



Photocatalytic Properties of Modified Carbon Nanotubes and Graphene in Environmental Remediation

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Abstract

Carbon-based nanomaterials (CBNMs), such as Graphene, Carbon Nanotubes (CNTs), Carbon Quantum Dots (CQDs), and Fullerenes, have gained significant attention within academic and industrial platforms due to their remarkable properties; specific properties include high surface area, high tensile strength, high electrical conductivity, and high chemical stability. Even though CBNMs present these valuable properties, there are potential limitations for using CBNMs in high-performance applications, such as poor dispersibility in select solvents or ineffective light-absorption properties in photocatalytic applications. Functionalization is one of the most important strategies to modify CBNMs by altering intrinsic properties and realizing their full potential; in particular, anti-corrosion technology, and photocatalytic augmented technology. Performing modifications take into account chemical reactivity, dispersibility, and creating custom functional groups to the surface area of CBNMs. The chemical functionalization of CBNMs is described as the covalent or non-covalent bonding of functional groups to the carbon lattice. For example, the oxidative processes that convert Graphene to Graphene Oxide results in higher density of oxygen-containing functional groups; these functional groups drastically increase the chemical dispersibility of CBNMs in water, and the large volume of functional groups create more opportunities for additional chemical modification.

Keywords:

Carbon, Nano, Materials, Anti-Corrosion, Photo Catalytic

Introduction

With the emergence of carbon-based nanomaterials (CNMs) such as Carbon Nanotubes (CNTs), Graphene, and Fullerenes, a new age for materials has been established due to their unique electronic, mechanical, and structural properties. As stated previously, many of these materials are quasi-1D (CNTs) and 2D (Graphene) and have exceptionally high surface area-to-mass ratios that can be advantageous in a host of applications including



sensing, catalysis, and drug delivery. However, the high surface area and chemically-inert nature of the pristine hybridized carbon lattice creates a substantial problem to tackle – their poor dispersibility in solvents and lack of unique chemical handles for directed interaction (Kumar, 2023).

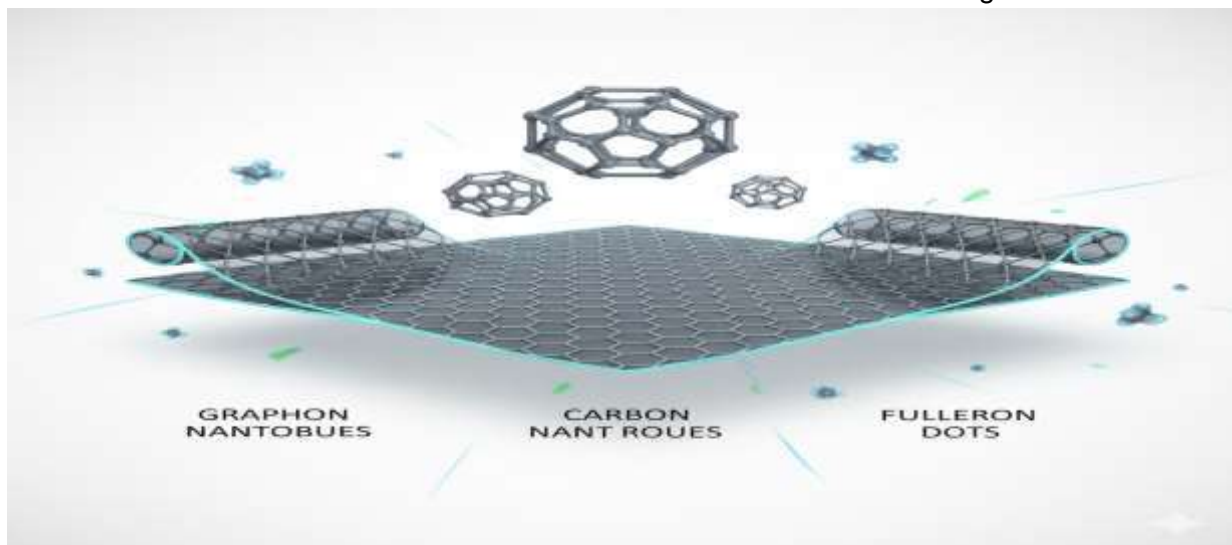
Chemical functionalization is an essential pathway to transform these inert, insoluble nanostructures into highly interactive, versatile chemical platforms. In fact, some modified CBNMs can also provide active protection. For example, functionalized Carbon Nanotubes, or Graphene sheets can be loaded with the molecules of a corrosion inhibitor. When there is localized damage to the coating, the corrosion inhibitor molecules are released into the corrosive environment (commonly acidic or neutral) and either self-heal the coating or passivate the exposed metal surface.

For example, Nitrogen-doped Graphene Oxide (N-GO) is more effective as an anti-corrosion pigment owing to the chemical interactions of the nitrogen functional groups with the metal substrate.

Photocatalysis is the process in which light energy can activate chemical reactions like organic pollutant degradation, like water splitting for hydrogen generation. While pristine CBNMs can provide a very high surface area, they will not be reactively active for most photocatalytic processes because they do not utilize visible-light as well (little light absorption), and the photogenerated electron-hole pairs combine extremely fast. Modification is designed to address these shortcomings.

The main role of CBNMs in photocatalysis is as a co-catalyst in a composite with a semiconductor. In this role, the CBNM can provide low resistance of electrical conductivity by acting as an electron sink or a transport pathway to collect and to shuttle photogenerated electrons from the conduction band of the semiconductor. Separating the photogenerated electron-hole pairs will increase the lifetime of the electron so that it can react in redox reactions and degrade the contaminants. The functional groups that were generated during the modification provide extremely strong anchoring sites, and strong contact, between the semiconductor and the carbon backbone, which is important for maximizing interaction for effective charge transfer and maximum lifetime. (Linic, 2020) Doping CBNMs or the majority semiconductor lattice with non-metals (e.g., N-doping) can decrease the band gap, allowing the material to absorb a larger portion of the available visible light instead of only the ultraviolet part of the spectrum. In addition, materials like Carbon Quantum Dots (CQDs) and Graphene Quantum Dots (GQDs) are (0D) varieties of CBNMs that show interesting quantum confinement effects in which their photoluminescence and light absorption properties become highly tunable. These properties make CQDs and GQDs highly effective sensitizers for photocatalysis driven by visible light.

The main reason for the chemical functionalization of CNMs is to change the surface



chemistry to gain certain, desired properties for specific applications. This can be generally separated into two approaches:

Covalent Functionalization: This is the formation of strong chemical bonds between the attached functional group(s) and the carbon lattice.

Defect Creation and Derivatization: The most common routes for chemical functionalization typically involve oxidation of the CNMs (like strong acids), which will introduce reactive functional groups like carboxylic acids at non-aromatic defect spacing, which may be the ends of the tubes. After such groups are attached to a defective site, those groups can undergo standard organic reactions such as esterification, amidation or silanization resulting in covalent binding of polymers, biomolecules or ligands.

For example, the introduction of carboxylic acid groups increases water solubility, which is vital for biological applications such as drug delivery. Although the method is suitable for making stable covalent bonds, it often alters the electronic structure of the graphene sheet or CNT sidewall, which can compromise electrical conductivity, and this trade-off should be taken into consideration depending on the end-use application.

Sensing - CNMs can be turned into selective chemical sensors by attaching specific receptor molecules (through functional group). When the analyte interacts with the functional group on surface modification, a measurable alteration in the electrical properties or optical behavior of the nanomaterial can be observed.

Biomedicine - The functionalization of CNMs allows/houses bespoke drug loading, improved water solubility, targeting capabilities and lower cytotoxicity, which renders CNMs fair candidates in theranostic applications (therapy + diagnostics).



Energy Storage - The use of functional groups is beneficial to enhance the performance and charge transfer kinetics in batteries and supercapacitors by enhancing electrode-electrolyte interfaces.(Wang, 2021)

Literature Review

Astruc et al. (2020): Hybridization or composite formation is the process of forming composites of CBNMs with other materials, including metal oxides, some polymers (epoxy, polyurethane), and additional inorganic nanoparticles through the combination of the synergistic properties of the components. This approach might be considered the most common means of a practical application of CBNMs.

According to Zhang et al. (2022): Corrosion is a global phenomenon and cost-intensive challenge to infrastructure and industrial settings. Therefore, CBNMs that have been modified are transforming anti-corrosion coatings and inhibitors through two mechanisms of action; improved formation of physical barriers, and active protection.

According to Wang et al. (2021): When introduced into polymer matrix coatings temporarily (epoxy/polystyrene or similar), the increased aspect ratio of CBNMs (Graphene, CNTs) results in a mass path preventing the diffusion of species (water, oxygen, chloride) to the metal substrate.

According to Linic et al. (2020): Functionalization is important to ensure an even dispersion in the polymer system to minimize clustering, as this promotes the durability of the barrier layer in addition to the properties that CBNMs offer in mechanical strength, and improve scratch resistance of the coatings that inhibit mechanical exposure of metals to corroding agents and species.

Experimental procedure

Some carbon nanostructures also generally displayed pronounced surface plasmon resonance (SPR) effects, which will enhance light absorption. Although SPR is generally in noble metal nanoparticles, it is now understood that localized surface plasmon resonance (LSPR) in carbons or doped or defective forms of carbon can be engineered to absorb light at specific wavelengths. The high surface-to-volume ratio of CBNs in porous configurations creates a large area of interaction with incoming photons. The geometric feature enables a greater degree of light trapping and scattering effect which extends the effective length of the light path through the device (i.e. a solar cell) increasing the probabilities of absorption, over a broader spectrum of light.

Result and Discussion

Carbon-based nanomaterials offer an unprecedented opportunity for mechanical enhancement because they promise materials that can be engineered with superior properties that can provide a performance advantage.

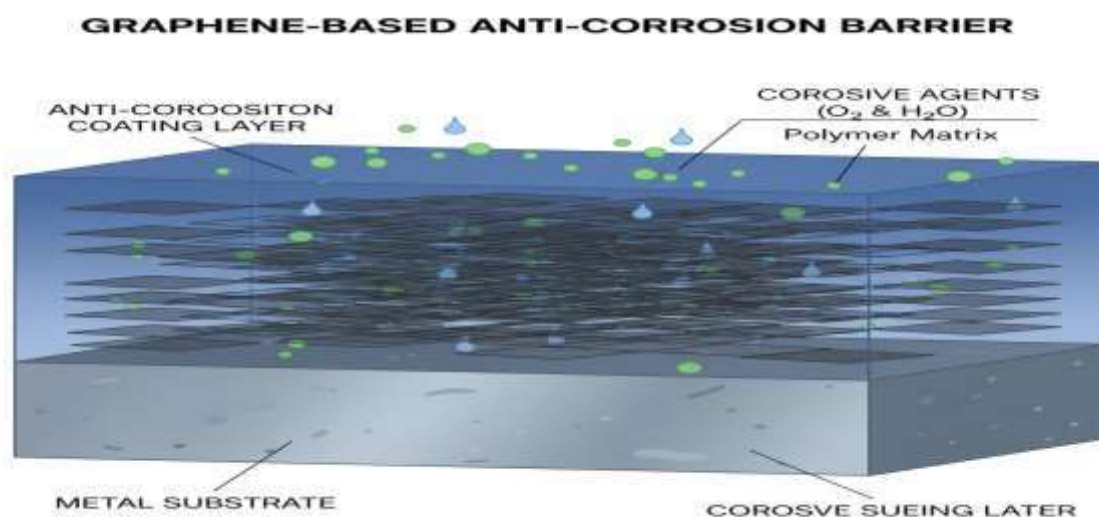
One of the key ways in which CBNs enhance light absorption is through their tunable band structures and unique quantum effects. In photocatalysis, conventional semiconductors such as titanium dioxide are combined with material such as graphene or carbon nanotubes which act as excellent electron acceptors and electron transporters. This method, utilizing a composite, not only allows for improved separation of photogenerated electron-hole pairs, but also, in addition to the prior example of the tuned band gap of CQDs, increased absorption of the composite material. Due to the near-zero bandgap and strong pi-electron conjugation, graphene has excellent absorption into high ranges of the solar spectrum.

It can capture photons that are generally bypassed by the main semiconductor catalyst before introducing these excited electrons into the conduction band of the semiconductor, essentially increasing the total light utilization from solar light.

In photovoltaics, carbon nanotubes (CNTs) have an interesting mechanism. In addition to being the charge transport material, certain arrangements of CNTs have been shown to induce a quantum effect, where it absorbs lower energy infrared light and re-emits it as higher energy visible light, in the latter case it is referred to up-conversion.

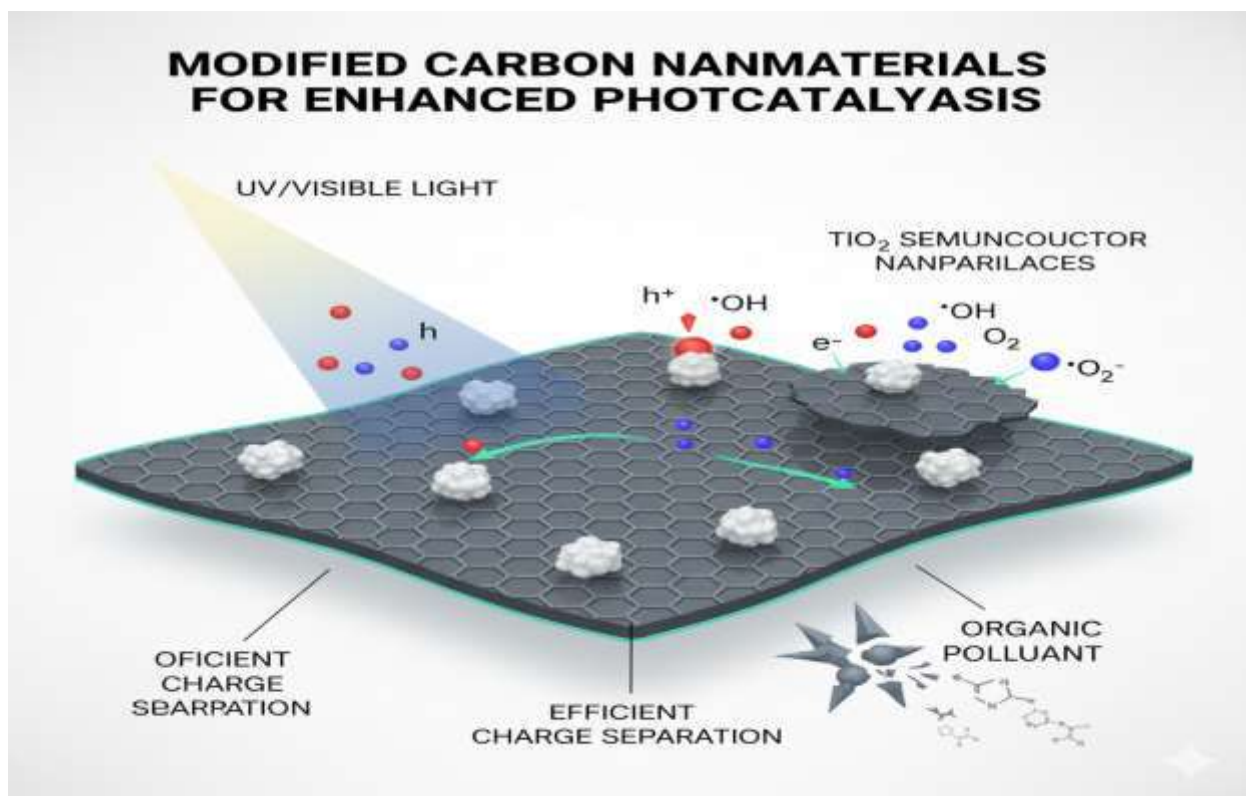
The capacity to convert typically wasted infrared light into valuable visible light holds tremendous potential for boosting the effectiveness of solar panels by capturing a previously unavailable region of the solar spectrum.

Although the inherent qualities of carbon nanomaterials are noteworthy, it is the chemical functionalization—the purposeful grafting of molecular handles—that allows these internal qualities to become customized, application-specific functionality. This surface engineering



is not just an optional step in the integration of CNMs into next-generation technologies, it is a required step.

The CBNs provide reinforcement not just as a simple addition but relies on a variety of



mechanisms on the nanoscale.

Conclusion

The modification of carbon-based nanomaterials is a clear example of the power of materials engineering and a compelling launching point for tuning properties to meet specific functional requirements. By carefully controlling their surface chemistry, electronic structure, and morphological integration into composites, researchers are modifying these building blocks into high-performing components. When it comes to anti-corrosion applications, modified CBNMs provide an advanced reliable, long-lasting mechanism of resistance through both passive barrier function and active self-healing capacity. Regarding photocatalysis, it has been demonstrated that CBNMs effectively facilitate charge transfer and enhance light harvesting, therefore increasing the efficiency of the environmental remediation and energy production processes. As sustainable synthetic protocols and scalability are establishing the way, modified carbon-based nanomaterials are emerging as core components towards developing next-generation materials for sustainable strategies.

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