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ABSTRACT

EXPERIMENTAL AND COMPUTATIONAL STUDIES OF FUNCTIONALIZED CARBON NANOTUBES FOR USE IN ENERGY STORAGE DEVICES AND MEMBRANES

by

Emine S. Karaman

Electrolytes with good interfacial stability are a crucial component of any electrochemical device. The development of novel gel polymer electrolytes (GEs) with good interface stability and better manufacturability is important for the development of the next generation electrochemical devices. Gel electrolytes are hybrid electrolyte materials, combining benefits of both liquid and solid systems. Compared with liquid and solid electrolytes, GEs open new design opportunities and do not require rigorous encapsulation methods. In this dissertation, studies on functionalized carbon nanotubes (fCNTs) and graphene oxide (GO) doped polyvinyl alcohol (PVA) based gel electrolytes (GEs) are reported. The ionic conductivity and mechanical strength of fCNT doped gel electrolyte (fCNTGE) is significantly improved, when compared to pure GE and graphene oxide doped gel electrolyte (GOGE). The ionic conductivity is significantly improved by introducing fCNTs into the PVA gel and reaches 6.9×10^{-2} S cm^{-1}, revealing that the diffusion and transport of ions into electrolyte are much better than the GE and GOGE. A significant enhancement in the gel mechanical properties is observed with Young's modulus (E = 2.3) and tensile strength (22.3 kPa) of fCNTGE. Furthermore, the composite Zn–Ag_{2}O batteries are made and tested using the fCNTGE, GE, and GOGE in three dimensional (3D) -printed battery casings.
However, questions remain about the origin of the property enhancement and the interactions between components of GEs. Density functional theory (DFT) calculations are employed to analyze the interactions between fCNT, PVA, and Zn ions. CNTs with increasing numbers of carboxyl (-COOH) functional groups and PVA chains with varying lengths are studied. Increasing the number of -COOH on the CNTs enhances the adsorption energies ($E_{\text{ads}}$) of PVA, and $E_{\text{ads}}$ also increase as the number of monomers increase. Strong fCNT-PVA interactions contribute to the enhanced mechanical strength and thermal stability, while the enhanced ionic conductivity is partly due to weak Zn adsorption.

Computational modelling is used to understand how fCNT displays better performance in membrane separation and investigate if the same trend could be seen for different pollutants as well. The nature of the interactions between the pollutants and raw and functionalized CNTs are studied on the atomic level by using DFT calculations. By determining the adsorption energies, DFT calculations theoretically confirm that pollutants interact more strongly with fCNTs than unfunctionalized CNTs, likely partly contributing to the observed some properties such as mass transfer coefficient, selectivity, and flux. It is demonstrated that this is due to enhanced charge transfer between the CNT and pollutants as the number of functional groups increases. Trends in the HOMO-LUMO gap and how they are affected by the functionalization of the CNT are also described. These calculations allow for better understanding of the influence of CNT functionalization on the properties of membranes.
EXPERIMENTAL AND COMPUTATIONAL STUDIES OF FUNCTIONALIZED CARBON NANOTUBES FOR USE IN ENERGY STORAGE DEVICES AND MEMBRANES

by
Emine S. Karaman

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This thesis is wholeheartedly dedicated to my beloved dad and my wonderful family who have been with me every step of the way through good times and bad. Thank you for all your endless love, sacrifices, prayers, and support.
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COMPUTATIONAL INVESTIGATION OF ENHANCED PROPERTIES IN FUNCTIONALIZED CARBON NANOTUBE DOPED POLYVINYL ALCOHOL GEL ELECTROLYTE SYSTEMS

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CHAPTER 1

INTRODUCTION

1.1 Objective

The objective of this dissertation is to study applications of functionalized carbon nanotubes (fCNTs) for energy storage devices and membranes.

First, fCNTs and graphene oxide (GOs), as components in gel electrolytes, have been used to improve ionic conductivity, electrochemical diffusion, mechanical strength and study the effectiveness of the GEs for Zn-Ag_2O battery system.

Second, computational modeling of the interactions between gel electrolyte components such as fCNTs, PVA, and the working ion has been studied. The nature of the interaction between PVA dendrimers, fCNTs, and Zn ions is investigated on the atomic level by using Density Functional Theory (DFT) calculations.

Third, computational modelling is used to understand how fCNT displays better performance in membrane separation and investigate if the same trend is observed for different pollutants as well. The nature of interactions between the pollutants and raw and functionalized CNTs were studied on the atomic level by using DFT calculations.
1.2 Background Information

1.2.1 Introduction to Gel Electrolyte Systems

Electrolytes, with good interfacial stability, are a crucial component in electrochemical devices. The development of novel gel polymer electrolytes (GEs) with good interface stability and better manufacturability is important for the development of next generation electrochemical devices. A gel electrolyte (GE) is a hybrid electrolyte material, which combines the beneficial characteristics of both liquid and solid systems [Ahamad, 2020 #96]. Compared with liquid electrolytes, GEs do not require safety encapsulation materials of high standard [2] and thus do not limit the battery geometry. This opens new design opportunities for energy storage. Also, they can provide high reliability without electrolyte leakage and volatilization and can be used in conformal and flexible batteries and in separator-free devices [4]. The development of novel gel electrolytes with low reactivity, flexibility, good interfacial stability, and better manufacturability are important for the development of the next generation of batteries [5]. In batteries, GEs have been used as ionic conductors as well as separator for lithium-ion [2, 6, 7], aluminum-air [8], magnesium-ion, [5], sodium-sulfur [9] and zinc-air battery systems [10, 11].

Gels can be obtained as a result of either a chemical or a physical cross-linking process (Figure 1.1). When gelation occurs, a dilute or a more viscous polymer solution is transformed into a system of infinite viscosity, i.e., a gel. A gelled solution does not exhibit any flow when a tube containing the solution is tilted.
Chemical cross-linking is a covalent bonding of polymer chains by a chemical reaction to form a certain number of tie or junction points, as presented in Figure 1a. Chemical gels are covalently crosslinked network polymers swollen in a large amount of solvent and covalent cross-linking leads to the formation of irreversible gels. In such gels, the number of tie-points essentially does not change upon variation of the external conditions such as temperature, concentration, or stress [12]. Physical gels are reversible and occur as a result of the intermolecular association by electrostatic, van der Waals, or hydrogen bonding interactions [13] (Figure 1.1 b-c).

Figure 1.1 Schematic Illustration of Gel Through A) Chemical Network with Junction Points, and B-C) Physical Network Having Junction Zones [14, 15].

A GE is a polymer swollen by a liquid electrolyte. These electrolytes exhibit high ionic conductivity at room temperature but have poor mechanical properties. To solve this problem, nanoparticles can be used to improve the electrochemical stability and mechanical properties without decreasing the ionic conductivity. A plasticizer can also change the polymer matrix in gel electrolyte systems as it makes segmental motion easier.
or gives liquid like character like that of a liquid electrolyte. These two together give rise to the high ionic conductivity in the gel electrolyte system. The ionic conductivity of a gel electrolyte is around $10^{-3}$ Scm$^{-1}$ at room temperature which is far above that of a solid electrolyte [16, 17].

Because of the mechanism of ionic conduction in these systems, the ionic conductivity can be improved by increasing the motion of the polymer segment. One of the typical preparation procedures of the GE electrolytes is dissolving the polymer and salts in a selective solvent to form a homogeneous solution. An illustration of ionic conduction mechanism in lithium is shown in Figure 1.2 [18]. The lithium salt dissociates and dissolves in the polymer matrix to initiate free ions. The lithium ion organizes with oxygen atoms with a fixed ratio in the PEO chain and the ionic conduction mostly occurs in the amorphous phase. Ions are transported easily in the amorphous region, thus improving the ionic conductivity [19]. These complex ions move with the segment of polymer chain. Thus, the cations move freely from one electrode to another while an electric field is applied across the polymer electrolyte. Generally, this motion can be increased through modification of the molecular structure, such as grafting, copolymerizing, mingling with more flexible polymers.

![Figure 1.2](image.png)

**Figure 1.2** Ion Conduction Mechanism in the Polymer Electrolyte [18].
1.2.2 Literature Review of Gel Electrolyte Systems

During the scale up of manufacture of battery from laboratory setup to full production, the mechanical strength of electrolyte needs to be improved for manufacturability by conventional large-scale coating processes. The use of different polymers, plasticizers, and modification to increase the ionic conductivity of GEs is reviewed here. Many different polymers have been used in GEs. A sample of different examples are described here.

The most common polymers used as the polymer matrix in gel polymer electrolytes include polyethylene oxide (PEO), Poly (p-phenylene oxide) PPO, polyacrylonitrile (PAN), poly (methyl methacrylate) (PMMA), poly (vinyl chloride) (PVC), poly (vinylidene fluoride (PVdF), poly (vinylidene fluoride-hexafluoro propylene) (PVdF–HFP), etc. The first proposed concept of the GE contained a small amount of organic liquid known as a plasticizer, such as chain-like ester and cyclic carbonic acid ester [20]. Until now, it has been the most common approach for enabling the ionic conductivity to reach the magnitude of $10^{-3}$ S/cm at room temperature; for example, plasticizer-containing PAN or PMMA polymer hosts were reported to provide very high ionic conductivity [21].

Flora et al. prepared a polymer blend electrolyte with various ratio of poly(acrylonitrile) (PAN) and poly (methyl methacrylate) (PMMA) as host polymers and lithium perchlorate (LiClO₄) as an ionic salt. Among the different concentrations, the polymer electrolyte film containing PAN/PMMA (75:25 wt.% ) was concluded to be a suitable candidate for the battery applications on the basis of ionic conductivity which showed the order of $0.019 \times 10^{-5}$ S cm⁻¹ [22].
Kucharskiet et al. prepared a PEO based polymer GE. The electrolyte demonstrated a conductivity of $10^{-4}$ Scm$^{-1}$ at room temperature [23]. When the salt concentration was increased to 10 wt %, the conductivity increased to $6.4 \times 10^{-3}$ Scm$^{-1}$, but the mechanical properties were poor due to deficient gel formation [23].

Zaghib et al. studied the performance characteristics of polymer GEs for C and LiFePO$_4$ cells [24]. In the GE, the polymer chain segments are highly mobile. By modifying the PEO structure with introduction of substituents and the synthesis of branched and network polymer matrices, the conductivity of the corresponding gel electrolytes was enhanced [24]. Although gel electrolytes based on PVDF and PVDF-HFP display high ionic conductivity, they have some disadvantages such as high cost and the overall yield of their synthesis [25].

Vickraman et al. studied polymer gel electrolytes based on PVC, which exhibited conductivity of an order of magnitude of $10^{-6}$ Scm$^{-1}$ at room temperature [26]. Furthermore, their matrix was modified using PVDF-HFP since mixing of various polymer components has a beneficial effect on the electro-chemical properties of gel electrolytes as will be discussed in more detail later. However, in this case, the ionic conductivity was decreased because of poor compatibility of polymers and their inability to hold the liquid electrolyte [26].

Kim and Oh found that ionic conductivity and the mechanical stability of polymer gel electrolytes based on PMMA modified with the interpenetrating polymer network components [27]. Ito et al. investigated the increase in ionic conductivity using PEG as plasticizer which was mainly attributed to the reduction in crystallinity as well as the increase in free volume of the system [28].
The PAN-based electrolyte offers homogeneity among the polymer hosts that are used for gel electrolytes. As reported by Abraham and Alamgir, a typical electrolyte comprising PAN showed an ion conductivity of $1.1 \times 10^{-3} \text{S/cm}$ at $-10 \degree \text{C}$ and $1.71 \times 10^{-3} \text{S/cm}$ at $20 \degree \text{C}$ [29].

PVDF has been chosen as a polymer host by virtue of its multifold appealing properties. PVDF-based polymer electrolytes are highly anodically stable due to the strongly electron-withdrawing functional group (C—F). Wang et al. studied the plasticized PVDF system and reported an increase in the ion conductivity. They explained that the ion conductivity of a polymer electrolyte depends strongly on the ionic mobility within the material [30].

Wang et al. reported a PMMA-based electrolyte for a lithium-ion battery with improved mechanical properties [30]. The lithium cell fabricated with this gel polymer electrolyte showed excellent electrochemical properties.

Zhu and Huang investigated the electrochemical properties of PVC and PMMA-based gel electrolytes [31]. Their results indicated that these electrolytes acquire a high ionic conductivity and a wide electrochemical stability window. However, their application in rechargeable lithium-ion batteries was hindered by the corrosion of the lithium electrode interface.

Next, fillers have been shown to affect both the conductivity and mechanical properties. Nanocomposites based on PMMA in GE systems were studied by Ahmad et al. [32]. The nanofiller GE composite exhibited better mechanical properties than the unfilled polymer electrolytes [32]. Another PEO-based nanocomposite GE system was studied by Nan et al. [33].
A net improvement in ionic conductivity and a very high Young’s modulus was obtained at room temperature, higher than the unfilled PEO electrolyte. This improvement in mechanical properties was found to correlate to a specific interaction between SiO$_2$ and PEO [33]. Gel nanocomposite polymer electrolytes based on PVDF-HFP were studied in another research [34] and it was found that the diffusion coefficient indicated reduction in both anion and cation mobilities by the presence of the filler [34].

Finally, the copolymerization or blending with polymers has been proposed to improve the performance of polymer electrolytes. PVDF, PVC, and PAN have been mostly used as matrix polymers in plasticized polymer electrolytes with ionic conductivity in the order of $10^{-3}$ S/cm at room temperature. However, they cannot completely fulfill the requirements for the high mechanical strength, long-term phase stability, and good adhesion to the electrode. Blending is more useful because of the ease of preparation and control of polymer electrolytes by changing the composition of blended polymer matrices.

For example, Park and co-workers investigated polymer electrolytes based on the blend of poly(vinylacetate) (PVA) and PVdF–HFP and the maximum ion conductivity reached $2.3 \times 10^{-3}$ S/cm at room temperature [35]. By increasing the amount of PVA content, the mobility and concentration of the free ions in the polymer electrolyte were reduced, showing a decrease in the ionic conductivity [35].

In another example, Oh and Kim attempted to develop a new gel electrolyte that exhibited a high ionic conductivity and excellent film formation ability [36]. They developed a polymer system consisting of a matrix polymer and a filling polymer for absorbing electrolyte solution and gelation of the microporous gel electrolyte for
sustaining the mechanical integrity [36]. Liu and colleagues also invented gel polymer films by mixing PMMA with PVDF–HFP, the latter showing better compatibility with the liquid electrolyte. [37].

There is a wide variety of GEs based on different polymers, and different methods such as adding fillers and blending have been used to improve their properties. In the next section, the use of functionalized carbon nanotubes as fillers will be discussed.

1.2.3 Functionalized Carbon Nanotubes (fCNT) in Gel Electrolyte Systems

Composite electrolyte with the idea of incorporating electrochemically inert fillers into polymer matrices can provide two advantages. One is to improve the stability at the interface with electrodes and the other is enhancement of ionic conductivity at low temperatures. Generally, high surface area particulate fillers such as chitosan [38], silica [39], CNTs [40] have been studied in polymer matrices [41].

Among them, CNTs are highly flexible which can improve the interaction and cross-linking with polymer molecules that further enhances morphological features and ionic conductivity of composite electrolytes. They have been used for energy storage devices because of their high specific surface area and mechanical elasticity of the tubular network [42]. Also, the superior electrical conductivity enables CNT as an additive to composite electrodes and facilitates activation of poorly conducting electrode materials making them electrochemically active [43].

On the other hand, CNTs have played an important role as sorbents for selective solute transport in different membrane applications which have promoted higher flux, selectivity, and reduced fouling in membrane systems [44, 45]. It was observed that
immobilization of CNTs on membrane surfaces has a great effect on the interaction between the membrane and solutes [46-48]. The surface areas of CNTs are between 100 and 1000 m²/g [49] which make them excellent candidates as sorbents.

However, while CNTs display high water permeability and good adsorptive capabilities [50], they also have some disadvantages such as weak van der Waals interaction [51], insolubility for adsorbing materials in aqueous solutions [52], and agglomeration [53]. Functionalized CNTs (or fCNTs) lead to improvements in hydrophilicity, specific charge transport and reducing agglomeration. Recently, CNTs functionalized by oxygen containing functional groups such as –COOH and –OH groups have become particularly promising material for a wide range of applications from electronics to biotechnology as they are easily synthesized using oxidative treatments [54]; they enhance adsorptive capabilities [41] and improve solubility [55].

CNTs can be functionalized by two methods: chemical and physical methods [56]. The characterization corresponding to these methods are summarized in Figure1.3. When CNT is bonded to the functional group using a chemical reaction, this is called chemical functionalization. If the modifier is adsorbed on CNT or stored in the hole of CNT, it is a physical method [57].

For covalent functionalization, introducing carboxylic groups on CNTs is usually the first step, generally prepared by microwave treatment with strong acids, refluxing, and sonication [58]. In an acid treatment, CNT is reacted with a concentrated acid solution such as sulfuric and nitric acid [59]. Commonly, the mixtures of the acid are 3/1 or 1/3 v/v of H₂SO₄/ HNO₃ solution [60]. Detailed procedures of acid treatment can be found in the literature. In summary, CNT is dispersed in an acid mixture at relatively
high temperature for a while. Afterwards, the CNT is washed, filtered, and dried. The treatment time, the strength of the reagents, and reaction temperature control the degree of functionalization in terms of the number of carboxylated groups.

Figure 1.3 Functionalization possibilities for CNTs: A) Defect-group Functionalization, B) Covalent sidewall functionalization, C) Non-covalent exohedral functionalization with surfactants, D) Non-covalent exohedral functionalization with polymers [61].

The chemistry of microwave treatment has been seen to be more efficient, ecofriendly, and faster than conventional methods so far [62]. Different types of reactions and organic syntheses with high yields under controlled pressure and temperature, and high-purity products due to the short residence times have been reported [63, 64]. Besides, the further polarization of the dipoles under microwave radiation can facilitate modification of chemical activation parameters [65].

The microwave treatment was observed to lead to increase in oxygen content with increasing carboxylation as well as significant tube damage [66]. Also, the surface
area was found to be increased since both acids and microwave treatment led to carbon-carbon bonds to break, leaving defects on CNTs [66].

1.2.4 Electrochemical Impedance Spectroscopy (EIS)

A direct current (DC) method cannot be used to calculate the resistance of a dielectric material due to the polarization of charges taking place at the phase boundaries of the sample or at the electrode-electrolyte interface. Therefore, other techniques are needed, one of which is Electrochemical Impedance Spectroscopy (EIS). Impedance measurement using EIS is performed by applying a low amplitude sinusoidal potential (AC voltage) over a range of frequencies to the sample. EIS measures the time response, which enables the evaluation or decoupling of small-scale polarization and conductance mechanism at the electrode interface and within the electrolyte. EIS results can be presented as a Nyquist plot or a Bode plot. For a Bode plot, the frequency is precise while for a Nyquist plot, the frequency is hidden.

GEs, consisting of an ionic salt dissolved in a polymer, can present both capacitive and resistive behavior as reflected from the real ($Z'$) and imaginary ($Z''$) parts of the complex impedance ($Z^*$). Figure 1.4 shows a schematic drawing of GE sandwiched in between two blocking electrodes and the possible equivalent circuit model, in which the resistance and capacitance are in parallel that can be distinguished using impedance spectroscopy over a range of frequencies.
Figure 1.4 (a) Schematic drawing of GE sandwiched between two blocking electrodes. (B) equivalent circuit (model) of GE sandwiched between two Blocking Electrodes [67].

The data plots of $Z'$ against $Z''$ of the impedance measured under AC over a range of frequencies, where the frequency is hidden, are illustrated in Figure 1.5. These plots are scientifically known as frequency dispersion spectrum or frequently called a Nyquist plot [68]. Each data point in the Nyquist plot represents the impedance of the electrolyte measured at a certain frequency. In fact, the plot is separated into frequency regions known as the high frequency region and the low frequency region. The high frequency region is plotted toward the origin of the figure whereas the low frequency region is plotted outward from the origin of both $x$- and $y$-axes. The value of the point of intersection between the plot and the $x$-axis represents the value of the bulk resistance ($R_b$) of electrolyte.
The ionic conductivity can be analyzed by using the following Equation 1.1 [70].

\[
\sigma = \frac{h}{R_b S}
\]

where \( R_b \) is the bulk resistance of polymer electrolyte, \( h \) is the distance between two electrodes and \( S \) is the total contact area of the electrolyte with electrodes.

### 1.2.5 Transference Number and Electrochemical Stability Window

The electrons and ions (cations and anions) can contribute to conduction processes in an ion conducting system. Thus, it becomes important to separate the current and distinguish how much is carried by each mobile species; this is referred as the measurement of the transference number. Ionic transference number is a technique used
to separate the different contribution of electrons and ions from total charge transport. It is a dimensionless parameter which gives information about the contribution of the charged species present in the bulk of electrolyte to the overall charge transport across the measured system.

GEs are placed between two blocking electrodes and current is monitored as a function of time by applying a small dc voltage. The current decreases with increase in time due to polarization of mobile ions at the electrodes. At the beginning, both the ionic and electronic components contribute but after a while, current either reaches a residual constant value (for mixed ionic/electronic conductor) or attain zero (for a pure ionic conductor). Therefore, the ionic transference number are calculated using Equation 1.2 [34]:

\[
t_{\text{ion}} = 1 - \frac{I_{\text{e}}}{I_{\text{t}}}
\]

where \( I_{\text{t}} \) is the total initial current or due to ions or as a combined result of ion and electron contribution while constant residual current \( I_{\text{e}} \) is due to electron contribution only.

A large transference number can reduce the concentration polarization of electrolytes during charge–discharge steps, and thus produce a higher power density. It is highly desirable that the transference number approaches 1 in an electrolyte system. However, many existing electrolyte systems, either liquid or polymeric, have transference numbers less than 0.5 [7].
The gel electrolyte is interposed between the cathode and the anode, and its chemical stability should not have undesired chemical reaction as the electrodes come into direct contact. In general, the electrochemical stability can be characterized by an electrochemical window measured via a linear sweep voltammetry (LSV) shown in Figure 1.6. The flat areas occurring in the figure represent the electrochemical window. LSV is voltametric method; the current at a working electrode is measured while the potential between the working electrode and reference electrode is swept linearly vs. time from lower to higher potentials.

The objective is to detect at which potential the GE will be oxidized/reduced and, thus, degraded. Oxidation or reduction of species is registered as a peak or trough in the current signal at the potential at which the species begins to be oxidized or reduced. Principally, when LSV is applied, a sudden increase in the current appears at a given potential and indicates oxidation (faradic current). Figure 1.7. shows an example of an experimental LSV profile. Experimental parameters include scanning rate, temperature, determination of the potential estimated as the beginning of the oxidation, or the minimum current value considered as a realistic value meaning that oxidation occurs.
1.2.6 Introduction of Density Functional Theory (DFT)

Ionic conductivities of gel electrolyte systems are recognizably raised by numerous orders of magnitude after adding plasticizers to the gel electrolyte system. According to the research, it can be concluded that the ionic mobility plays a key role in the achievement of higher ionic conductivity in polymer electrolytes. However, high
compatibility between electrolyte components should be assured to obtain a homogeneous membrane and enable the polymer to dissolve.

Recently, some modifications have been carried out to enhance the efficiency in membrane technology. For example, immobilizing nanomaterials such as carbon nanotubes (CNTs) [73], silica [74], and polymers [75] have shown improvement in flux and stability of the membrane [76]. Furthermore, sorbate and sorbent interaction in membrane systems can be affected by the capillary forces in nanotubes, presence of defects, or polarizability [77, 78], all of which directly influence the separation performance. For instance, deposition of dissolved elements on the membrane pores can cause membrane fouling [79] and capillary forces have been shown to produce bending during the drying process [80]. At this point, understanding interactions at the membrane interface as well as electrolytes is becoming a very important parameter for correlation of components [81].

On the other hand, the electrochemical stability at the electrode/electrolyte interface is the most important criteria for an energy storage device with a highly oxidizing cathode material before a reliable gel electrolyte battery with long life cycle can be realized. Modern computational approaches can provide accurate energies of surface chemical reactions which is important to design and optimize new materials for energy storage devices [82].

Density Functional Theory (DFT) is an approach to quantum chemistry where a system of interacting electrons is mapped onto a system of non-interacting ones in an effective potential [83]; it can provide accurate and valuable information on molecular geometries and properties. It can also be used to compute the electronic properties of
transition metals and compounds faster and more accurately [84] over classical quantum mechanics.

For a molecule or system, it is critical to know the changes in energy when the atoms move around. The configuration of atoms that gives the lowest energy is considered to be the most stable state (“ground state”). This can be done by solving the Schrodinger equation 1.3 [85].

\[ H\Psi = E\Psi. \]  

(1.3)

In this equation, H is defined as the Hamiltonian operator and \( \Psi \) is a set of solutions, or eigenstates, of the Hamiltonian. Each of these solutions, \( \Psi_n \) has an associated eigenvalue, \( E_n \), a real number that corresponds the eigenvalue equation [86].

The terms making up the Hamiltonian are the:

- ion-electron potential energy
- ion-ion potential energy
- electron-electron energy
- kinetic energy
- exchange-correlation energy

If the nuclei positions are defined with \( R_1, \ldots, R_m \), the ground state energy as a function of the positions of these nuclei will be \( E(R_1, \ldots, R_m) \), which is called potential energy surface of the atoms [87]. On the other hand, for defining atoms’ location, both
its nucleus and electrons position must be determined. Since the atom nuclei are much heavier than individual electrons, those electrons can respond to changes in their surroundings much faster than the nuclei. As a result, the physical question can be solved for a fixed position of the atomic nuclei, which the equations explain via the movement of electrons.

According to Born-Oppenheimer approximation, the wave functions of atomic nuclei and electrons in a molecule can be treated separately and the lowest energy state is accepted as the ground state of electrons [88]. Therefore, the energy terms describing the energy of the nuclei are approximately zero.

With these terms removed; the Schrödinger equation can be defined by the following formula containing only electron terms [89].

\[
\left[ \frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i=1}^{N} V(\mathbf{r}_i) + \sum_{i=1}^{N} \sum_{j<i} U(\mathbf{r}_i, \mathbf{r}_j) \right] \psi = E \psi.
\] (1.4)

Here, \( m \) is the electron mass, the first term in brackets is the kinetic energy of each electron, the second term is the interaction energy between each electron and the collection of atomic nuclei, and the third term is the interaction energy between different electrons. \( \Psi \) is the electronic wave function, and \( E \) is the ground state energy of the electrons which is independent of time. This is the time independent electronic Schrödinger equation. However, this equation still cannot be solved for a real system with interacting electrons. To move forward, DFT is utilized.
DFT is based on a fundamental mathematical theorem explained by Hohenberg and Kohn in the 1960s. According to their first theorem, the ground state energy from Schrödinger’s equation is a unique functional of the electron density [90]. To understand the importance of this result, it is required to explain what a functional is: a functional is a function of a function [88].

Thus, Hohenberg and Kohn’s theorem can be stated as the ground-state energy $E$ that can be expressed as $E(n(r))$, where $n(r)$ is the electron density. The Hohenberg and Kohn theorem declares that the electron density of any system determines all ground state properties of the system. In this case, the total ground state energy of a many-electron system is a functional of the density. By knowing the electron density functional, the total energy of our system can be determined [90]. By focusing on the electron density, it is possible to derive an effective one-electron-type Schrödinger equation.

Figure 1.8. Density Functional Theory (DFT) abandons the many-particle electron reality in favor of electron density [91].
This theorem also explains the one-to-one correlation between the ground state electron density and ground state wave function [92]. Because the ground-state electron density uniquely determines all properties, including the energy and wave function of the ground state, there is an exact dependence between the ground-state wave function and the electron density. This allows to reduce the complexity from $3N$ dimensions to just $3$ dimensions. While many body wave function relies on all spatial coordinates in electron system, the electron density only depends on three spatial coordinates (Figure 1.8). Thus, electron density makes object simply computationally, which is the foundation of desirable computational properties of DFT.

However, the first Hohenberg and Kohn theorem does not generate information on how to find the functional. The second Hohenberg and Kohn theorem expresses a critical property of the functional and states that “the electron density that minimizes the energy of the overall functional is the true electron density corresponding to the full solution of the Schrödinger equation” [93].

If the true functional form is known, the minimum energy can be found by varying the electron density to find the ground state electron density. Once the ground state electron density is known, all the properties can be calculated. This variational principle is used in practice with approximate forms of the functional. After this, Kohn and Sham showed how to turn the system of interacting electrons to the system of non-interacting electrons [94]. The total energy functional can be re-written as the sum of different interactions as:
\[ E[n(r)] = \int V(r)n(r)dr + T[n(r)] + E_H[n(r)] + E_{XC}[n(r)] \] (1.5)

The first term is the potential energy, the second term is the kinetic energy, the third term is the Hartree energy (it describes the interaction of the electron density with itself), and the fourth term is the exchange-correlation energy (describing all the other electron-electron interactions). Up to now, density functional theory has been exact, and all terms except for the exchange-correlation energy can be solved by choosing a trial charge density and iterating on it until minimization; however, because there is no exact formula for the exchange-correlation energy, which contain all the electron-electron interaction information, assumptions must be made.

To approximate the exchange-correlation energy, different “functionals” have been developed and are used to calculate this contribution to \( E(n(r)) \). The one used in this work is B3LYP (Becke, 3-parameter, Lee, Yang, Parr), which is one of the most used in the world [95, 96].

\[ E_{xc}^{B3LYP} = (1 - a)E_{xc}^{LSDA} + aE_{xc}^{HF} + b \Delta E_{xc}^B + (1 - c)E_{xc}^{LSDA} + cE_{xc}^{LYP} \] (1.6)

Here, \( a, b, \) and \( c \) are three parameters, while the other terms are other different approximations of the exchange-correlation energy. Now with these functionals, density functional theory calculations can be performed quickly and reliably.
1.2.7 Conclusion

The need for efficient and clean energy storage devices is more important today and providing power to numerous portable consumer electronic devices such as laptops, mobile phones, personal digital assistants (PDAs), or for implantable medical applications will be a massive task. Gel electrolytes are obligatory for these developments. They are expected to take the place of liquid electrolytes in the future since they have many advantages over their liquid and solid counterparts. During the past 30 years, revolutionary progress has been made in the preparation, characterization, and electrochemical evaluation of various gel electrolytes. However, for the state-of-art technology of gel electrolytes, there are still several technical limitations to be improved. In any case, GEs are a developing trend for both electrochemistry science and polymer science and is a very attractive field to perform research.
CHAPTER 2
FUNCTIONALIZED CARBON NANOTUBE DOPED GEL ELECTROLYTES
WITH ENHANCED MECHANICAL AND ELECTRICAL PROPERTIES FOR
BATTERY APPLICATIONS

2.1 Introduction
Several polymers including poly(acrylonitrile) (PAN) [97, 98], poly(vinyl alcohol) (PVA) [99-102], poly(ethylene oxide) (PEO) [2, 103], poly(methyl methacrylate) (PMMA) [76, 104], and copolymer poly(vinylidene fluoride-hexafluoropropylene) (P(VDF-HFP)) [5, 105] have been used to make gel electrolytes (GE) for solar cells [106-109], membranes [110, 111], and supercapacitors [4, 100, 112, 113].

GEs can be limited by their ionic conductivity [7, 114] and poor mechanical properties [7, 115]. In an effort to improve the mechanical and electrical properties of GE, nanosized inorganic fillers have been used which have altered crystallinity [116] and stabilized the conductive amorphous phase [117]. Moreover, its electrochemical properties strongly affected the battery performance in terms of rate capability and cyclability [76].

PVA is a semi-crystalline hydrophilic polymer with high capacity for holding water and salts. Fillers such as GO [111, 118, 119], chitosan [38], silica [39], CNTs [40] have been added to PVA to generate gel composite electrolytes. The fillers which have abundant oxygen functional groups [113] are readily dispersible in water [120] and can interact with polar functional groups within polymers [121]. PVA simultaneously interacts with these fillers via both -inter and -intra chain hydrogen bonds which make it a unique polymer [122]. For instance, GO fillers [123] in PVA provide good interfacial interaction and dispersion due to the interaction of OH
CNTs are highly flexible which might improve the interaction and cross-linking with polymer molecules that further enhance morphological features and ionic conductivity of composite electrolytes. It has been used for energy storage devices because of its high specific surface area, mechanical elasticity of the tubular network and superior electrical conductivity [42]. Furthermore, functionalized CNTs (or fCNTs) lead to improvements in hydrophilicity, specific charge transport and reduction in agglomeration. Using fCNT with high surface area and oxygen-containing functional groups should be a wise strategy as an additional material to improve performance of GE and the incorporation of fCNT into gel as GE for batteries has not been reported so far. The functionalized carbon nanotubes (fCNTs) may also generate gel structure with improved mechanical properties [125].

The objective of this research is to use fCNTs and GOs as components in gel electrolytes to improve ionic conductivity, electrochemical stability, mechanical strength and study the effectiveness of the GE for Zn-Ag$_2$O battery system.

2.2 Experimental Description

2.2.1 Preparation of polymer gel electrolytes (GE), fCNT and graphene oxide (GO) doped polymer gel electrolytes

Raw multiwalled CNTs were treated for 5, 10, 30, 60, and 120 min respectively under microwave radiation to produce fCNTs. The GE (PVA-KOH polymer gel electrolytes) were prepared by dissolving the appropriate weight of PVA in water. The KOH solution was added to PVA solution drop wisely and continuously stirred (at 80 °C for 2 hours) till a homogeneous viscous liquid. Concentration of PVA and
KOH solutions for the polymerization reaction were adjusted and it was found that an appropriate composition of the PVA-KOH-H₂O solution could be prepared with 80% H₂O, 6% PVA, and 14% KOH by weight. The gelation of PVA–KOH–H₂O was allowed to proceed at room temperature for another 2 hours. The fCNTGE was prepared with 0.018% fCNTs, 80.52% H₂O, 6% PVA, and 13.45% KOH. A similar formulation was used for GOGGE.

2.2.2 Preparation of electrodes

The battery anode paste was prepared by mixing 4% PEO, 94% zinc, 2% Bismuth (III) oxide in DI water; and the cathode paste was prepared by mixing 82% silver oxide, 8% carbon and 10% PEO in DI water. Silver paste on polyethylene terephthalate (PET) substrates was used as the current collector. Battery electrode inks were pasted onto current collectors and dried. The effective working area for each electrode was calculated as 3.98 cm². The typical mass of a cathode was 0.05 g, and mass for anode was 0.1 g (in excess).

2.2.3 Materials and Treatment

PVA (molecular weight: 75,000; Aldrich), KOH (Aldrich), polyethylene oxide (PEO; Aldrich; molecular weight: 400,000), zinc powder (>98.5; Fluka), silver (I) oxide (Aldrich), bismuth (III) oxide (Aldrich), and graphene oxide (Graphenea) were used as received without further treatment. Raw multiwall carbon nanotubes (rCNTs, purity 95%, diameter 20-30 nm, length 10-30 µm) were purchased from Cheap Tubes. fCNTs were obtained by microwave irradiation method from raw CNTs [66, 126]. Raw CNTs were treated in CEM Mars microwave reactor with a mixture of concentrated acid (H₂SO₄ and HNO₃) at 140 °C for 5, 10, 30, 60, and 120 min.
respectively. Resulted products were filtered through a 0.3 μm membrane filter, then washed with Milli-Q water to a neutral pH and finally dried under vacuum at 65 °C to a constant weight.

2.2.4 Characterizations

The samples were characterized using a scanning electron microscope (SEM, JSM-7900F, JEOL). The ionic conductivity (σ) of samples were measured using an electrochemical impedance spectroscopy (EIS, Gamry Instruments, Reference 600+). The electrochemical testing was performed through cyclic voltammetry (CV) on a Homiangz 320C electrochemical analyzer versus a standard Ag-AgCl electrode. Galvanostatic discharge measurements were carried out using an MTI Battery Analyzer (Richmond, CA). Thermo-gravimetric analysis (TGA) was carried out by a thermal analyzer (PerkinElmer TGA 8000) and the melting temperature was investigated using differential scanning calorimetry (PerkinElmer, DSC 6000). X-ray diffraction (XRD, Philips EMPYREAN X-Ray Diffractometer) measurement was performed to examine their crystallinity characteristics. The polymerization was obtained by Fourier transform infrared (FTIR, Agilent Technologies Cary 600 Series). Rheological behaviors and mechanical properties of samples were evaluated with a rotational viscometer (Malvern, Kinexus).
2.3 Results and Discussion

2.3.1 Structural Characterization of GE, fCNTGE, and GOGE

The functionalization via microwave treatment of CNTs in acids introduced oxygen-containing groups, especially hydrophilic carboxylic groups (–COOH) [62, 127] leading to high aqueous dispensability of the products. The water content of the gel electrolyte is an important parameter to maintain the hydration of ions for better ionic transport. Various functionalization times were used to determine the optimum ionic conductivity of the polymer gel. The elemental analysis was carried out by EDX and shown in Table 2.1. As the treatment time was increased, there was a noticeable increase in oxygen to carbon ratio, although the increase was less significant after 30 min. Impedance spectroscopy measurements were used to evaluate the effect of the altered degree of functionalization on ionic conductivity (σ) of the gel electrolytes (Table 2.1.).

Table 2.1 Ionic Conductivity of Gel Electrolytes with Different Degree of Carboxylation

<table>
<thead>
<tr>
<th>Gel Electrolyte Samples</th>
<th>CNT treatment time (min)</th>
<th>Carbon content in fCNTs % by weigh</th>
<th>Oxygen content in fCNTs % by weigh</th>
<th>Carbon to Oxygen Ratio</th>
<th>σ (10⁻² S cm⁻¹)</th>
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<tbody>
<tr>
<td>fCNTGE-5</td>
<td>5</td>
<td>92.2</td>
<td>7.3</td>
<td>16.9</td>
<td>5.3</td>
</tr>
<tr>
<td>fCNTGE-10</td>
<td>10</td>
<td>89.4</td>
<td>9.6</td>
<td>12.5</td>
<td>5.5</td>
</tr>
<tr>
<td>fCNTGE-30</td>
<td>30</td>
<td>87.9</td>
<td>12.1</td>
<td>9.8</td>
<td>6.2</td>
</tr>
<tr>
<td>fCNTGE-60</td>
<td>60</td>
<td>86.8</td>
<td>12.8</td>
<td>9.1</td>
<td>6.9</td>
</tr>
<tr>
<td>fCNTGE-120</td>
<td>120</td>
<td>85.8</td>
<td>13.3</td>
<td>8.6</td>
<td>6.8</td>
</tr>
</tbody>
</table>
Figure 2.1 The picture of a) GE, b) fCNTGE, c) GOGE; SEM images of d) GE, e) fCNTGE, f) GOGE; g) cathode material; h) anode material.

The pictures of GE, fCNTGE, and GOGE are shown in Figure 2.1a-c. No free flow of liquid was observed after the gelling process. SEM images are presented in Figure 2.1.d-h. The surface morphology of GE in Figure 2.1d showed rough structure with a 3-D network which allowed KOH to be entrapped in the PVA matrix. fCNTs were observed to be embedded in the electrolyte in Figure 2.1e. While tube damage increased with treatment time, the circle in inset of Figure 2.1e corresponding to tubular structure of fCNT remained. Figure 2.1f shows the porous morphology of the GO-doped gel electrolyte. The electrodes and gels were dried during SEM sample
preparation. The pores and holes observed in dried gels were formed during the removal of water. In the original gels, these pores and holes held water contents and allowed ion movement.

![Figure 2.2](image)

**Figure 2.2** Ionic Conductivity of fCNTGE samples with fCNTs containing different oxygen contents.

As shown in Figure 2.2, the ionic conductivity was increased by increasing the oxygen content of fCNTs in gel electrolytes gradually. Overall, an optimized high ionic conductivity of about $6.9 \times 10^{-2}$ S cm$^{-1}$ was achieved when 60-minute treated fCNTs were used to prepare fCNTGE (Table 1). Therefore, 12.8% oxygen was chosen as an optimal oxygen content level for fCNT-PVA-KOH gel electrolyte (fCNTGE) and was used for further evaluations.

The increase in ionic conductivity was attributed to the fCNTs serving as dielectric materials or a redox shuttle. It was observed that higher treatment time generated smaller particle sizes and less agglomeration in water [126, 128]. This led to the –COOH groups to enhance dissociation of KOH and facilitated ion transport in the fCNT-doped gel electrolyte. When the oxygen level was low, fCNTs could not
accomplish well as redox shuttle, and the conductivity of the gel electrolyte was reduced. The fCNT bundles covered with hydroxyl groups (OH⁻) of PVA could absorb both KOH and H₂O molecules. Accordingly, the OH⁻ ions can be transferred readily in the fCNTGE, which might contribute to the increase in ionic conductivity [129]. Moreover, hydrophilic properties of fCNTs [125] helped to conduct OH⁻ through its microchannel, which could also contribute to increased ionic conductivity. The proposed schematic gel mechanism representation was shown in Scheme 2.1. Suitable amounts of fCNTs were uniformly dispersed in the PVA matrix and the PVA grafted fCNTs chains were oriented, resulting in strengthening their interfacial bonding. Segmental motions of the PVA grafted fCNTs might cause the increase of conductivity [130]. When the fCNTs were added into the gel, due to the abundant oxygen containing functional groups, the fCNTs interacted with the copolymer to form amorphous phase and decreased the degree of crystalline in fCNTGE.

Scheme 2.1 Proposed gelation mechanism of fCNT-PVA-KOH mixtures
Table 2.2 Calculated Thermal and Mechanical Properties, Ionic Conductivity, Transference Number, Specific capacity, and Energy

<table>
<thead>
<tr>
<th></th>
<th>GE</th>
<th>fCNTGE</th>
<th>GOGGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_d$ (°C)</td>
<td>150</td>
<td>202</td>
<td>189</td>
</tr>
<tr>
<td>$\Delta H_m$ (J/g)</td>
<td>271</td>
<td>167</td>
<td>270</td>
</tr>
<tr>
<td>Young’s Module (kPa)</td>
<td>0.9</td>
<td>2.3</td>
<td>0.2</td>
</tr>
<tr>
<td>Tensile Strength (kPa)</td>
<td>9.3</td>
<td>22.3</td>
<td>5.8</td>
</tr>
<tr>
<td>$\sigma$ ($10^{-2}$ S cm$^{-1}$)</td>
<td>5.1</td>
<td>6.9</td>
<td>6.2</td>
</tr>
<tr>
<td>Ionic Transference Number</td>
<td>0.55</td>
<td>0.90</td>
<td>0.87</td>
</tr>
<tr>
<td>Electronic Transference Number</td>
<td>0.45</td>
<td>0.10</td>
<td>0.13</td>
</tr>
<tr>
<td>Electrochemical Stability window (V)</td>
<td>3.04</td>
<td>3.6</td>
<td>3.02</td>
</tr>
<tr>
<td>Specific Capacity (C/20, mAh g$^{-1}$)</td>
<td>205.4</td>
<td>204.3</td>
<td>108.3</td>
</tr>
<tr>
<td>Specific Energy (mWh g$^{-1}$)</td>
<td>235.2</td>
<td>234.9</td>
<td>212.8</td>
</tr>
</tbody>
</table>

FTIR spectra were used to determine the interactions within PVA, GE, GOGGE and fCNTGE and results were displayed in Figure 2.3. All major peaks related to acetate and hydroxyl groups were observed. PVA exhibited strong stretching broad peaks of $-\text{OH}$ groups at about 3200 cm$^{-1}$ to strong intermolecular and intramolecular hydrogen bonds [131]. Peaks from C-O groups at about 1095 cm$^{-1}$ and C-H wagging and stretching vibrations from alkyl CH$_2$ groups at 2937 cm$^{-1}$ [132, 133] were observed. These peaks were also seen in the FTIR spectrum of GE, fCNTGE, and GOGGE which indicated the existence of bonds and functional groups. While an additional weak the absorption peak at about 1105 cm$^{-1}$ in the fCNTGE spectrum can be attributed to the absorption of carboxyl C=O groups of the surplus MWCNT–COOH traces [129, 134], the band at 1365 cm$^{-1}$ was associated with secondary bending vibration of O-H [135]. GO has a broad and strong deformation vibration -OH band at 1365 cm$^{-1}$ due to extensive oxidation [136]. The peak at about 1729 cm$^{-1}$ belongs to stretching of C–O and C=O from acetate group remains [137].
Figure 2.3 FTIR Spectra of pure PVA, fCNTGE, GE and GOGE.

The peaks show the interactions between hydroxyl groups of the PVA macromolecule and carboxyl groups of CNTs. The complex structure between the PVA polymer, KOH and doped fCNTs could be verified with the peaks shifting and peaks intensity changes in the FTIR spectra such as stretching and bending vibration of O-H group. The intensity increases of stretching O-H and broadening bending vibration of O-H may confirm that the PVA monomers were polymerized and grafted successfully onto the GO and CNT fibers in the gel electrolyte.
The X-ray diffraction (XRD) characterization studies have been carried out to determine the crystallinity and phase structure of the PVA only, GE, GOGE and fCNTGE polymer electrolytes. As shown in Figure 2.4., PVA shows a broad amorphous halo centered peak at the diffraction angles (2θ) value of 11.2° as well as a prominent peak at 2θ° = 19.4° and 2θ = 40.7° for all samples, indicating the coexistence of mixed amorphous and crystalline regions. The amorphous peaks correspond to (100) and crystalline peaks (-101), (-111) orientation planes, respectively [138]. Also, the peak of 2θ = 40.7° is invisible for GE, GOGE, and fCNTGE showing no other crystalline complex formed.
To improve the ionic conductivity and ion transport more easily, amorphous characterization of gel electrolytes should be improved [101]. All crystalline peaks and amorphous peaks were expanded, and their intensities decreased sharply after the PVA was treated with KOH solution, GO and fCNT. The GE, GOGGE and fCNGTE samples displayed similar crystalline diffraction patterns but the intensity of fCNGTE peak was a little lower than GE and GOGGE implying that amorphous nature of fCNGTE increased compared with GE, GOGGE, and PVA only.

![Figure 2.5](image.png)

**Figure 2.5** TGA curves of pure PVA, GE, GOGGE and fCNGTE.

The thermal behavior and stability of samples were investigated using thermogravimetric analysis (TGA) in Figure 2.5 and differential scanning calorimetry (DSC) in Figure 2.6. The initial weight loss (≈5 wt.%) has occurred about 40 °C for GE, GOGGE, and fCNGTE, which may be due to the removal of electrolyte moisture. This result was compatible with others that stated water removal starts at lower temperature for PVA gel systems [139, 140]. The decomposition temperature of pure
PVA is \( \sim 350 \, ^{\circ}\text{C} \). A weight loss for the GE which contains only KOH is observed at \( \sim 150 \, ^{\circ}\text{C} \) which is smaller than PVA only since complex form of \(-\text{OH}\) groups in PVA backbone with salt cation causes a decrease in decomposition temperature [101, 141]. When fCNTs were added to the PVA-KOH gel electrolyte, the decomposition temperature and thermal stability of nanocomposite electrolytes increased from 150 °C to 206 °C and from 150 °C to 189 °C with adding GO (Table 2), which was high enough for potential applications such as electrolyte in energy storage devices.

The thermal stability and melting temperature \( (T_m) \) are important parameters to assess in-situ performance of the samples in the battery especially while the operating temperature is increased.

![Figure 2.6](image.png)

**Figure 2.6** Differential Scanning Calorimetry (DSC) thermogram of GE, GOGE and fCNTGE.
GE exhibits a strong endothermic peak at around 126.4 °C. When fCNT were added, the melting temperature of GE shifted to slightly lower temperature from 126.4 °C to 124.9 °C. Also, the melting enthalpy value is reduced with introduction of fCNTs into GE, suggesting the addition of fCNT promote amorphicity in gel electrolyte.

2.3.2 Mechanical Properties of GE, fCNTGE, and GOGGE

GE, GOGE, and fCNTGE were used as electrolyte and separator between electrodes in the battery fabrication process. Mechanical properties of polymer electrolytes based on rheological techniques play important roles to understand the relationship between internal structural changes and constitutional variations by an input stress.

![Stress-Strain curves of GE, GOGE, and fCNTGE samples.](image)

**Figure 2.7** Stress-Strain curves of GE, GOGE, and fCNTGE samples.
Typical stress-strain curves of GE, GOGE and fCNTGE samples are shown in Figure 2.7. For mechanical tests, the samples were cast on a rectangular mold having dimensions for $5 \times 5 \times 2.5$ mm$^3$ and then measured 4 times, with the average values calculated and reported here. fCNTGE exhibited higher mechanical properties such as Young’s modulus calculated from the slopes of curves in the early stage of linear portion and ultimate tensile strength compared to GE and GOGE. The Young’s modulus and tensile strength was 2.3 and 22.3 kPa for fCNTGE, 0.9 and 9.3 kPa for GE, and 0.22 kPa and 5.8 kPa for GOGE, respectively are shown in Table 2.2. The fCNTs had strong interaction with the PVA matrix and showed dramatic improvements over the pure PVA gel as well as GOGE.

The viscoelastic mechanical properties of fCNTGE were further tested as a function of shear strain at constant frequency (1 Hz) and shown Figure 2.8. GOGE was not tested further because it showed lower mechanical strength. It was observed that the dynamic mechanical properties of storage modulus ($G'$) and loss modulus ($G''$) decreased with increase in shear strain indicating typical gel-like behavior [142]. $G'$ dominated over the $G''$, explained that the elastic properties dominated over the viscous properties till the crossover point. The $G''$ dominated the $G'$ at high shear strain value by the fact that 3-D network of gel might be broken and consequently the viscous modulus was greater than the elastic modulus. In the GE, crossovers occurred at strain amplitudes of 0.5 % while the crossover of fCNTGE appeared at 1.5 %, which was about three times greater than GE.
2.3.3 Electrical Properties of the GE, fCNTGE, and GOGE

Electrochemical impedance spectroscopy (EIS) tests using two-electrode configuration was carried out at open circuit potential with AC potential amplitude of 5 mV, and the frequency ranged from 100 Hz to 1 MHz to evaluate the efficient ion migration channel of GE, GOGE as well as fCNTGE. It was observed that the ionic conductivity of the PVA-KOH system was $5.1 \times 10^{-2} \text{ S cm}^{-1}$ (no fCNT content), lower than that of PVA-KOH-fCNTs (fCNTGE) system. When 17.5 mg of GO or fCNTs were introduced, the ionic conductivity values of the gel electrolytes increased to $6.2 \times 10^{-2} \text{ S cm}^{-1}$ for GOGE and $6.9 \times 10^{-2} \text{ S cm}^{-1}$ for fCNTGE, according to the Equation. (2.1). The ionic conductivity of the gel electrolytes ($\sigma$, S cm$^{-1}$) was evaluated by the Nyquist plot representing the imaginary and the real part of the

**Figure 2.8** The Dynamic shear modulus of (a) GE and (b) fCNTGE with strain.
impedance and calculated by the equation;

\[ \sigma = \frac{L}{R_b \cdot A} \]

where \( L \) (cm) is the distance between the two-platinum inner electrode, \( R_b \) (ohms) is the bulk resistance calculated from the point of intersecting with the x-axis, \( A \) (cm\(^2\)) is the contact area of the electrolyte with platinum during the experiment.

From Figure 2.9, it can be seen that GE, GOG, and fCNTGE exhibit a small inclined line at the middle frequency, which is related to Warburg or diffusive resistance of ions in the bulk electrode. Conductivity is significantly improved by introducing fCNTs into PVA gel, revealing that the diffusion and transport of ions into electrolyte were much better than GE and GOG. It was explicit that \( R_b \) calculated from the point of intersecting with x-axis in the range of high frequency decreased with embedding fCNTs into the gel. The increase of conductivity can be explained as addition of the fCNTs promoting segmental motion of PVA grafted fCNTs, which ease ions to migrate in material.
Figure 2.9 The Nyquist plots for the GE, GGE and fCNTGE.

The cyclic voltammetry (CV) behavior was compared for GE, GGE and fCNTGE at scan rate 50 mV s$^{-1}$ in Figure 2.10a. Silver oxide electrode was used as a working electrode, platinum as a counter electrode, and Ag/AgCl as a reference electrode. The voltammogram showed well-defined anodic peaks at 0.33 V for GE and at 0.37 V for fCNTGE from the oxidation of silver (I) at 50 mV s$^{-1}$. The cathodic peaks at 0.19 V for GE, 0.23 V for fCNTGE, and 0.25 V for GGE were attributed to the reduction of silver (I).

Figure 2.10 CV curves of a) GE and fCNTGE, at 0.05 mV s$^{-1}$ scan rate; b) GE, c) fCNTGE, d) GGE with different scan rates.
The addition of fCNTs led to increase in the size of oxidation and reduction peaks, suggesting a better utilization of electrodes. Figure 2.10. b-d. Shows the CV curves for GE, GOGE and fCNTGE at different scan rates from 10 to 100 mV s⁻¹. The electrode current density increased with scan rate and the shape of CV did not change considerably and exhibited acceptable electrochemical reversibility [95].

2.3.4 Transference Number and Electrochemical Stability Window Measurements

Transference number is an important parameter described as the ratio of the ionic conduction to the total charge transport. Here, the transference number of gel electrolytes was measured by chronoamperometry and calculated the residual electronic current passing through the electrolyte using Wagner’s polarization technique [143, 144]. The stainless steel/gel electrolyte/stainless steel cells were polarized fully with a fixed DC potential of 1.5 V and the current flow passing through the cells was monitored as a function of time. The polarization current versus time plotted for GE, fCNTGE, and GOGE was shown in Figure 2.11a. The following formulas was adopted to calculate transference number (t):

\[
t_{\text{ion}} = \frac{I_T - I_e}{I_T}
\]  

(2.2)
where $t_{\text{ion}}$ is ionic transference, $t_e$ is electronic transference number. Initial total current $I_T$ can be defined as the sum of ionic ($I_i$) and electronic ($I_e$) currents. Electronic current $I_e$ after polarization were measured as a final current. $I_T - I_e$

**Figure 2.11** a) DC polarization curve; b) Linear sweep voltammograms at scan rate 0.05 mV/s for GE, fCNTGE, and GOGE.
The ionic transference number of GE, GOGE and fCNTGE was calculated as 0.55, 0.87 and 0.90, respectively. Both ionic and electronic transference numbers are shown in Table 2.2. The decrease in current with time in Figure 2.11a suggested that the total conductivity and charge transport in the electrolyte systems were predominantly due to ions, accompanied by mass transport [145] and electronic contribution could be neglected. $T_{\text{ion}}$ gradually increased (up to 0.90) upon addition of fCNT nanoparticles. Consequently, this proved that KOH salt has provided OH$^-$ ions as mobile species more in fCNTGE than GOGE and GE.

One of the main drawbacks for aqueous electrolytes is the narrow electrochemical windows due to the electrolysis of water [146]. In order to determine the electrochemical stability window, linear sweep voltammetry (LSV) technique was conducted by a sweep voltammetry on the stainless steel/gel electrolyte/stainless steel cell configurations. A standard Ag-AgCl was used as the reference electrode. LSV was performed between 0 V and 3 V at a scan rate of 0.05 mV s$^{-1}$ presented in Figure 2.11b.

As can be seen, the current flow was stable within the voltage range of approximately -1.72 to +1.9 for fCNTGE and -1.14 to +1.9 for GOGE and GE and they begin to rise with continuous increase in voltage. Redox peaks for fCNTGE appeared at 1.3 V and it was relatively wide and weak. The onset of current flow which refers to anodic decomposition voltage [145, 147] starts at about 1.9 V which refers to OH$^-$ anions. The cathodic voltage was observed for fCNTGE at -1.72 V, for GE at -1.14 V, and for GOGE at -0.9 V.
Thus, there is an improvement in the voltage stability window in fCNT-containing gel electrolyte which is ~3.6 V. The electrochemical stability window for GE was found ~3.04 V, and ~3.02V for GOGGE, shown in Table 2.2.

2.3.5 Galvanostatic Discharge (GCD) Analysis of GE, fCNTGE, and GOGGE

Crescent shape prototype batteries were fabricated using 3-dimentiononal printed (3D) acrylonitrile butadiene styrene (ABS) casings. In a typical cell, the silver oxide cathode, which was the limiting reagent, was firstly inserted in the casing. Then, the gellable electrolyte was poured onto the electrodes to fulfill the gelation reaction. In this way, the electrolyte could penetrate the vacancies of the electrode materials and exclude bubbles on the surfaces. Thus, the electrode-electrolyte interface can significantly improve. After that, zinc anode was added, and the components were capped to make it a cell (Figure 2.12d.).

The SEM images and the picture of electrodes are shown in Figures 2.1j-k. and 2.12c., respectively. The performance of zinc-silver oxide batteries with GE, GOGGE and fCNTGE in a 3D printed system discharged at C/20 and C/10 was shown in Figure 2.12a-b. The specific capacity (C/20, calculated based on Ag₂O) and specific energy was displayed in Table 2.2. For the fCNTGE the curves showed more stable voltages than GOGGE and GE. The voltage plateau region for fCNTGE was to be higher than GE and GOGGE. Furthermore, the voltage plateau region for GOGGE and GE turned out to be less unstable and fluctuated especially for the case of GOGGE. One possible reason might be that GO got reduced by zinc, causing aggregation of graphene and short circuits.
Figure 2.12 Discharge curves under different rates a) C/20, b) C/10; c) Zinc anode (grey) and silver cathode (black), d) 3D-printed Ag-Zn batteries.

2.4 Conclusion

A novel fCNTs gel electrolyte (fCNTGE) with PVA as the polymer matrix is prepared and tested inside Zn-Ag2O batteries. The formulation was optimized with fCNTs having different degrees of functionalization. The results show improved ionic conductivity of PVA-KOH gel by doping fCNTs into the gel because of ionic channels provided by the fCNTs. The ionic conductivity of the GE (no fCNT content) system is 5.1×10⁻² S cm⁻¹. After the addition of GO (17.5 mg) or fCNTs, the ionic conductivity increases to 6.2×10⁻² S cm⁻¹ (GOGE) and 6.9×10⁻² S cm⁻¹ (fCNTGE). A significant enhancement in the mechanical properties is also observed as the tensile strength increased to 22.3 kPa for fCNTGE which is 2.5-fold enhancement as compared to the GE and 3.5-fold enhancement compared to the GOGE. The
electrochemical performance of the electrolytes is evaluated by the batteries using Zn-Ag2O electrode material. Experimental results from the battery containing fCNTGE show more stable voltages, desired plateau region and promising application ability in the Zn-Ag2O batteries.
CHAPTER 3
COMPUTATIONAL INVESTIGATION OF ENHANCED PROPERTIES IN FUNCTIONALIZED CARBON NANOTUBE DOPED POLYVINYL ALCOHOL GEL ELECTROLYTE SYSTEMS

3.1 Introduction

Although electrolytes with good interfacial stability are a crucial component of any electrochemical device, electrode materials accompanied by electrolyte decomposition or electrolytes’ loss due to leakage can cause detrimental reactions in batteries. Liquid electrolytes have been used traditionally for a long time owing to their excellent electrochemical properties, but there are some disadvantages such as material defects [82], low operating temperature range [148] and the necessary encapsulation of a liquid [149] which are risky elements for cell operation. To this end, gel electrolytes (GE) utilizing a liquid phase in a solid polymer matrix are becoming widely studied for such systems because they have higher ionic conductivity than completely solid-state electrolytes while being safer and more compact than liquid ones and can be prepared in any configuration in soft casings [150].

Although GEs offer many improvements over solid polymer electrolytes, there are still enhancements to be made, such as increasing their ionic conductivity, mechanical properties, and thermal stability [151]. Using additives in GE systems is a wise strategy to improve their performance in electrochemical devices [152]. However, the nature of the interactions between the different electrolyte components and how they influence various properties such as ionic transport remains an area of active study [153].
In Chapter 2, the development of a hybrid GE consisting of functionalized carbon nanotube-doped poly (vinyl alcohol) (PVA) polymer and using 3D printed Zn-Ag$_2$O batteries was shown [154]. The potassium hydroxide (KOH) liquid electrolyte was trapped in the GE and COOH functionalized carbon nanotubes (fCNTs) were used as an additive to improve the hydrophilicity, ionic transport, and mechanical strength of the electrolyte. The influence of the fCNT additives in the GE was determined by electrochemical and mechanical characterization. However, questions remain about the atomistic origins of the enhancement of the properties in this system.

In this work, these questions through computational modeling of the interactions between fCNTs, PVA, and the working ion were answered. The nature of the interaction between PVA dendrimers, fCNTs, and Zn ions was investigated on the atomic level by using density functional theory (DFT) calculations.

First, by determining the adsorption energies, DFT calculations theoretically confirmed that PVA chains interact more strongly with fCNTs than non-functionalized CNTs, likely partly contributing to the observed higher mechanical properties. It was demonstrated that this is due to enhanced charge transfer between the CNT and PVA as the number of functional groups increases. Next, it looked at trends in the HOMO-LUMO gap and how they are affected by the functionalization of the CNT. Finally, the interaction of Zn ions with the fCNT-GE complex was studied and found that the enhanced ionic conductivity is partly because the Zn ion does not adsorb strongly. These calculations allowed us to better understand the influence of CNT functionalization on the properties of GEs.
3.2 Computational Methods

Modern computational approaches can provide accurate energies of molecules and can be used to design and optimize new materials for energy storage devices [83]. Here, density functional theory (DFT) was utilized, in which the system of interacting electrons is mapped to non-interacting ones moving in an effective potential [155]. DFT provides valuable information on molecular geometries and properties and can be used to determine the electronic properties of compounds fast and accurately [84].

The adsorption processes of the Zn atom on pristine and fCNT loaded PVAs are investigated in this way. The DFT calculations were performed in the ORCA computational package [156]. The B3LYP functional was applied in this work to carry out all the computations. A def2-SVP functional was used for the CNT, while the def2-TZVP basis set was used on the COOH functional groups, PVA molecules, and Zn atoms [157]. This approach has been shown to be appropriate for studying the adsorption of compounds with H-terminated CNTs [158]. A D3BJ dispersion correction was used [159], along with a RIJCOSX approximation for Coulomb integrals [160]. A sample of the input file and output file of all samples was added to Appendix A and B.

A single-wall armchair (5,5) carbon nanotube terminated by hydrogen atoms was considered and the (5,5) SWCNT containing 70 carbon atoms and 20 hydrogen atoms was selected for this purpose. The diameter of the nanotube is 6.99 Å, the length of the nanotube is 7.34 Å, and the average C-C bond length is 1.42 Å. The most favorable adsorption position for PVA was determined by calculating the energy of a variety of configurations relative to the CNT and functional group and finding the lowest energy one. The adsorption binding energy was computed to measure the
adsorption energies (\(E_{\text{ads}}\)) of fCNT-PVA-Zn structures. In every case the ionic positions were fully relaxed with an energy convergence criterion of \(5 \times 10^{-5}\) Ha (NormalOpt in ORCA). To evaluate the interaction between the PVA molecule with the pristine CNT and fCNT, their adsorption energies (\(E_{\text{ads}}\)) were calculated using Equation 3.1 and Equation 3.2, respectively. It was defined as the energy difference between the adsorbed CNT-PVA or fCNT-PVA system and the isolated CNT species and PVA, and can be expressed as:

\[
E_{\text{ads}} = E_{\text{CNTPVA}} - (E_{\text{PVA}} + E_{\text{CNT}}) \tag{3.1}
\]

\[
E_{\text{ads}} = E_{\text{fCNTPVA}} - (E_{\text{PVA}} + E_{\text{fCNT}}) \tag{3.2}
\]

where \(E_{\text{CNTPVA}}\) is the total energy of the PVA molecule adsorbed on the pristine CNT, \(E_{\text{fCNTPVA}}\) is the total energy of the PVA molecule adsorbed on the functionalized CNT, \(E_{\text{fCNT}}\) is the total energy of the functionalized CNT, and \(E_{\text{PVA}}\) is the total energy of the PVA molecule. To estimate the interaction between the Zn molecule and fCNT-PVA, their adsorption energy (\(E_{\text{ads}}\)), is calculated as Equation 3.3.

\[
E_{\text{ads}} = E_{\text{fCNTPVAZn}} - (E_{\text{fCNTPVA}} + E_{\text{Zn}}) \tag{3.3}
\]

where \(E_{\text{fCNTPVAZn}}\) is the total energy of the Zn molecule adsorbed on the functionalized CNT and \(E_{\text{Zn}}\) is the total energy of the Zn molecule. A negative value of \(E_{\text{ads}}\) indicates a spontaneous process leading to a stable structure. With this definition, a negative binding energy shows that the binding interaction is favored, with a more negative
indicating a more favorable interaction.

The charge density and orbital interactions were evaluated using natural bond orbital (NBO) analysis and the JANPA code [161]. NBO was used to calculate the charge difference before and after adsorption of the Zn and PVA molecule on CNTs and fCNTs on the optimized structures. NBO analyses were also performed at the previously described level of theory for all atoms. Charge transfer is a key factor in the adsorption process to find if the adsorbate and functional groups act as electron donors or acceptors and how strongly the components interact. The charge transfer (ΔQₑ) is defined with Equation 3.4 and 3.5.

\[
\Delta Q_e (PVA) = Q(PVA)_{\text{after ads.}} - Q(PVA)_{\text{before ads.}} \quad (3.4)
\]

\[
\Delta Q_e (Zn) = Q(Zn)_{\text{after ads.}} - Q(Zn)_{\text{before ads.}} \quad (3.5)
\]

where \(Q_{\text{after ads.}}\) is the total charge adsorbing on the CNT and fCNT surface and \(Q_{\text{before ads.}}\) is the total charge in the free case.
3.3. Results and Discussion

3.3.1 PVA Interaction with Pristine and Functionalized CNTs

CNTs have a structure formed with a hexagonal network of covalent sp$^2$ C-C bonds and a very high length-to-diameter ratio. For the solubilization of carbon nanotubes, the attachment of relatively large functional groups to the nanotubes is required. The functionalization breaks the nanotube bundles, which is essential to the solubility [162]. Since pristine CNTs are insoluble, functionalization enhances their solubility or dispersion [163, 164].

In a previous chapter, fCNTs were produced by microwave treatment of carbon nanotubes to alter the degree of the carboxylic terminal group (-COOH) [165]. The functionalization of CNTs introduced oxygen-containing groups, especially hydrophilic -COOH, leading to high aqueous dispensability of the products [154]. It has also been previously reported that modification of CNTs leads to improved interactions with small molecules with considerable binding energy [166]. Moreover, the strength of the carbon-carbon bonds gives carbon nanotubes excellent mechanical properties [167]. As such, it was first studied the CNT structure with increasing numbers of functional groups. The optimized geometries of the computational models of the pristine CNT and functionalized CNT with 1, 2, and 3 COOH functional groups (denoted fCNT, ffCNT, and fffCNT, respectively) are displayed in Figure 3.1.
In a GE, a polymer network is created in which a solvent and a salt are incorporated in a polymer matrix and rely on the well-documented ability of the repeating vinyl alcohol unit to coordinate alkali cations. Hence, both the polymer network and the solvent often contain PVA oligomer segments. In this study, two and three monomer ethanol (vinyl alcohol) CH$_2$CH(OH) matrixes have been adopted to determine how these PVA species interact with the -COOH functional groups and coordinate the alkali cations. To determine the PVA interactions with pristine CNT, fCNT, ffCNT, and fffCNT, it was first adsorbed a one monomer polyvinyl alcohol (denoted (PVA)$_1$) molecule on the surface of each structure (Figure 3a-d). It was also tested the effect of polymer length by adsorbing two and three monomer long molecules (denoted (PVA)$_2$ and (PVA)$_3$, respectively) on these different CNT structures. Figure 3.2e-h and Figure 3.2i-k show the optimized geometry of the CNTs with two and three PVA monomer chains, respectively. In each case it was computed the adsorption energy of PVA with the CNT substrate as described previously, the results of which are summarized in Table 3.1.
Figure 3.2 Optimized geometry of one monomer (PVA)$_1$ interaction with (a) CNT, (b) fCNT, (c) ffCNT, and (d) fffCNT; two monomer (PVA)$_2$ interaction with (e) CNT, (f) fCNT, (g) ffCNT, and (h) fffCNT; three monomer (PVA)$_3$ interaction with (i) CNT, (j) fCNT, and (k) ffCNT.
Table 3.1 Adsorption energy ($\Delta E_{\text{ads}}$, units of eV) of PVA and charge transfer ($\Delta Q_e$, units of electrons, $e$) to PVA in each CNT-PVA complex.

<table>
<thead>
<tr>
<th>Structure</th>
<th>$\Delta E_{\text{ads}}$ PVA (eV)</th>
<th>$\Delta Q_e$ PVA ($e$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNT-(PVA)$_1$</td>
<td>-0.51</td>
<td>0.006</td>
</tr>
<tr>
<td>fCNT-(PVA)$_1$</td>
<td>-0.67</td>
<td>-0.004</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_1$</td>
<td>-0.84</td>
<td>-0.001</td>
</tr>
<tr>
<td>fffCNT-(PVA)$_1$</td>
<td>-1.52</td>
<td>0.011</td>
</tr>
<tr>
<td>CNT-(PVA)$_2$</td>
<td>-0.72</td>
<td>0.019</td>
</tr>
<tr>
<td>fCNT-(PVA)$_2$</td>
<td>-0.97</td>
<td>0.046</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_2$</td>
<td>-1.15</td>
<td>0.027</td>
</tr>
<tr>
<td>fffCNT-(PVA)$_2$</td>
<td>-2.23</td>
<td>0.069</td>
</tr>
<tr>
<td>CNT-(PVA)$_3$</td>
<td>-0.66</td>
<td>0.021</td>
</tr>
<tr>
<td>fCNT-(PVA)$_3$</td>
<td>-0.52</td>
<td>0.007</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_3$</td>
<td>-1.40</td>
<td>0.049</td>
</tr>
</tbody>
</table>

On the pristine CNT, the PVA molecule orient horizontally with small adsorption energies ranging from approximately -0.5 to -0.7 eV, indicating some weak interaction between them. In the functionalized CNT cases, the PVA chain prefers to orient horizontally next to the -COOH group in almost every case. As the number of functional groups increase, $\Delta E_{\text{ads}}$ become more negative, indicating a stronger interaction with the PVA molecule regardless of the length of the PVA chain. Furthermore, the interaction between PVA and the functionalized CNTs becomes stronger as the chain length increases from one to two. Two monomer PVA on fffCNT provided the most negative interaction energies (Table 1) among all cases. Although three monomer PVA with three functional groups on CNT could not be employed because of computational infeasibility, the adsorption energy follows a similar trend on CNT, fCNT, and ffCNT. As expected, this indicates that increasing the number of functional groups on the CNT (such as through the aforementioned microwave process [165]) enhances its interaction with the PVA polymer matrix of the GE. These stronger interactions can contribute to the increased mechanical strength and thermal
stability of the fCNT-PVA system.

Then the charge transfer occurring between each CNT-PVA complex (Qₑ, as defined previously) were computed to help explain these observed trends in adsorption energy. Because the -COOH functional groups act as electron withdrawing, the charge on the PVA is generally positive. In the (PVA)₁ case, the charge on the PVA does not change significantly until the case of three functional groups, at which point it jumps from near 0 to 0.01 e. In the (PVA)₂ and (PVA)₃ cases; however, more charge transfer is observed. In general, increasing the number of functional groups caused an increase in the amount of charge transfer from the PVA to the CNT substrate, similarly partially contributing to the observed increasing trends of the adsorption energies. The charge transfer from the PVA goes from 0.02 e to 0.04 e to 0.07 e as the number of functional groups goes from 0 to 1 to 3 in (PVA)₂ case, but the charge transfer is only 0.03 e for two functional groups, slightly bucking the trend. The charge transfer does not track exactly the trends in adsorption energy, but in general more charge transfer occurs for the (PVA)₂ and (PVA)₃ molecules as the number of -COOH functional groups increase. Moreover, the charge transfer in all cases is quite small, indicating that strong bonds are not formed between the PVA molecules and CNT structures.

The visualization of the charge density in these complexes (Figure 3.3) also corroborates these findings. The charge density of (PVA)₁, (PVA)₂ and (PVA)₃ on CNT with increasing number of functional groups are shown in Figure 3.3a-d, 3e-h, and 3.3i-k, respectively. From these figures, it is clear that as the number of functional groups increases, increasing amounts of charge density is present on both the COOH group and the surface of the CNT. Interestingly, in the case of ffCNT and fffCNT, it
appears that most of the charge is concentrated within one of the -COOH functional
groups rather than split evenly between all of them. This implies that the interaction
of the head group of the PVA molecule with one of the functional groups is most
important in determining the adsorption properties.

![Diagram showing electron density of different CNT-(PVA) complexes](image)

Figure 3.3 Electron density of (a) CNT-(PVA)$_1$, (b) fCNT-(PVA)$_1$, (c) ffCNT-
(PVA)$_1$, (d) fffCNT-(PVA)$_1$, (e) CNT-(PVA)$_2$ (f) fCNT-(PVA)$_2$, (g) ffCNT-(PVA)$_2$
(h) fffCNT-(PVA)$_2$, (i) CNT-(PVA)$_3$, (j) fCNT-(PVA)$_3$, and (k) ffCNT-(PVA)$_3$.

Finally, the highest occupied molecular orbitals and lowest unoccupied
molecular orbitals ($E_{HOMO}$ and $E_{LUMO}$) in these complexes (Table 3.2) and the energy
gap between them ($E_g$) were reported. Although DFT is well-known to underestimate
the energy gaps, the overall observed trends in the gaps can still give useful insights.
In agreement with previous computational results involving hydrogen terminated
CNTs, the systems in this study exhibited HOMO-LUMO gaps ranging from approximately 0.4 to 1 eV [158]. First, increasing the number of functional groups was observed to have the largest effect on the HOMO-LUMO gap. Increasing the number of functional groups from 0 to 1 and to 3 steadily increased the HOMO-LUMO gap from approximately 0.8 to 0.9 to 1 eV. However, the drop of gap to 0.4 eV needed to be investigated in the case of two functional groups. Next, increasing the number of monomers in the PVA chain were found little effect on the magnitude of the HOMO-LUMO gap in the case of fCNT, ffCNT, and fffCNT, which increases only 0.02 eV when increasing from (PVA)$_1$ to (PVA)$_3$. This was an expected result since there is no significant bonding between the CNTs and PVA molecules although the adsorption energies between them is non-negligible.

<table>
<thead>
<tr>
<th>Structure</th>
<th>$E_{\text{HOMO}}$ (eV)</th>
<th>$E_{\text{LUMO}}$ (eV)</th>
<th>$E_g$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNT</td>
<td>-4.10</td>
<td>-3.32</td>
<td>0.78</td>
</tr>
<tr>
<td>CNT-(PVA)$_1$</td>
<td>-4.06</td>
<td>-3.27</td>
<td>0.78</td>
</tr>
<tr>
<td>fCNT-(PVA)$_1$</td>
<td>-4.19</td>
<td>-3.32</td>
<td>0.87</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_1$</td>
<td>-3.97</td>
<td>-3.54</td>
<td>0.43</td>
</tr>
<tr>
<td>fffCNT-(PVA)$_1$</td>
<td>-4.45</td>
<td>-3.25</td>
<td>1.19</td>
</tr>
<tr>
<td>CNT-(PVA)$_2$</td>
<td>-4.07</td>
<td>-3.26</td>
<td>0.80</td>
</tr>
<tr>
<td>fCNT-(PVA)$_2$</td>
<td>-4.15</td>
<td>-3.31</td>
<td>0.84</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_2$</td>
<td>-3.95</td>
<td>-3.52</td>
<td>0.43</td>
</tr>
<tr>
<td>fffCNT-(PVA)$_2$</td>
<td>-4.23</td>
<td>-3.17</td>
<td>1.06</td>
</tr>
<tr>
<td>CNT-(PVA)$_3$</td>
<td>-4.18</td>
<td>-3.39</td>
<td>0.79</td>
</tr>
<tr>
<td>fCNT-(PVA)$_3$</td>
<td>-4.16</td>
<td>-3.28</td>
<td>0.87</td>
</tr>
<tr>
<td>fffCNT-(PVA)$_3$</td>
<td>-3.96</td>
<td>-3.55</td>
<td>0.41</td>
</tr>
</tbody>
</table>
3.3.2 Zn Ion Interaction with Pristine and Functionalized CNT-(PVA)$_n$ Complexes

The other aspect of this study is the modelling of the coordination situation around the Zn ion in polymer gel electrolytes where amorphous long-chain PVA plays a central role. It is therefore interesting to investigate how Zn cations are coordinated to the solvent molecules and functionalized CNT and thereby gain insights about the vinyl–ion complex interaction in these systems. The DFT-optimized geometry of (PVA)$_1$, (PVA)$_2$, and (PVA)$_3$ with different functionalized CNTs and a Zn ion is shown in Figure 3.4a-c, 3.4d-f, and 4g-i, respectively. In each case, the lowest energy configuration for the Zn ion (Table 3.1) is to be coordinated to the COOH group with the PVA molecule above it. It was also found that the PVA chains and functionalized CNTs generally interact weakly with the Zn ions (an average of -0.4 eV), allowing for facile transport and likely partly contributes to the observed high ionic conductivity in this gel electrolyte. Indeed, the $\Delta E_{\text{ads}}$ for the Zn ion are significantly lower than that of any PVA molecule (Table 3.1). This small $\Delta E_{\text{ads}}$ are known to be needed to get good ionic conductivity in electrolytes [163].

Although favorable adsorption (*i.e.*, a negative $\Delta E_{\text{ads}}$), is necessary for good ionic conductivity, too strong of interactions between Zn and the system can lead to immobilization of the ions in the electrolyte, preventing their movement. It is therefore important that $E_{\text{ads}}$ of Zn is not so strong that the ions preferentially bind to the system and do not diffuse (in particular, not stronger than that of PVA).

Furthermore, in contrast to the PVA-only case, there is no significant trend in the adsorption energy for the Zn ion. The $\Delta E_{\text{ads}}$ of PVA in these complexes is similar or slightly higher compared to the case without the Zn ions. This indicates that the
introduction of Zn ions to the system does not significantly disrupt the interactions between the PVA and CNT, which is an ideal situation for a gel electrolyte system.

<table>
<thead>
<tr>
<th>Structure</th>
<th>$\Delta E_{\text{ads}}$ (eV)</th>
<th>$\Delta E_{\text{ads}}$ (eV)</th>
<th>$\Delta Q_e$ (eV)</th>
<th>$\Delta Q_e$ (eV)</th>
<th>$E_{\text{HOMO}}$ (eV)</th>
<th>$E_{\text{LUMO}}$ (eV)</th>
<th>$E_g$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNT-(PVA)$_1$-Zn</td>
<td>-0.87</td>
<td>-0.36</td>
<td>-0.002</td>
<td>0.026</td>
<td>-4.19</td>
<td>-3.40</td>
<td>0.78</td>
</tr>
<tr>
<td>fCNT-(PVA)$_1$-Zn</td>
<td>-0.84</td>
<td>-0.17</td>
<td>-0.040</td>
<td>0.086</td>
<td>-4.23</td>
<td>-3.36</td>
<td>0.87</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_1$-Zn</td>
<td>-1.23</td>
<td>-0.39</td>
<td>0.050</td>
<td>0.059</td>
<td>-4.05</td>
<td>-3.58</td>
<td>0.47</td>
</tr>
<tr>
<td>CNT-(PVA)$_2$-Zn</td>
<td>-1.09</td>
<td>-0.57</td>
<td>0.020</td>
<td>0.030</td>
<td>-4.19</td>
<td>-3.42</td>
<td>0.78</td>
</tr>
<tr>
<td>fCNT-(PVA)$_2$-Zn</td>
<td>-1.06</td>
<td>-0.08</td>
<td>-0.010</td>
<td>0.061</td>
<td>-4.24</td>
<td>-3.37</td>
<td>0.86</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_2$-Zn</td>
<td>-1.84</td>
<td>-0.69</td>
<td>0.063</td>
<td>0.077</td>
<td>-3.96</td>
<td>-3.52</td>
<td>0.44</td>
</tr>
<tr>
<td>CNT-(PVA)$_3$-Zn</td>
<td>-1.21</td>
<td>-0.55</td>
<td>0.014</td>
<td>0.035</td>
<td>-4.04</td>
<td>-3.25</td>
<td>0.79</td>
</tr>
<tr>
<td>fCNT-(PVA)$_3$-Zn</td>
<td>-1.47</td>
<td>-0.95</td>
<td>0.003</td>
<td>0.079</td>
<td>-4.18</td>
<td>-3.32</td>
<td>0.86</td>
</tr>
<tr>
<td>ffCNT-(PVA)$_3$-Zn</td>
<td>-1.50</td>
<td>-0.10</td>
<td>0.018</td>
<td>0.069</td>
<td>-3.94</td>
<td>-3.48</td>
<td>0.46</td>
</tr>
</tbody>
</table>

The charge transfer to the PVA molecule ($\Delta Q_e$) and Zn ion on various functionalized CNTs were investigated. As before, the -COOH species act as electron withdrawing groups, imparting a slight positive charge to both adsorbates. In each case, the charge transfer from the Zn ion to the functional group is larger than from the PVA molecules; this is expected since the lowest energy configuration occurs with the Zn ion closest to the -COOH group. Furthermore, the charge transfer on the Zn ion on fCNT and ffCNT is 2 to 4 times larger than on the pristine CNT, as in the case of PVA alone. However, there is no clear trend for the adsorption energy of PVA molecules in combination with Zn, likely due to the fact that now there are interactions to consider with both the Zn ion and the functionalized CNTs. Moreover, the PVA molecules are closer to the Zn ion than to the actual CNT surface. Finally, as with the
pure PVA case, adding Zn ions to the system does not significantly change the HOMO-LUMO gap (Table 3.3). As described before, the Zn ion does not interact strongly with the functionalized CNT-PVA systems, and as such little change in the HOMO-LUMO gap is to be expected.

Figure 3.4 The adsorption configuration of a Zn ion with a (a) CNT-(PVA)$_1$, (b) fCNT-(PVA)$_1$, (c) ffCNT-(PVA)$_1$, (d) CNT-(PVA)$_2$, (e) fCNT-(PVA)$_2$, (f) ffCNT-(PVA)$_2$, (g) CNT-(PVA)$_3$, (h) fCNT-(PVA)$_3$, and (i) ffCNT-(PVA)$_3$ complex.

3.3.3 Discussion

It was now placed our results in the broader context of gel electrolyte systems with additives. Although the atomic level interactions between the electrolyte components contribute to the electrolytes’ characteristics, it was recognized that the extended structure of the CNT-polymer network is also critically important; unfortunately, such studies are well beyond the scope of the type of DFT calculations performed here. For
example, in addition to the additives, the cross-linking of the polymer chains also contributes significantly to the mechanical properties and transport properties [168]. Furthermore, low $E_{\text{ads}}$ for Zn ions is not the only requirement for increased ionic transport, as non-functionalized CNTs have been shown to increase the ionic conductivity in GEs by creating a 3D conducting network in the electrolyte [169]. In this work, functionalizing the CNT with -COOH groups is observed to increase the interactions with PVA while not affecting the interactions with Zn, which can contribute to the observed enhanced properties.

The mechanical properties of composites rely on the dispersion state of fillers, alignment, a high aspect ratio, and interfacial interactions between the CNTs and the polymer matrix. Physical and chemical functionalization of CNTs has been shown to enhance the interfacial adhesion, the modulus, and strength as well as fracture resistance of nanocomposites. DFT remains one of the most efficient methods of quantitatively predicting and rationalizing the mechanical properties for materials. Our experimental results in a previous study showed that a significant enhancement in the mechanical properties in terms of the Young's module ($E = 2.3$) and tensile strength (22.3 kPa) of fCNTGE which was 2.5-fold higher than a typical GE. Although these mechanical properties cannot be calculated directly using this implementation of DFT, it can be described how these enhancements are influenced by the interactions between various components (i.e., through $E_{\text{ads}}$). DFT calculations confirmed that PVA chains interact more strongly with fCNTs than unfunctionalized CNTs and the interaction between PVA and the functionalized CNTs becomes stronger as the chain length increases from one to two to three. The increase in charge transfer with the number of functional groups are attributed to increase adsorption
energies and consequently better mechanical properties.

Furthermore, low $E_{\text{ads}}$ for Zn ions is not the only requirement for increased ionic transport, as non-functionalized CNTs have been shown to increase the ionic conductivity in GEs by creating a 3D conducting network in the electrolyte [Fan, 2020 #112]. In this work, functionalizing the CNT with -COOH groups was observed to increase the interactions with PVA while not affecting the interactions with Zn, which can contribute to the observed enhanced properties.

3.4 Conclusion

In summary, the nature of interaction between PVA dendrimers, functionalized carbon nanotubes, and Zn ions is investigated at the atomic level using DFT. The most favorable adsorption positions for PVA are determined by calculating the energy of a variety of configurations relative to the CNT and functional group and finding the lowest energy one; similar calculations were then performed for Zn-PVA complexes. DFT calculations theoretically confirms that various monomers of PVA interact with non-functionalized CNT but more strongly as the number of functional groups increased (i.e., enhancing $\Delta E_{\text{ads}}$). Then, it is investigated the effect of polymer length by adsorbing two and three monomers long PVA on the different CNT structures. The interaction between PVA and the functionalized CNTs becomes stronger as the chain length increases from one to two to three. The increase in charge transfer with the number of functional groups likely results in these increased adsorption energies and better mechanical properties. Finally, it is demonstrated that a Zn ion weakly adsorbs to the CNT-PVA complex, which is good for ionic conductivity. Furthermore, Zn does not disrupt the interactions between the PVA and functionalized CNTs. These
insights into this gel electrolyte system can explain the atomic level reasons for the observed experimental properties.
CHAPTER 4

COMPUTATIONAL STUDY OF ADSORPTION OF WATER POLLUTANTS ON A FUNCTIONALIZED CARBON NANOTUBE-BASED MEMBRANE

4.1 Introduction

Water and air are the most important factors for life and every organism on Earth depends on them. Unfortunately, these resources are in danger due to continued industrial growth and the advancement of technology causing discharge of pollutants into the environment [170]. The contamination of water and air by pollutants causes harmful effects in the human body and results in both short- and long-term problems [171]. Some contaminants are from geological materials in nature [172] and some of them are man-made by-products of industry [41]. Although some contaminants can be detected by odor, color, and taste, most require testing if water or air is contaminated or not followed by removal. Recent solutions to remove the contaminants from the environment include various treatment methods such as adsorption [173], ion exchange [174], and membrane technology [175]. Of these, membrane technology has gained interest because it can be processed in mild conditions using low energy with requirement of relatively small size equipment and it can be used with other separation techniques together [176, 177]. However, there are also downsides such as low lifetime, concentration of polarization, and fouling [178, 179].

Among recent materials, CNTs have played an important role as sorbents for selective solute transport in different membrane applications which have promoted higher flux, selectivity, and reduced fouling of the system [44, 45]. It was observed
that immobilization of CNTs on membrane surfaces has a great effect on the interaction between the membrane and solutes [46-48]. CNTs’ surface areas are between 100 and 1000 m²/g [49] which make them excellent candidates as sorbents. However, CNTs display high water permeability and good adsorptive capabilities [50], they also have some disadvantages such as weak van der Waals interaction [51], insolubility for adsorbing of materials in aqueous solutions [52], and agglomeration [53].

Recently, CNTs functionalized by oxygen containing functional groups such as –COOH or –OH groups have become particularly promising materials for such applications as they are easily synthesized using oxidative treatments [54] enhance adsorptive capabilities [41] and improve solubility [55]. For example, such functionalized CNTs have been used in membranes for water desalination [180, 181], and removal of pollutants such as heavy metals [182], organic dyes [183] and endocrine disrupting chemicals [184]. In two recent studies, bare CNT and those functionalized with –COOH groups (denoted from here on as fCNT) immobilized membranes were used for both ammonia and methyl tert-butyl ether (MTBE) separation from water, and the fCNT immobilized membrane showed significantly better performance than bare CNT [45, 185]. The influence of the fCNT additives in the membrane was evaluated by mass transfer coefficients, selectivity, and flux [45]. The fCNT immobilized membrane showed extraordinary transport and adsorption of solutes, higher selectivity, and flux, as well as enhanced separation of organic solvents from water [185].

Density functional theory calculations (DFT) were used to understand how –COOH functionalized CNTs bind to and interact with these pollutants and investigate
if the same trend for different pollutants would be seen, as well. Our studied contaminants include a variety of atmospheric and aqueous pollutants, specifically mercury (Hg), nitric oxide (NO), ozone (O₃), sulfur dioxide (SO₂), peroxyacyl nitrate (PAN), ammonia (NH₃), polytetrafluoroethylene (PTFE), perfluorooctanoic acid (PFOA), and perfluorooctanesulfonic acid (PFOS). The nature of the interaction between the pollutants and bare and fCNTs were studied on the atomic level by using DFT calculations. First, by determining the adsorption energies, calculations confirmed that these pollutants interact more strongly with fCNTs than non-functionalized CNTs, likely partly contributing to the observed improved properties such as mass transfer coefficient, selectivity, and flux. It was demonstrated that this is due to enhanced charge transfer between the CNT and pollutants as the number of functional groups increases. It was also looked at trends in the HOMO-LUMO gap and how they are affected by the functionalization of the CNT. These calculations allowed us to better understand the influence of CNT functionalization on the properties of membranes.

4.2 Methods

The adsorption processes of the water pollutants on CNT and fCNT loaded membranes are investigated using density functional theory (DFT), which provides valuable information on molecular geometries and electronic properties of compounds [84]. The DFT calculations were performed in the ORCA computational package [166]. The B3LYP functional was applied in this work to carry out all the computations. A def2-SVP basis set was used for the C and H atoms in the CNT, while the def2-TZVP basis set was used on pollutants and -COOH functional groups, an appropriate approach for studying the adsorption of compounds with H-terminated
CNTs [158]. A D3BJ dispersion correction was used to include van der Waals interactions [168], along with a RIJCOSX approximation for Coulomb integrals [169].

Presented results are based on a single-wall armchair (5,5) (SWCNT) carbon nanotube terminated by hydrogen atoms. The (5,5) SWCNT contains 70 carbon atoms and 20 hydrogen atoms. The diameter of the nanotube is 6.99 Å, the length of the nanotube is 7.34 Å, and the average C-C bond length is 1.42 Å. One and two carboxyl functional groups were attached to a carbon on the external surface of the CNT based on experimental functionalization; it was denoted these systems as fCNT and ffCNT, respectively.

The most favorable adsorption position was determined by calculating the energy of a variety of configurations of each pollutant relative to the CNT and functional group and finding the lowest energy one. In every case the ionic positions were fully relaxed with a convergence criterion of $5 \times 10^{-5}$ Ha (NormalOpt in ORCA). To evaluate the interaction between samples with the pristine CNT and fCNT, their adsorption energies ($E_{\text{ads}}$) were calculated using Equation (1) and Equation (2), respectively. Adsorption energy ($E_{\text{ads}}$) is the change in energy that occurs when an adsorbate interacts with a surface. A negative value of $E_{\text{ads}}$ indicates a spontaneous process leading to a stable structure. With this definition, a negative binding energy shows that the binding interaction is favored, with a more negative $E_{\text{ads}}$ indicating a more favorable interaction. It is expressed as the energy difference between the adsorbed CNT or fCNT system and can be defined for each system as:
\[ E_{\text{ads}} = E_{\text{system}} - (E_{\text{CNT}} + E_{\text{pollutant}}) \]  
(4.1)

\[ E_{\text{ads}} = E_{\text{system}} - (E_{\text{fCNT}} + E_{\text{pollutant}}) \]  
(4.2)

where \( E_{\text{system}} \) is the total energy of the water pollutant molecules adsorbed on the bare CNT and fCNT, \( E_{\text{CNT}} \) is the total energy of the functionalized or non-functionalized CNT, \( E_{\text{fCNT}} \) is the total energy of the functionalized CNT, and \( E_{\text{pollutant}} \) is the energy of the pollutant molecule.

The solvation energy is calculated based on the following Equation 4.3.

\[ E_{\text{sol}} = E_{\text{system}} - (E_{\text{CNT}} + E_{\text{pollutant}}) \]  
(4.3)

\[ E_{\text{sol}} = E_{\text{system}} - (E_{\text{fCNT}} + E_{\text{pollutant}}) \]  
(4.4)

The charge density and orbital interactions were evaluated using natural bond orbital (NBO) analysis and the JANPA code [83]. NBO was used to calculate the charge difference before and after adsorption of the water pollutant molecules on CNTs and fCNTs on the optimized structures. NBO analyses were also performed at the previously described level of theory for all atoms. Charge transfer is a key factor in the adsorption process to find if the adsorbate and functional groups act as electron donors or acceptors and how strongly the components interact. The charge transfer (\( \Delta Q_c \)) is defined with Equation 4.5.

\[ \Delta Q_c(\text{pollutant}) = Q(\text{pollutant})_{\text{after ads}} - Q(\text{pollutant})_{\text{before ads}} \]  
(4.5)

where \( Q_{\text{after ads}} \) is the total charge adsorbing on the CNT and fCNT surface and \( Q_{\text{before ads}} \)
ads is the total charge in the free case.

Moreover, the HOMO/LUMO gap (Eg) is resulted as the Equation 4.6.

\[
E_g = E_{\text{LUMO}} - E_{\text{HOMO}}
\]  

\textit{(4.6)}

ELUMO and EHOMO signify the energies of the Lower Unoccupied Molecular Orbital and Higher Occupied Molecular Orbital.

The effect of an aqueous environment was included by a conductor-like polarizable continuum model (CPCM) as implemented in ORCA. A dielectric constant of 80.4 was used to simulate water.

\section*{4.3 Results and Discussion}

\subsection*{4.3.1 Pollutant interactions with functionalized CNT in gas phase}

The strength of the interactions between bare CNT and CNT functionalized with multiple -COOH groups with the various aforementioned pollutants were investigated. First, the atomic positions of a bare CNT, and CNT with one and two -COOH groups (fCNT and ffCNT respectively) were fully optimized. Next, the interaction of each pollutant with CNT, fCNT, and ffCNT was investigated by determining the most energetically favorable configuration in each case; this is summarized in Figure 4.1 (non-PFAS pollutants) and Figure 4.2 (PFAS pollutants) which show the corresponding lowest energy CNT/pollutant configuration after structural optimizations. Generally, most of them prefer to orient horizontally next to the functional group (-COOH) in almost every case except PFOS and PFOA with ffCNT configuration.
Figure 4.1 DFT optimized geometry for (a) CNT-Hg, (b) fCNT-Hg, (c) ffCNT-Hg (d) CNT-NO, (e) fCNT-NO, (f) ffCNT-NO, (g) CNT-O₃, (h) fCNT-O₃, (i) ffCNT-O₃, (j) CNT-NH₃, (k) fCNT-NH₃, (l) ffCNT-NH₃ (m) CNT-SO₂, (n) fCNT-SO₂, (o) ffCNT-SO₂ (p) CNT-PTFE, (q) fCNT-PTFE, (r) ffCNT-PTFE (s) CNT-PAN, (t) fCNT-PAN, (u) ffCNT-PAN.
Figure 4.2. DFT Optimized Geometry for (a) CNT-PFOS (b) ffCNT-PFOS (c) CNT-PFOA (d) ffCNT-PFOA.
In total, twenty-five different adsorption configurations were investigated in this work (nine pollutants with bare CNT, fCNT, and ffCNT). A stable optimized configuration and bonding is achieved by a favorable functionalization which keeps the system together. As expected, the adsorption of each pollutant on the functionalized CNTs occurred near the carboxyl group above the surface of CNT. The adsorption energy values are presented at Table 4.1. All the calculated adsorption energies are negative, indicating spontaneous adsorption on the surface. The more
negative the adsorption energy leads to the stronger adsorption between the CNTs and the pollutant molecule. On bare CNT, Hg, NO, and NH$_3$ are the weakest binding pollutants all with similar $E_{\text{ads}}$ of only -0.23 to -0.24 eV, in agreement with the fact that non functionalized CNT is not very good at NH$_3$ separation. Next, PTFE, SO$_2$, and O$_3$ bind slightly more strongly, each with $E_{\text{ads}}$ of approximately -0.4 eV. Finally, PAN, PFOS, and PFOA are the strongest binding pollutants to bare CNT, with $E_{\text{ads}}$ ranging from -0.72 to -0.85 eV. These weaker interactions between the pollutants with bare CNT are unlikely to provide chemisorption; this is a well-known problem with adsorbate interactions with bare CNT surfaces [186].

With the introduction of -COOH functional groups on the CNT, much stronger adsorption energies were found, and the results showed that the functionalization of CNTs with –COOH molecules leads to stronger adsorption of some adsorbents. The three most weakly binding adsorbents on bare CNT (NH$_3$, NO, Hg) remained the most weakly bound after the introduction of one functional group; of these, only NH$_3$ increased by any significant amount (from -0.22 to -0.38 eV) but remains relatively weak. Interestingly, this agrees with the previously mentioned experimental observation that functionalization helps in removal of NH$_3$ [45]. This puts the adsorptive capability of fCNT towards NH$_3$ on the same level as PTFE. In this case, however, $E_{\text{ads}}$ of PTFE only increase by 0.01 eV on fCNT. For SO$_2$, O$_3$, and PAN, $E_{\text{ads}}$ increased in each case by 0.1 to 0.2 eV, indicating stronger binding of these pollutants upon functionalization.
Finally, in contrast to fCNT, the introduction of a second -COOH group increased the interaction strength of the CNT with all pollutants. Hg and PTFE remained the most weak bound, although both of their $E_{\text{ads}}$ increased by approximately 0.1 eV. Both NH$_3$ and NO became more strongly bound as well, with the $E_{\text{ads}}$ of NH$_3$ increasing by nearly 0.5 eV, again in agreement with the increase in NH$_3$ removal ability. Moreover, another study showed how functionalization of CNT with oxygen-based groups increases its interactions with NOx species, also in agreement with these results [187]. SO$_2$ and O$_3$ became more strongly bound by 0.1 eV. Interestingly, the adsorption energy of PFOS and PFOA became significantly more negative at -1.25 and -1.3 eV, respectively.

4.3.2 Pollutant Interactions with Functionalized CNT in Aqueous Phase

Next, the adsorption of each pollutant molecule with CNT, fCNT and ffCNT were investigated by re-optimizing the geometries in an implicit aqueous environment, as assessing the impact of solvent at the pollutant-liquid interface is required to predict numerous interfacial processes. The solvated adsorption energy ($E_{\text{sol}}$) was calculated using Equation. (3)-(4) and results are presented for different complexes in Table 1. Negative values of $E_{\text{sol}}$ signify the stability of the studied complexes in the aqueous medium and show that adsorption remains a spontaneous process. In general, all the calculated adsorption energies become weaker when an implicit aqueous medium is included in the simulations. On bare CNT, the only significant change observed was for PAN, PFAS, and PFOS, for which the solvation environment resulted in a weakening of $E_{\text{sol}}$ compared to $E_{\text{ads}}$ by around 0.1 eV. $E_{\text{sol}}$ of all the other pollutants remained within 0.01 or 0.02 eV of their $E_{\text{ads}}$ value on CNT. Furthermore, the ranking
of all the pollutants by their solvated adsorption energy ($E_{\text{sol}}$) matches that of the non-solvated one ($E_{\text{ads}}$).

However, the situation changes on the functionalized CNTs. On fCNT, the adsorption energy of NO remains very weak while Hg is nearly halved in the solvation environment. For each of the other compounds $E_{\text{sol}}$ decreases only slightly; interestingly, NH$_3$ shows the largest decrease in agreement with experimental results that functionalization of CNT improves its adsorptive properties towards this molecule. Finally, the presence of two –COOH groups strongly affects the adsorption of NO, SO$_2$, and Hg, the $E_{\text{sol}}$ of which decreases by around 0.2 eV each. The $E_{\text{sol}}$ of the other pollutants is not strongly affected by this further functionalization, decreasing only by 0.01 to 0.02 eV. These results show that, although functionalization of CNT improves its adsorptive capability in an aqueous environment, especially towards NH$_3$ and Hg, the effect is not as strong as in the gas phase; also, although it improves NO and SO$_2$ adsorption, these compounds typically form nitric acid and sulfurous acid in water and so would likely not be present.

4.3.3 Charge Transfer in the Pollutant-functionalized CNT Systems

The charge transfer from pollutants to CNT, fCNT, and ffCNT were investigated since it influences the adsorption strength of molecules to surfaces. Generally, increasing the number of functional groups causes an increase in the amount of charge transfer from the pollutants to the membrane, contributing to the observed increasing trends of the adsorption energies. From the calculated charge transfer ($\Delta Q_e$, Table 1), it can be can observed that some of the molecules behave as electron donors and others behave as electron acceptors. One bare CNT, $\Delta Q_e$ of the three weakest binding
pollutants (NH₃, PAN, and NO) are nearly 0. As expected, the absolute magnitude of the charge transfer increases for the next set of more strongly binding pollutants, PTFE (ΔQₑ = 0.02e), SO₂ (ΔQₑ = -0.05e), and O₃ (ΔQₑ = -0.24e). Interestingly, the charge density for the two most strongly binding pollutants (PFOS, and PFOA) show a different trend. The ΔQₑ for PFOA is very weak (~0.002e) while that of PFOS is significant (0.62e). This shows that, while important, charge transfer is not the only factor affecting adsorption. It could not been gotten any results in terms of charge transfer for Hg pollutants owing to the different basis set required for use on Hg.

On fCNT, the charge transfer of NO and PAN remained very weak (0.006e) while NH₃ increased to 0.04e. This likely leads to the observed increase in the adsorption energy when compared to bare CNT. The charge transfer values for SO₂ and PTFE decreased on fCNT while it did not change for O₃ significantly. With the introduction of ffCNT, all pollutants' charge transfer value has shown increase while the highest negative value (~ -0.4e) was seen on O₃ and the lowest value (0.004e) belongs to the PFOA. On the other hand, SO₂, NH₃, and PFOS have relatively higher increases with approximately ~0.1e, in agreement with the observed increase in E_ads for these compounds when adding a second functional group. PAN and PTFE have weaker increases in the charge transfer value with ~0.02e. For PAN and PTFE this is somewhat expected as E_ads only decrease by 0.04 eV and 0.09 eV, respectively. For NO, the charge transfer becomes three times larger (0.006e to 0.018e), correlating with its substantial increase in E_ads (~0.06 eV to -0.49 eV) when going from one to two functional groups on the CNT.
Figure 4.3 Electron density of (a) CNT-NO, (b) fCNT-NO, (c) ffCNT-NO, (d) fCNT-SO₂, (e) ffCNT-SO₂, (f) CNT-SO₂, (g) CNT-O₃, (h) fCNT-O₃, (i) ffCNT-O₃, (j) CNT-PAN, (k) fCNT-PAN, (l) ffCNT-PAN, (m) fCNT-NH₃, (n) ffCNT-NH₃, (o) ffCNT-NH₃, (p) CNT-PTFE, (r) fCNT-PTFE, (q) ffCNT-PTFE.

Figure 4.4 Electron Density of (a) CNT-PFOS (b) 90°ffCNT-PFOS (c) CNT-PFOA (e) 90°ffCNT-PFOA.
4.3.4 HOMO-LUMO

The energy of the highest occupied molecular orbitals ($E_{\text{HOMO}}$) and lowest unoccupied molecular orbitals ($E_{\text{LUMO}}$) were computed. While HOMO defines electron donating behavior of composite, LUMO defines its electron accepting behavior. That means higher $E_{\text{HUMO}}$ shows greater electron donating capacity and lower $E_{\text{LUMO}}$ values indicates easier electron accepting capacity [188]. $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$ values and the energy difference between the HOMO and LUMO orbitals (HOMO-LUMO gap, $E_g$) were reported for the bare CNTs, fCNTs, and ffCNTs models in Table 4.2. Energy gap values displayed a zigzag pattern because of possible effects of curvature character of nanotubes. Previously, it was shown that band gap decreases with decreasing diameter of nanotubes with saw tooth-like periodicity and functionalizing with carboxyl can cause a change in diameter [55].
Unlike the previous chapter in which the HOMO-LUMO gap followed some general trends, in this case the gap does not seem to follow such nice trends. However, it can be made some general observations. On raw CNT, most of the adsorbates (NO, NH₃, PFOS, PTFE, PAN, Hg, and O₃) result in a similar gap of approximately 0.8 eV while the other two (PFOA and SO₂) both have gaps of nearly half that (approximately 0.4 eV). However, the magnitude of the gap does not correlate with either the

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adsorption energy or amount of charge transfer; as such it is more useful to look at changes in $E_g$ only between the same adsorbates as the number of functional groups increase. However, one interesting point is that even though PFOS and PFOA have the same adsorption energy, the $E_g$ of PFOS is 0.79 eV while that of PFOA is 0.44 eV; this increase for PFOS is likely due to the fact that it withdraws charge from the CNT (0.624 $e$) while PFOA does not (0.002 $e$).

When a carboxyl functional group is introduced, the gaps with NH$_3$, PAN, PTFE, and Hg all slightly increase by an average of 0.08 eV from raw CNT to fCNT. The lack of change is likely since the $E_{ads}$ of these species do not substantially change (see discussion in section 4.3.1). In the case of SO$_2$ the gap increases from 0.38 eV on raw CNT to 0.87 eV on fCNT; there is also an increase in the adsorption energy from -0.41 eV on raw CNT to -0.60 eV on fCNT. With NO, the gap decreases substantially from 0.81 eV to 0.32 eV while the adsorption energy also decreases from -0.23 eV to -0.06 eV. It is interesting to note that it would be expected the HOMO-LUMO gap to decrease as interactions between the adsorbate and CNT become stronger (i.e., as $E_{ads}$ becomes more negative; it will be shown this is the case for ffCNT), which is the opposite observation for SO$_2$ and NO on fCNT, a discrepancy that deserves further study.

Upon introduction of a second functional group, the band gaps of NH$_3$, PAN, PTFE, and Hg now show substantial changes, all decreasing to nearly the same value of 0.43 eV; in each of these cases, this drop corresponds to an increase of $E_{ads}$ to more negative values. On ffCNT the gap of SO$_2$ follows a similar trend, decreasing to 0.40 eV with $E_{ads}$ becoming more negative at -0.88 eV; however, as noted above, this is opposite to what is observed when going from CNT to fCNT. Interestingly, NO
behaves differently again while following the same trend it did when going from CNT to fCNT, with the band gap increasing from 0.32 eV to 0.8 eV from fCNT to ffCNT even though there is an increase in $E_{\text{ads}}$ from -0.06 eV to -0.49 eV. Finally, it is interesting to note that the gaps of ffCNT with PFOS and PFOA did not change by any significant amount (0.01 eV) from the raw CNT values. Therefore, while most pollutants show somewhat expected trends in the HOMO-LUMO gap with $E_{\text{ads}}$, the anomalous case of NO deserves more study.

4.4 Conclusion

In this chapter, the ability of -COOH functionalized to adsorb different pollutants in gas phase and aqueous phase was investigated by computing adsorption energies, charge transfer, and HOMO-LUMO gaps. It was found that increasing the number of functional groups increases the strength of the interactions with the pollutants. Furthermore, the interactions are weakened when an implicit solvation model is introduced, indicating weaker adsorption in water. Then the adsorption strength to the charge transfer between the adsorbates and functionalized CNTs were correlated. Finally, it was shown how changes in the HOMO-LUMO gap can also correlate with changes in adsorption strength, with strong adsorption generally resulting in decreases in the gap, although adsorption of NO does not seem to follow this trend. Overall, these results provide a better understanding of the nature of the interaction of functionalized CNTs with air and water pollutants of interest for environmental remediation.
APPENDIX A

INPUT FILE FOR ffCNTPVAZn

The ORCA Input file contains a collection which show how to easily do various tasks using the many methods and approximations. As an example, the input file of ffCNTPVAZn sample is given.

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nprocs 64
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*

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APPENDIX B

OUTPUT FILE FOR SAMPLES

Geometry optimizations were studied to find the geometry that minimizes the total energy for the given method. After a geometry optimization was run, a file named samplename.xyz can be printed with the final geometry coordinates that can be used in various calculation. These are the xyz files for samples used in computational studies.

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