Surface Engineering of Graphene and Graphene Quantum Dots for Industrial and Medical Applications

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CHAPTER 1

AN INTRODUCTION TO SURFACE CHEMISTRY

BEHESHTEH SOHRABI

Why is it important to research interface theory and properties? First, to comprehend numerous natural processes, and second, to provide one with a more comprehensive understanding of how to logically build and alter desirable interfaces, given the significant role of interfaces in industries. On the same ground, we must examine the precise meaning of the term "surface free energy" and its connection to interfacial tension, as well as comprehend the pertinent theoretical links. For many medicinal and industrial uses, it is also vital to understand the variables that impact the chemical and physical characteristics of the surface.

1.1 Surface Chemistry-Fundamentals

The two key ideas in surface science are interface and surface. The boundary between two phases, such as solid, liquid, and gas, is referred to as the interface. Liquid-solid, solid-gas, and liquid-gas interfaces are three possible combinations of the interfaces. Two immiscible liquids, such as water and oil, and two solid phases are divided by liquid-liquid interfaces and solid-solid interfaces, respectively. The contact type known as a surface, on the other hand, has air as one of its phases.

According to Park and Seo, surface free energy, also known as interfacial free energy or surface energy, quantifies the breaking of intermolecular connections caused by the formation of a surface (Park and Seo 2011). However, in this instance, a greater surface energy value results in a wettable surface whereas a lower value results in a non-wettable surface (Jothi Prakash and Prasanth 2021).

Because the atoms on the surface of a material contain more energy than the atoms within the material's bulk, surfaces should be fundamentally less energetically favorable than the material's bulk, according to solid-state physics. As a result, a driving force is required to generate a surface by taking away the majority of a substance. Therefore, surface energy may be characterised as the excess energy present on a material's surface relative to its volume or as the amount of effort necessary to create a certain surface area. Another way to describe surface energy is as the effort necessary to split one surface into two, creating two new surfaces.

A solid's bonds are broken during cutting, which also increases surface area and surface energy. The energy used in the cutting process will be equal to the energy present in the two newly produced surfaces if the cutting is done in a way that is reversible. As a result, a material's surface energy is equal to half of its cohesion energy. In other words, atoms are stable and have an even distribution of bonds and interactions with their neighbors in the bulk of a substance. In contrast, the inadequate interactions between surface atoms will result in unstable binding energies. Actually, surface energy is a measure of the energy present on the surface as a result of this broken link. How many particles interact with one another in a material's bulk and how much surface area is exposed to the substance affect the amount of this energy. As a result, the surface energy will be greater if the bulk interactions are stronger or if the surface accessibility is greater.

Every surface strives to have as little energy as possible. This can be accomplished by absorbing something with less energy on its surface. The number of exposed surface atoms with high surface energy is reduced and replaced by low-energy atoms or molecules during the adsorption process. Because of the weak interactions between their molecules, liquids frequently have lower surface energies than solids. Surface energy, which is frequently expressed in terms of J/m^2, may be defined as the energy needed to expand the size of a surface by a unit.

The size of the surface's constituent particles, the materials used to cover it, the temperature, and the degree of surface roughness are only a few of the factors that affect the surface's free energy. The energy of the surface changes depending on the type of material and how it interacts with the surface when we cover it with a variety of layers. For instance, a material's surface energy changes depending on whether its molecules are attracted to or repellent to one another. The adhesive force holding atoms together weakens as temperature rises, which also causes an increase in atomic oscillation. Because the surface energy is dependent on the net force of internal adhesion, it falls as the temperature rises. According to studies, the surface energy of several metals, including copper, gold, and silver, drops by approximately 0.5 mJ/m^2. K^{-1} as temperature rises.

The contact angle measurement, which characterises surface hydrophilicity or hydrophobicity depending on several factors, such as surface energy and roughness (Adamson and Gast 1990, Bhushan 1999, Bhushan and Ko 2003, Israelachvili 1992, Nosonovsky and Bhushan 2008a), is one of the straightforward but fundamental approaches to preparing interfaces. When a liquid drop is put on a solid surface for contact angle research, the molecular attraction lowers the energy of the two separated surfaces. This shift in energy is expressed by the Dupré equation:

$$W_{ls} = \gamma_{\mathrm{lg}} + \gamma_{sg} - \gamma_{ls} \quad (1\text{-}1)$$

where W_{ls} is the work of adhesion per unit area, γ_{sg} and γ_{ls} are the surface energies of the solid against gas and liquid, and γ_{lg} is the surface energy of liquid against gas (Adamson and Gast 1990, Bhushan 1999, Israelachvili 1992). Once a droplet is on the surface, it spreads to create an interface with the solid surface. After reaching an equilibrium state, a characteristic angle called the static contact angle θ_y (see Figure 1) is measured, which provides important information about the interfacial interactions and the surface characteristics. If a liquid droplet is spread on a hydrophilic surface, the value of the measured contact angle is $0^\circ \leq \theta \leq 90^\circ$, while if it is spread on the hydrophobic one, the value of the measured contact angle is $90^\circ < \theta \leq 180^\circ$. Although the terms "hydrophilic" and "hydrophobic" specifically refer to liking or disliking water, they may also be used to describe the interaction and contact of any liquids on a solid surface. Surfaces consisting of non-polar molecules are low-energy and hydrophobic, whereas surfaces comprised of polar molecules are hydrophilic and have high surface energy. Superhydrophobic surfaces are those that have a contact angle with the drop of between 150 and 180 degrees. As a result of fewer links between neighbouring atoms or molecules on liquid or solid surfaces, they possess more energy than equivalent atoms and molecules in bulk. This extra energy is equivalent to the free surface energy, also known as surface tension, needed to form a unit area of a surface at constant pressure and temperature. The contact angle can be determined by minimizing the net surface free energy of the system (Adamson and Gast 1990, Bhushan 1999, Israelachvili 1992). The total energy E_{tot} is given by

$$E_{tot} = \gamma_{\mathrm{lg}}\left(A_{\mathrm{lg}} + A_{ls}\right) - W_{ls}A_{ls} \quad (1\text{-}2)$$

where A_{ls} and A_{lg} are the contact areas of the liquid with the solid and air, respectively. It is assumed that the volume and pressure are constant so that the volumetric energy does not change. At the equilibrium $dE_{tot} = 0$, which yields

$$\gamma_{\mathrm{lg}}\left(dA_{\mathrm{lg}} + dA_{ls}\right) - W_{ls}dA_{ls} = 0 \quad (1\text{-}3)$$

For a droplet of constant volume, it is easy to show using geometrical considerations that

$$\frac{dA_{\mathrm{lg}}}{dA_{ls}} = Cos\,\theta_y \quad (1\text{-}4)$$

Combining (1), (3), and (4), the well-known Young equation for the contact angle is obtained

$$Cos\,\theta_y = \frac{\gamma_{sg} - \gamma_{ls}}{\gamma_{\mathrm{lg}}} \quad (1\text{-}5)$$

Eq. 1-5 provides an expression for the static contact angle for given surface energies.

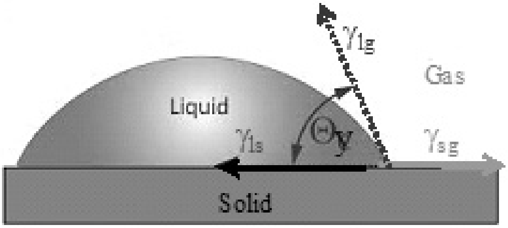

Figure 1 The schema of surface tension vectors for the joint contact surface of liquid-gas (γ_{lg}), liquid-solid (γ_{ls}) and solid-gas (γ_{sg}) phases.

In addition to their high contact angle, superhydrophobic surfaces also need to have a very low contact angle hysteresis for applications requiring self-cleaning qualities and low surface tension. The lotus effect is a type of self-cleaning property that these surfaces exhibit when water droplets roll off and transport impurities. The difference between the advancing and receding contact angles is shown by a contact angle hysteresis (Figure 2a), which is created when the contact angle in front of the drop (the advancing contact angle) is larger than the contact angle behind the drop (the receding contact angle). The contact angle hysteresis occurring due to surface heterogeneity and surface roughness shows that the wetting/dewetting cycle is irreversible. The Wenzel and Cassie-Baxter models are depicted in Figures 2a and 2b. The Wenzel model is used to explain surfaces where, in addition to being rough, the substance of the surface also contributes to the drop's increased adhesion to the surface, causing the droplets to penetrate and stick to the surface's rough structures. In other words, the surface will be sticky. As opposed to the rough surface that is impermeable to liquid droplets described by the Cassie-Baxter model. In this instance, the air is trapped behind the droplets because they are positioned on top of the uneven surface structures. In addition to regulating the amount of roughness, a surface should be coated with a layer composition that lessens the adherence of the drop to the surface and produces a slippy surface in order to produce a surface that adheres to the Cassie-Baxter model (Bharat 2004).

On flat surfaces, we can employ strategies to create surfaces that are superhydrophobic and self-cleaning. In reality, there are methods that help roll the drop and cause the surface to self-clean by altering the geometric dimensions of the surface's roughness.

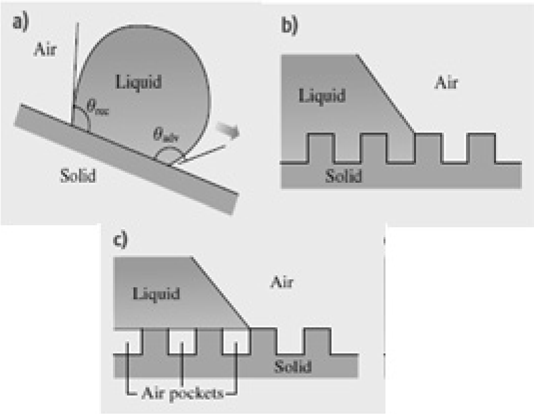

Figure 2 (**a**) Schematics of a droplet on a tilted substrate showing advancing (θ_{adv}) and receding (θ_{rec}) contact angles. The difference between these angles constitutes the contact angle hysteresis. Configurations described by (**b**) the Wenzel equation for the homogeneous interface (Extrand 2002), (**c**) the Cassie–Baxter equation for the composite interface with air pockets (Nosonovsky and Bhushan 2007).

A rough surface can be built in a regular (engineered surface), random (irregular rough surface), or intermediate condition (hierarchical rough surface), according to thorough research (Feng et al. 2002). A true superhydrophobic surface with a high contact angle (> 150°) and a low hysteresis angle (sliding angle) may be designed using any of the aforementioned methods when utilized to produce a rough surface (Li and Amirfazli 2007). Huang et al.'s study showed that patterned surfaces have special benefits for superhydrophobicity because of the homogeneity of the large-scale surface. Significantly, they draw inspiration from the "lock and key" paradigm as an illustration of patterned surfaces made up of dense arrays and employ microfabricated PDMS lenses (as locks) and bowls (as keys) for wettability and modifying the adhesion force.(Huang et al. 2009). In this way, they were able to achieve They were able to accomplish their objective in this manner without the need for silanization, which is the conversion of hydrophobicity to superhydrophobicity and the alteration of high adhesion force to anti-adhesion force. These microlens-designed surfaces can exhibit hydrophobic behaviour that is dimension-dependent. Additionally, their research demonstrated that these surfaces are entirely distinct from chemically produced hierarchically rough surfaces (Guo and Liu 2007) and aligned nanotube films (Jin et al. 2005). The microbowl-arrayed surfaces, as shown in Figure 3, exhibit a high contact angle and anti-sticking behaviour in accordance with the Cassie-Baxter model, where a droplet sits on the surface peaks and air fills the interstices.

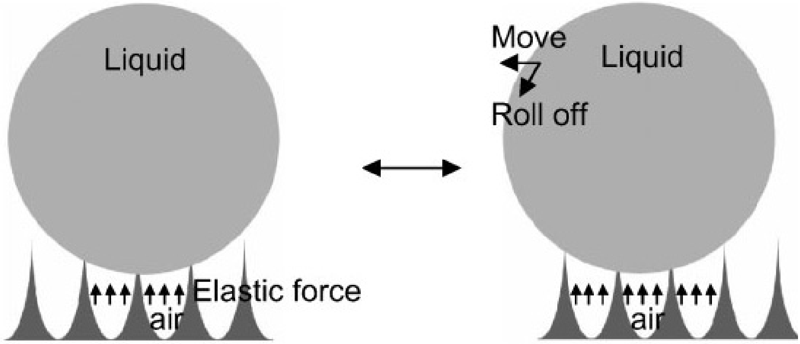

Figure 3 The superhydrophobic surface with low surface free energy (Huang et al. 2009).

1.2 Surface Forces and Methods used to Study them

It is crucial to investigate surface forces because they have a significant impact on how basic systems, particularly more complicated systems such as gases, liquids, and solids, behave. Extensive research reveals that some of these intricate structures are layers of nanoparticle-coated surfaces. Investigating the interactions between these surfaces and coated nanoparticles can help with surface design for several businesses and in the medical field. In the sections that follow, we'll look at the hydrophobicity and hydrophilicity of surfaces whose surface energy is influenced by the kind of coating material applied to them as well as the degree of surface roughness. Surface forces are therefore a very wide topic in physics, chemistry, chemical engineering, and biology, all of which have made enormous strides in recent years. Separate examples of these developments may be found in medicine and numerous industries. The interactions that take place between the molecules of a substance are what are employed to establish its macroscopic qualities, such as its physical state, viscosity, and boiling point. The kind of interaction, polarizability, and molecular contact area all affect how strong these interactions are. Given that this book is about the usage of graphene and its derivatives in both industries and medicine, it will attempt to look at the many sorts of interactions and how they affect the operation of these systems. According to studies, hydrogen bonding and the π-π interaction are the intermolecular interactions that are crucial for the non-covalent functionalization of graphene.

When two electronegative substances with a single pair of electrons, such as oxygen or nitrogen, are in close proximity to one another, such interactions are known as hydrogen bonds (Chauhan, Maekawa, and Kumar 2017). Less than 20 kJ mol-1 is the energy associated with the electrostatic nature of these interactions, which is lower than the energy in chemical bonds, which is 250 kJ mol^{-1}. Hydrogen bonds can be as powerful as certain covalent bonds if their quantity increases.

Dispersion forces are interactions between non-polar molecules, and π-π interactions are a sort of dispersion force between aromatic compounds. Since nonpolar molecules with a homogenous charge distribution lack permanent or partial dipoles, there is no electrostatic contact when two of them are first introduced close to one another. But at a specific time, the concentration of electrons in a particular area of the molecule increases. This will cause a temporary dipole to form in the molecule and spread to nearby molecules because one half will have a partial negative charge and the other will have a partial positive charge. Due to the polarizability of this instantaneous dipole, the electron cloud in the molecule may deviate; the degree of this deviation depends on the close proximity of the molecules (Matthews, Welton, and Hunt 2014). In essence, non-covalent functionalization via interactions is a technology that has promise since it permits the attachment of functional groups to graphene without disrupting the electronic structure of the material (Karousis and Tagmatarchis 2010). Some scientists create novel materials based on graphene using these non-covalent interactions (Kemp and Kim 2016, Niu et al. 2019). In graphene, there are typically two kinds of π-π interactions between electron-rich and electron-poor areas, and these interactions have an impact on how other molecules or nanomaterials interact with graphene. According to Figure 4 in graphene, these interactions usually occur in a face-to-face or edge-to-face arrangement.

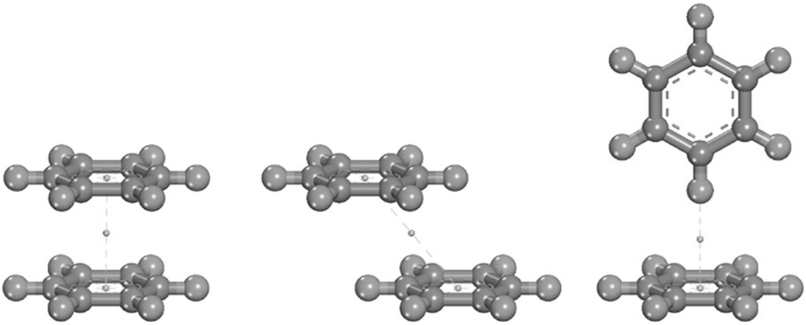

Figure 4 The interactions of C-H···π type (right), slip (middle) and face-to-face π-π stacking (left) corresponding to benzyl molecules. In this figure, gray atoms represent carbon and orange represent hydrogen for benzene or other atoms for various derivatives (Kemp and Kim 2016).

Similar interactions between tiny molecules and graphene and graphene oxide are seen, and they may be utilized to alter the characteristics of graphene and its derivatives to make them suitable for usage in a variety of fields, including medicine and industry. Figure 5 shows, in general, the many kinds of π-π interactions seen in graphene. A hydrogen atom or phenyl rings oriented perpendicular to the graphene surface can be used to manage the CH···π interactions that could additionally happen at the edge of graphene in addition to these other interactions.

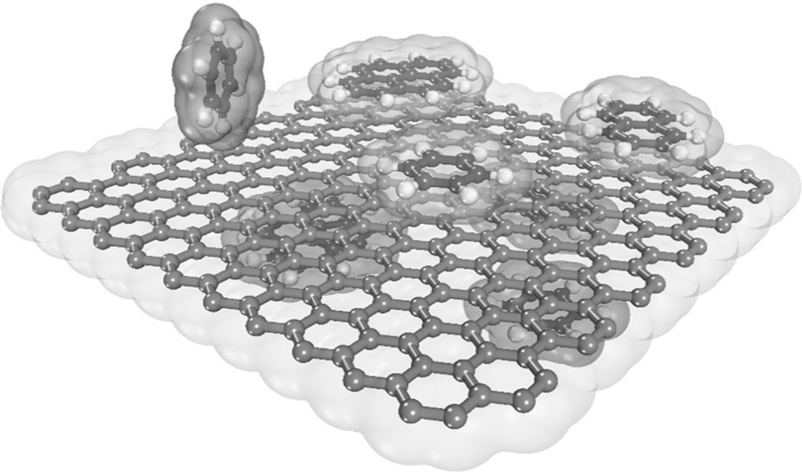

Figure 5 Representation of π-π or C-H····π interactions at the top and bottom of the graphene sheet (Kemp and Kim 2016).

The base plate of graphene oxide is comparable to graphene in many ways; however, flaws have been introduced because of epoxide and hydroxide groups bonded to carbon atoms on the surface. Because of this, interactions resembling those in graphene are probably present there. The oxygen groups on GO may mostly be found at or on the edges, as seen in Figure 6, and they may contribute to the interactions at the edge.

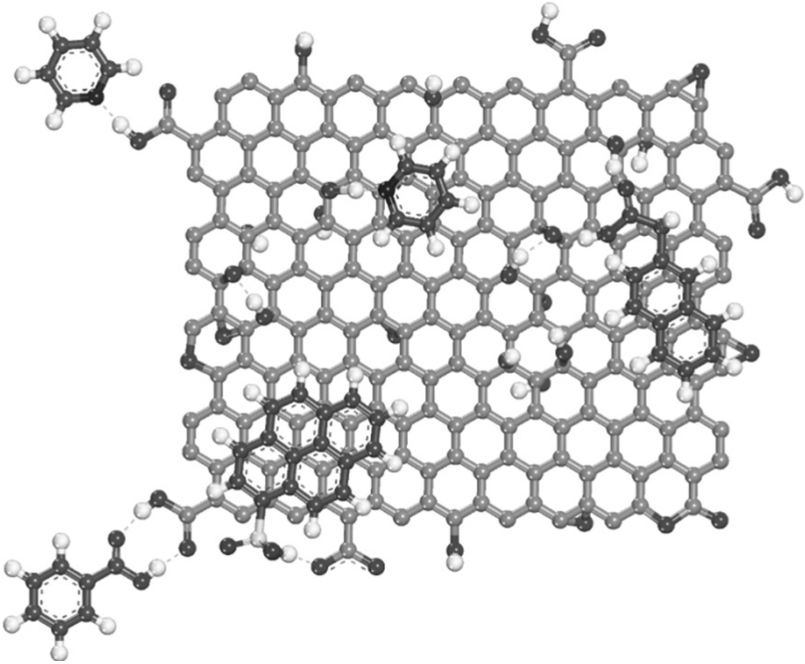

Figure 6 Scheme of two interactions of π-π stacking and hydrogen bonding with GO (Kemp and Kim 2016).

It is possible to use scanning tunneling spectroscopy (STS) and scanning tunneling microscopy (STM) to look at the non-covalent interactions between molecules that have been adsorbed on the surface of graphene and its derivatives. Without the use of light or electron beams, pictures of the surface and its interactions at the atomic scale are produced using the scanning tunneling microscope imaging technique (Hossain, Walsh, and Hersam 2010). The electrical structure of surfaces may be quickly and with atomic precision examined using scanning tunneling spectroscopy (STS) (de Parga and Miranda 2015). A strong method for measuring different forces, such as magnetic forces, adhesion strength, and mechanical characteristics of diverse surfaces, including graphene, is the atomic force microscope (AFM). Almost every surface type, including polymers, ceramics, composites, glass, and biological materials, may be imaged using this method. Chapter 5 will provide a thorough examination of several microscopic techniques and how they might be used to examine surface interactions, particularly those involving graphene and its derivatives. Furthermore, theoretical research that will be covered in greater detail in the next chapters demonstrates that molecules on the surface of graphene at the solid-liquid, atmosphere-solid, or solid-vacuum interfaces may be exploited to modify the characteristics of graphene (De Feyter and De Schryver 2003, Kozlov, Viñes, and Görling 2012, Zhang, Huang, and Yang 2011).

1.3 Surface Engineering

Surface engineering is the application of technology to change a surface's physical or mechanical characteristics so that it may be employed in a variety of industrial settings. In other words, surface engineering would allow for the creation of a structural modification on the surface using a variety of methods in addition to coating the surface to alter the surface energy.

In addition to the mechanical modification of the surface (producing a substrate with variable geometric forms), some materials may be used to alter the free energy of the surface. This can be done to affect the physical qualities of each surface, including its hydrophilicity and hydrophobicity.

Materials' surface energies may be categorised into three groups: high, medium, and low surface energies. In materials with a high surface energy, surface molecules are so strongly attracted to one another that liquid molecules can also be drawn to them with ease. Thus, these materials absorb moisture rather quickly. In interaction with liquids, metals and glass that have a surface energy of roughly 100 or 1000 dynes/cm are quickly moistened. Materials with medium surface energy range in energy from 36 to around 300 dynes/cm. Surface energies in this range are common in well-designed polymers. Additionally, natural materials having a medium surface energy include wood, stone, and concrete. There is extremely minimal attraction for each molecule in this type of material, especially for the molecules that are in direct contact with the surface, and the molecules on the surface are fully free. Low-surface-energy materials are particularly difficult to attach to surfaces and have a surface energy of less than 36 dynes/cm. This group of materials includes polyolefin polymers like polypropylene and polyethylene as well as "non-stick" surfaces like polytetrafluoroethylene (PTFE). Therefore, by altering the surface's free energy, these materials may be utilised to change each surface's physical characteristics (Darband et al. 2020, Zhao and Law 2012). For this reason, the function of graphene and graphene quantum dots will be examined in chapters 2 and 3. Additionally, chapters 6 and 7 will discuss techniques for altering the surface's physical composition for application in medicine and other fields. We'll also look into how to apply these techniques to physically alter the surface that has been covered with graphene or graphene quantum dots.

1.4 History of the Surface Engineering (Inspiring the Nature)

Design that is biologically inspired, naturally adapted, or derived from nature is called biomimetics. Otto Schmitt first used the Greek word biomimesis to define this concept in 1957 (Patterson 2003). Our forefathers turned to nature for inspiration and the invention of diverse materials and gadgets centuries ago, even though the word "biomimetics" is very new. Essentially, biomimetics is a method of learning from nature that may be applied to find more effective and affordable answers to the issues we now face. It may contribute significantly to a wide range of fields, including engineering, architecture, materials science, and medicine. Even if this strategy is changing, changes still need to be made. You can find more in chapter 8.

Due to their hierarchical structures (the nanoroughnesses on the microhigh posts) and the presence of a waxy covering, some plant leaves, such as lotus, are water-resistant, superhydrophobic, and self-cleaning in nature (FEYMAN 1960, Nosonovsky and Bhushan 2008b). Due to the structure of these leaves, surfaces that are superhydrophobic and self-cleaning may be created, such as dishes, roof tiles, fabrics, self-cleaning windows, self-cleaning windows for automobile fronts, exterior colours of buildings, and navigational boats. Energy conversion and conservation are further uses for surfaces that appear to be superhydrophobic (Nosonovsky and Bhushan 2009).

1.5 Application of Surface Engineering in different Fields

Friction between two surfaces causes wear and perhaps breaks over time as they come into contact and move on top of one another. In a number of sectors, this might result in catastrophic financial losses. As a result, designed surfaces are highly favoured for dealing with friction and minimising wear.

The production of self-cleaning glass for the construction and automotive industries, the production of waterproof doors, the reduction of air and water friction with aircraft and ship hulls, and other industries all make use of superhydrophobicity and superhydrophilicity today. They can also be used to increase the effectiveness of solar cells and supercapacitors. Additionally, they may be used to create nanobioreactors, treat cancer cells, and create drug delivery systems. These phenomena can be utilised in the creation of biosensors in addition to being employed for treatment, diagnosis, and prevention.

1.6 The Capacity of Computational Chemistry in Surface Chemistry

How to determine and create a surface's chemistry with the best qualities for a particular purpose has been a persistent difficulty in applied physical and chemical sciences for engineering surfaces. The identification and characterization of new structures that have potential for societal benefit make up a significant portion of surface chemistry research. However, the majority of advancements are still typically credited to costly and time-consuming trial-and-error experimentation. But using the experimental methods at hand, this question is difficult to address. In order to understand surface and interface behaviors at the molecular level and throw light on various surface phenomena, new approaches are therefore required. Faster, better, and less expensive research and development initiatives are critically needed in light of the present global concerns. Modern computational chemistry techniques offer paradigm shifts in the way surface chemistry phenomena are conceptually understood and developed for particular applications. These techniques show the orientation and/or conformation of materials in a variety of processes, including adsorption, adhesion, wetting, and friction, which are all greatly influenced by surface chemistry and raise intriguing questions about how the process actually modifies the molecular structure of materials. Perhaps the most effective technique for directly examining molecule-level interactions right now is molecular modelling. Numerous force field-based molecular modelling programmes have been created as a result of improvements in computer capability and molecular simulation methods, and they have the potential to produce precise quantitative data for the study of surface chemistry.

The user's representation of the system, or how the user chooses to characterise the system, is essential to any computational chemistry investigation. A solid-liquid interface or a complex of biomacromolecules are examples of complicated and ambiguous computational chemistry representations. These representations can span a variety of time and length scales, ranging from simple (for example, a precise chemical system comprises a water molecule) to complex and ambiguous.

Different molecular modelling approaches scaling from ab initio quantum mechanics (QM) to molecular dynamics (MD), Monte Carlo (MC) methods, and out to mesoscale (MS) techniques cover a broad range of both length and time scales to study surface chemistry (Aminpour, Montemagno, and Tuszynski 2019, Haghgoo, Ansari, and Hassanzadeh-Aghdam 2022, Mert, Deniz, and Baykasoglu 2020, Sattar 2021, Sethi, Kadian, and Manik 2022, Vacher and de Wijn 2022, Yang et al. 2022). Due to rapidly escalating computing costs, QM approaches have practical size constraints of a few hundred atoms but may give excellent precision when getting the electron distribution of any molecular system.

Along with describing the potentials of various molecular modelling approaches that have recently been used to study graphene surface chemistry and engineering, as well as various applications of graphene, we will also summarise recent studies that have examined the molecular modelling approaches for graphene applications in this book. We present an overview of the key design concepts for cutting-edge multifunctional graphene-based systems, demonstrating how graphene surface chemistry may offer exceptional platforms for use in a wide range of applications. We offer a road map outlining the advantages and disadvantages of using predictive multiscale molecular modelling tools to hasten the development of systems based on graphene.

1.7 Organization of the Book

This book consists of three parts and eight chapters; each has about 25 figures and several equations depending on the chapter's contents and the fundamental theory.

The first chapter will review the basic concepts of surface chemistry. Next, these concepts will be used for the surface engineering of graphene and its derivatives for use in various industries and medicine. Moreover, Surface forces and the methods used to study them will be explained. Since this chapter will cover the basics of surface chemistry, the number of equations presented in this chapter will be higher than in the other chapters. Part I is "Graphene and Graphene Quantum Dots," formed from two chapters (chapters 2 and 3).

In the second chapter, a comprehensive study of graphene structure and bonds will be introduced. In addition, graphene is produced by many methods, which are categorised into two main groups: top-down and bottom-up. Most of the methods will be discussed in this chapter. Moreover, the properties of graphene will be introduced, and the ferromagnetic properties of graphene will be presented individually. The many applications of GQDs in industry, electronics, and medicine have led us to collect the properties, synthesis, and identification of graphene quantum dots and make them available to everyone as a complete and accessible source. Therefore, in the third chapter of the book, we will discuss the properties, synthesis methods, and identification of graphene quantum dots in detail. Part II of the book is about characterization methods and has been organised from chapters 4 and 5. In chapter 4, we will start with spectroscopic insight via spectroscopic results, including Raman, FT-IR, UV-Vis, and XPS on graphene and graphene quantum dots, to clarify and confirm its synthesised molecular structures. Raman spectroscopy is now evolving into one of the most important tools for nanoscience and nanotechnology. Fourier Transform Infrared Spectroscopy, or FT-IR, is another powerful tool to detect chemical functionalities in oxidised carbons. Fundamentally, optical techniques (normally using infrared and UV-Visible wavelengths) are nondestructive and noninvasive because they use the photon as a probe. XPS is at most a semi-quantitative analysis technique, and this kind of analysis goes beyond the resolution limit of the instrument. Since the transmission electron microscope (TEM), scanning electron microscope (SEM), and atomic force microscope (AFM) are very useful instruments for the characterization of a large variety of materials, in chapter 5, these techniques for identifying and studying graphene and its derivatives will be introduced and discussed in detail. Part III is related to Graphene and GQD applications formed from chapters 6–8. Spintronics is a promising technology to employ the spin degree of freedom for information processing and storage with high-speed and low-power computing. Graphene, due to the long spin lifetime of its carriers combined with its high electron velocity, shows great potential for spintronics applications. In the first section of Chapter 6, we will present crucial spin-dependent characteristics of graphene and GQDs for spintronic devices based on recent experimental and theoretical studies. Finally, we will refer to some challenges and future directions in this field. In continuation, it will be tried to investigate the latest achievements reported in electronic devices based on graphene and GQDs, such as graphene transistors in integrated circuits (ICs), transparent electronic devices, graphene electrodes for touch screens, flexible electronics, memristors, photodetectors, light-emitting diodes (LEDs), and solar cells.

Recently, due to worsening global environmental issues related to population and a severe energy crisis, intense requests for discovering outstanding power and energy devices and novel energy storage have become persistent. In this regard, more variable materials are being used for energy storage. Among these materials, supercapacitors consisting of pseudo-capacitors (PsCs) and electrochemical double-layer capacitors (EDLCs) have gained more attention. The energy density characteristics of supercapacitors can be improved by graphene, which has interconnected porous network structures. Considering the combination of various special physical and chemical properties of GQDs, it is reasonable to expect them to be an ideal EDLC electrode material supercapacitor with high capacitance and stability. As a result, in a section of Chapter 6, we will discuss the use of graphene and its derivatives in this field. With the rapid growth of the population and the development of various industries, and due to the lack of clean water resources, environmental pollution and its elimination are significant challenges. Wastewater produced from residential, commercial, industrial, and hospital sites is mixed with groundwater and surface water. Since a significant portion of wastewater enters the environment without treatment, it will have a negative impact on quality of life, freshwater resources, ecosystems, and the economy. In this regard, the use of graphene and its derivatives in efficient and cost-effective methods of water treatment is being developed.

For this purpose, in the continuation of Chapter 6, we will examine the potential of graphene and its derivatives-based membranes for water treatment as well as water and oil separation. Our studies have demonstrated that graphene and its derivatives are used in agriculture as carriers of pesticides and chemical fertilisers. They are also used in the transportation industry to prevent corrosion and prepare composites to strengthen the fuselages of aircraft, ships, and spacecraft, as well as to reduce the weight of this equipment. On the other hand, graphene and its derivatives are used in the packaging industry to maintain freshness and increase the shelf life of food. All these applications led us to devote a part of Chapter 6 to the study of its important applications in this type of industry to pave the way for various other applications of this substance in these industries and other industries. Next, Chapter 7 is devoted to the medical applications of graphene and its derivatives. Undoubtedly, the discovery of graphene revolutionised many areas of medicine, including treatment, diagnosis, and prognosis. Interestingly, it has many other applications beyond these ones. Significantly, in all aspects of medicine where antiseptics are required, its antimicrobial properties might be useful. Additionally, its ability to be attached to different chemically active groups has allowed researchers to build graphene-based sensors to identify biochemical molecules (and eventually selected cells). For example, sensors for physical signals, such as the electrical activity of the heart, have also been suggested. Interestingly, graphene can also act as a sensor for blood sugar levels, blood pressure, and nitric oxide. The unique nanostructure of this material and its resulting physical properties (mechanical strength, elasticity, and large surface area) make it a very promising material for scaffolds used in tissue regeneration. Several studies have examined the potential benefits of graphene coating for endovascular implants, such as stents or valves. Studies on graphene hydrophilization have also shown new potential for use in cell culture. GQDs are also emerging materials that have growing applications in medicine. Until now, they were mostly used in fluorescence, photoacoustic, and magnetic resonance imaging, multimodal, photothermal (PTT), and photodynamic therapy for cancer. In this chapter, we aim to investigate the various applications of these two valuable materials in detail. At the end, a concluding comment section is added, which discusses the possible role of these two emerging materials in the future development of medicine. At first glance, it seems that there is no correlation between industrial and medical applications of graphene and graphene quantum dots. However, considering the invention story of many effective industrial instruments, it is clear that inspiring medicine had a huge impact on the birth of the original idea. The best example is the design of artificial intelligence, inspired by the complex circumstances in the brain. Interestingly, there are lots of these kinds of similarities between various sections of industry and medicine. Comparison of a cancer cell unit to a solar cell or a cell membrane to a supercapacitor are some examples. Over the past few decades, research on the GQD has seen explosive growth due to their diverse applications in fields ranging from optoelectronic devices to third-generation solar cells. These materials are suitable for use in solar cell design due to their efficient photoelectron transfer capability from one material to another. In this regard, the transfer of electrons to the oxygen in the cell can be compared to a solar cell. In cancer cells, the goal is to kill the tumors so that no cancer cells can be detected in the blood. One of these methods is the production of reactive oxygen species in cancer cells. Due to the high ability of GQDs to efficiently transfer photoelectrons from one substance to another, they may be able to be used as molecules and, of course, as efficient carriers for drug delivery simultaneously. Finding these kinds of similarities helps scientists inspire the industrial development of graphene and graphene quantum dots for applications in medicine and inversely. In this book, for the first time, we have gathered both industrial and medical applications of graphene and graphene quantum dots in order to benefit from similarities between the fields. In the same vein, we investigate these similarities thoroughly in one section, "Confrontation of Industrial and Medical Applications of Graphene and Graphene Quantum Dots.". This chapter will contain two sections: "Inspiring the medical applications of graphene and graphene quantum dots in industry" and "Inspiring the industrial applications of graphene and graphene quantum dots in medicine". In these two sections, we aim to examine the common points of medical and industrial applications of these two substances to find out as many applications as possible in these fields.

An ongoing challenge in applied physical and chemical sciences to engineer surfaces has been answering the following question: how can one identify and design a surface's chemistry with optimal properties for a given purpose? A substantial part of research in surface chemistry concerns the discovery and characterization of novel structures that can be beneficial for society. However, most advances are still generally attributed to trial-and-error experimentation, which requires significant time and cost. This question, however, is complicated to answer using the available experimental techniques. Therefore, additional methods are needed to study surface and interface behaviours at the molecular level and shed light on different surface phenomena. Due to current global challenges, faster, better, and cheaper research and development efforts are urgently required. Computational chemistry methods have significantly improved over time, and they promise paradigm shifts in how surface chemistry phenomena are fundamentally understood and designed for specific applications. In this regard, we have decided to add a computational part to each chapter. It is necessary to explain that at the end of each chapter, the conclusion of the whole chapter and a look to the future for more diverse applications of graphene and its derivatives will be presented. Also, at the end of each chapter, we will present a separate set of references for that chapter.

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