, it's critical to develop innovative methods for transmitting economical and precautionary batteries.

V. CONCLUSIONS

This work will clear another direction in the PIB region by organizing the K and Ti doped carbon nanotubes and K adsorption on carbon nanotubes in 1D material for the anode design in the PIBs applications. At last by performing CASTEP study optical properties of 1D carbon nanotubes with K and Ti doped and K adsorbed are analyzed. Conductivity and Density of state of materials were investigated after different chemical process, it is possible to conclude that the results of the calculations are promising and can serve as a foundation for additional research and inquiry.

As per our results, the K adsorption on carbon nanotubes possess the better electronic properties, band gape energy levels reduces0~2eV, conductivity increased and density of state remain non zero for different values of energy levels eV, Similarly, the charge carrying capacity will increased and it shows that among other configurations, the K adsorption anode combination in K-Ion can be a potential element for improving the energy storage capabilities of the K-Ion battery.

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