



Atomistic Modeling of Graphene Oxide and Epoxy Resin Composite for Wind Turbine Applications

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Abstract

This study integrates classical all-atom molecular dynamics (MD) simulations and density functional theory (DFT) calculations to explore bisphosphate interactions in carbon fiber reinforced polymers (CFRP) composed of graphene oxide and epoxy resin for wind turbine applications. This research addresses the growing need for durable and reliable materials in renewable energy technologies. MD simulations reveal favorable interaction energies between bisphosphate and the graphene oxide/epoxy resin composite, suggesting improved molecular compatibility and structural stability. Radial distribution function (RDF) analysis and MD snapshots provide a detailed view of bisphosphate's spatial arrangements and interactions within the composite matrix. Complementary DFT calculations highlight optimized energy configurations and electronic structures, emphasizing bisphosphate's electron-donating and accepting capabilities. These findings underscore bisphosphate's potential to enhance the performance and resilience of graphene oxide and epoxy resin composites under demanding environmental conditions. By offering atomistic insights into material behavior, this study supports the development of advanced composite materials for wind turbine technologies, contributing to the sustainability and efficiency of renewable energy infrastructure. Further experimental validation is recommended to translate these computational findings into practical applications.

Keywords: Wind turbine; Graphene oxide; Epoxy resin; Composite material; Computational work.

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1. Introduction

Renewable energy sources, such as wind energy, offer significant advantages over traditional fossil energy sources, including coal, hydrocarbons, and petroleum. Unlike fossil fuels, which are finite and contribute to greenhouse gas emissions, renewable energy is sustainable, environmentally friendly, and reduces carbon footprints. Renewable energy technologies play a critical role in advancing sustainable energy solutions, encompassing a range of applications such as batteries, capacitors, solar cells, and fuel cells.^[1-9] Wind energy, in particular, is a clean and abundant resource, making it a key component in the transition toward a low-carbon economy. These benefits underscore the importance of

developing advanced materials, such as graphene oxide and epoxy resin composites, to enhance the performance and durability of wind turbine applications. The rapid expansion of wind energy, with its capacity doubling approximately every three years, highlights its position as one of the fastest-growing renewable energy sources.

This impressive growth trajectory is especially prominent in regions such as Europe, North America, China, India, and other developing nations. As the global transition to sustainable energy accelerates, wind power is set to become a cornerstone of future energy systems. At the heart of this renewable revolution are wind turbines, which harness kinetic energy from wind to produce electricity. Unlike traditional windmills used for mechanical tasks, modern wind turbines are designed to generate electricity on a large scale, often as part of wind farms consisting of multiple turbines.^[10-15]

Wind turbines are classified based on their axis of rotation (horizontal or vertical), power generation capacity, and installation location (onshore or offshore). Horizontal axis wind turbines (HAWTs) are the most prevalent type, characterized by blades that rotate parallel to the wind

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direction. HAWTs offer significant advantages, including high efficiency, increased power density, and cost-effective energy production, making them the preferred choice for large-scale applications. In contrast, vertical axis wind turbines (VAWTs) can capture wind from any direction without requiring a yaw control system, which simplifies tower design and construction. This makes VAWTs suitable for specific environments, such as urban settings or areas with variable wind directions.^[16-20]

Offshore wind farms are gaining traction due to the higher wind speeds and more consistent wind availability over open water, which results in reliable and efficient power generation. However, offshore installations also present unique challenges, including higher production and maintenance costs, as well as technical complexities related to marine environments. Onshore turbines, while easier to install and maintain, must contend with varying wind patterns and land-use constraints. Despite these advancements, wind energy faces challenges such as intermittent wind availability, the need for optimized aerodynamic designs to maximize energy capture, and the high initial costs of turbine production and maintenance. Overcoming these obstacles requires continued innovation in turbine technology, materials, and energy storage solutions. As wind energy technology evolves, it holds tremendous potential to contribute to a sustainable and decarbonized energy future, addressing both global energy demands and environmental concerns.^[14-23]

The development of graphene oxide (GO)-epoxy resin composites presents an innovative approach to overcoming challenges in material performance and sustainability. GO, synthesized using environmentally friendly solvents like Deep Eutectic Solvents (DES), offers several advantages over traditional organic solvents. These include lower cost, reduced toxicity, and biodegradability, making DES a sustainable alternative for GO production.^[10-21] When incorporated into epoxy resin matrices, GO enhances critical properties, such as mechanical strength, electrical conductivity, and thermal stability. These improvements enable better heat dissipation and increased structural reliability, making GO-epoxy composites highly suitable for demanding applications.^[22-32] According to the literature, significant efforts have been made to enhance the interfacial microstructure and properties of carbon fiber-reinforced unsaturated polyester composites, including approaches such as chemically grafting carbon nanotubes onto carbon fibers using poly(acryloyl chloride) and utilizing sizing agents containing carbon nanotubes to improve interfacial strength.^[33-36]

Wind turbine blades are predominantly made from composite materials due to their favorable mechanical properties, which include high strength-to-weight ratios and resistance to environmental degradation. The most common composites are summarized in Table 1.^[37-41]

Table 1 highlights the diverse applications of composite materials in wind turbines, emphasizing their tailored properties for specific needs. Glass fiber composites are

widely used for cost-effectiveness in small to medium turbines, while carbon fiber composites enable longer blades in large turbines due to their high strength-to-weight ratio. Aramid fiber composites offer excellent impact resistance, ideal for applications requiring toughness, whereas basalt fiber composites provide a lightweight, stronger alternative to glass fibers, gaining popularity in emerging designs. Hybrid composites leverage multiple fiber properties, enabling advanced, weight-efficient turbine designs.^[28-41] This underscores the need for innovative composites, like GO-epoxy systems, for next-generation turbines. Unlike previous research focusing on traditional composites like glass, carbon, or hybrid fibers, this study leverages atomistic modeling to explore the unique properties of GO-epoxy resin composites. Recent studies have primarily investigated macroscopic properties or simpler epoxy systems, whereas our work provides detailed molecular-level insights into the structure-property relationship of these advanced composites. This approach not only bridges the gap in understanding but also offers a pathway for optimizing materials for enhanced performance in wind turbine applications.

Table 1: Application of composite materials in wind turbines.

Material type	Properties	Applications	Ref.
Glass Fiber Composites	Cost-effective, moderate strength	Common in small to medium-sized wind turbines	[37]
Carbon Fiber Composites	High strength-to-weight ratio	Large turbines require longer blades	[38]
Aramid Fiber Composites	Excellent impact resistance	Specialized applications where toughness is critical	[39]
Basalt Fiber Composites	Stronger and lighter than glass fibers	Emerging applications in small wind turbines	[40]
Hybrid Composites	Combination of properties from different fibers	Used in advanced turbine designs for weight savings	[41]

This study utilizes classical all-atom molecular dynamics (MD) simulations and density functional theory (DFT) calculations to investigate the molecular interactions within GO/epoxy resin composites, with a focus on bisphosphate molecules. By exploring these interactions at the atomic level, the research seeks to optimize the integration of GO into epoxy matrices. The findings are particularly relevant for wind turbine applications, where material durability and performance are paramount.

The incorporation of GO into epoxy composites has the potential to significantly enhance the lifespan and efficiency of wind turbine components. These improvements align with the growing demand for sustainable and reliable renewable energy solutions. By enhancing the mechanical and thermal properties of the composite materials, the study contributes to

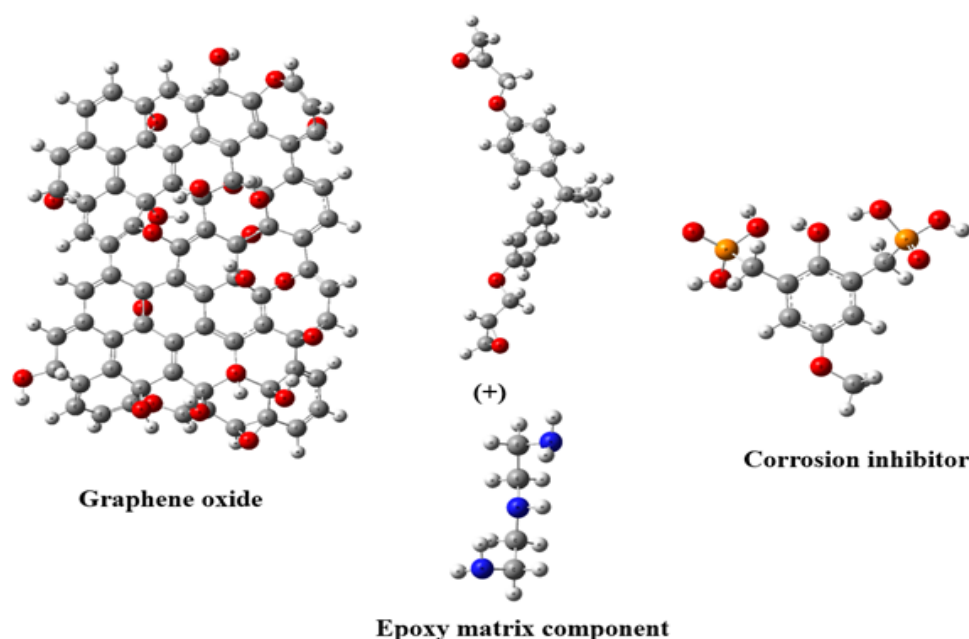


Fig. 1: Representations of GO, epoxy matrix components, and corrosion inhibitor. Color key: white (hydrogen); orange (phosphorus); grey (carbon); blue (nitrogen); and red (oxygen).

the development of wind energy technologies capable of withstanding the harsh environmental conditions turbines often face.

Ultimately, this research supports the advancement of sustainable energy technologies by providing atomistic insights that inform the design of more resilient materials. The integration of GO into epoxy resin composites not only improves material performance but also promotes environmentally friendly practices in material synthesis, aligning with global efforts to transition to a greener energy future. These advancements in material science are critical for ensuring the efficiency, reliability, and sustainability of wind energy systems.

2. Materials and methods

2.1 Theoretical models

A small segment representing GO, EPON-828, diethylenetriamine (DETA), and bis-phosphonic acid was chosen as the theoretical model for the GO, composite GO, and epoxy resin, and corrosion inhibitor component for classical all-atom MD simulations and DFT calculations, as can be seen in Fig. 1.

Fig. 1 provides visual representations of key components central to this study, including GO and the components of the epoxy resin matrix. The figure illustrates the specific molecular structures and arrangements crucial to understanding the processes investigated in this research. Additionally, Fig. 1 includes the structure of GO itself, offering insights into its atomic arrangement and functional groups. Understanding these structural characteristics is essential for evaluating GO's compatibility and interactions within the epoxy resin matrix.

The epoxy resin matrix, as a critical component of composite materials, is studied in conjunction with GO to assess their combined suitability for wind turbine applications. By providing a detailed visualization of the molecular configurations and interactions, Fig. 1 highlights the integration of GO into the epoxy resin matrix and its potential to enhance the mechanical, thermal, and structural properties of composite materials, which offers a comprehensive overview of the molecular structures and configurations relevant to this study, focusing on the structure of GO and its integration with the epoxy resin matrix for advanced composite applications in wind turbine technologies.

The GO layer has a sheet size of approximately 14.80 Å in length and 10.04 Å in width. The ratio of EPON-828 to DETA in the epoxy resin used in the simulations is 5:2, providing essential details for understanding the chemical structure of the polymer matrix. Chloride ions were selected for this study due to their corrosive nature, which is crucial for understanding their impact on the system's stability and interactions within the polymer matrix. GO serves as the nanoscale filler in the composite, while bis-phosphonic acid acts as an anticorrosive protective coating. EPON-828 is an undiluted, clear, difunctional bisphenol A/ A/epichlorohydrin-derived liquid epoxy resin monomer, and diethylenetriamine (DETA) functions as the curing agent. Together, EPON-828 and DETA form the epoxy resin matrix, which enhances the composite's mechanical and chemical stability.

2.2 Classical all-atom MD simulations

In classical all-atom MD simulations, the potential energy of the system is fundamentally determined by the positions of the atoms. This potential energy serves as a crucial input for

initiating molecular dynamics simulations, as it defines the forces acting on the molecules in Eq. (1).

$$V_{\text{TOT}} = V_{\text{TOT}}(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N) \quad (1)$$

Subsequently, the forces on each atom can be derived from the potential energy function, and the acceleration can be determined using Newton's second law (Eq. (2)). According to Newton's second law, the force acting on a particle is equal to the product of its mass and acceleration.

$$\vec{F}_i = -\frac{\partial V_{\text{TOT}}}{\partial \vec{r}_i} = m\vec{a}_i = m\frac{\partial^2 \vec{r}_i}{\partial t^2} \quad (2)$$

From Eq. (2), the forces are determined based on the potential energy. This process results in a large set of coupled second-order ordinary differential equations, as each atom contributes to the system. By applying variable transformations, these second-order equations can be simplified into first-order ordinary differential equations, which can then be solved using numerical algorithms.

Fig. 1 depicts a segment model representing GO, EPON-828, DETA, and bisphosphonic acid. The model illustrates the formation of GO and its integration with the epoxy matrix, which are crucial aspects for understanding their potential application in wind turbine technologies. To establish the molecular configurations, Lennard-Jones (LJ) parameters were derived from the GROMOS force field, while force field parameters (including dihedrals, angles, bonds, and partial charges) and coordinates for functional groups were sourced from the ATB database.^[40-44]

Representative sections of the GO (2 molecules)/epoxy matrix (215 molecules of EPON-828 and 86 molecules of DETA) systems were set up for MD simulations. The energy optimization process involved initial configuration optimization using the steepest descent approach for 0.1 ns. This was followed by NPT and NVT equilibrations for 1 ns each at 298 K and 1 bar pressure, resulting in an equilibrated box size of $8 \times 8 \times 8 \text{ nm}^3$. Subsequently, MD simulations were conducted under the NVT ensemble for 10 ns at 298 K and 1 bar after achieving equilibrium. During the simulations, all bonds were constrained using the LINCS algorithm, and a 1.0 nm cut-off was applied for coulombic short-range interactions and LJ interactions. Long-range interactions were calculated using Particle Mesh Ewald summation with fourth-order interpolation and a 0.16 nm grid spacing. Temperature control utilized the V-rescale technique while pressure was maintained using Berendsen pressure coupling.^[44,45] Periodic boundary conditions were applied in all directions.

The MD simulations were performed using the GROMACS software.^[46] This detailed simulation and analysis approach provides valuable insights into the interactions and behaviors of the GO and epoxy matrix systems, contributing to advancements in wind turbine technology.

2.3 DFT calculations

The Schrödinger equation is shown in Eqs. (3) and (4) serve

as the foundation of quantum mechanics (QM) for systems consisting of multiple atoms.

$$H \times \psi(\{r_i \dots\}, \{R_i \dots\}) = E \times \psi(\{r_i \dots\}, \{R_i \dots\}) \quad (3)$$

$$H = \hat{T} + \hat{V} \quad (4)$$

where H is the Hamiltonian operator, ψ is the wave function, E is the energy, r_i is the position of electrons, and R_i is the position of the nucleus.

Next, the concept of electron density, derived from DFT, plays a crucial role. DFT methods, widely utilized in computational chemistry, are primarily based on approximate solutions to the Schrödinger equation. The electron density, which is a three-dimensional quantity, is defined in terms of the wave function as shown in Eq. (5).

$$n(r) = \psi(\{r_i\}) * \psi(\{r_i\}) \quad (5)$$

After Hohenberg and Kohn theorems, Eq. (3) can be rewritten as Eq. (6):

$$\left[\frac{-\hbar^2}{2m_i} \nabla^2 + V(r) + V_H(r) + V_{XC}(r) \right] \psi_i(r) = \varepsilon_i * \psi_i(r) \quad (6)$$

where $\frac{-\hbar^2}{2m_i} \nabla^2$ is kinetic energy term, $V(r)$ is potential energy term, and $V_H(r)$ is Hartree potential, $V_{XC}(r)$ is exchange correlation potential.

The Kohn-Sham iteration method forms the foundation of most DFT calculations and is employed to solve the aforementioned Eq. (6).

For our DFT calculations, we employed the B3LYP functional,^[47] which has been validated in the literature as accurate for estimating binding energies in systems similar to ours. The results obtained from DFT calculations were verified by their consistency with the outcomes from classical all-atom MD simulations, providing cross-validation between computational methods. Future work will include experimental validation to map these computational results.

In our DFT calculations, we modeled a typical structure of epoxy resin and bisphosphonic acid, as depicted in Fig. 1. The investigation focused on both covalent and noncovalent interactions within the composite material. Utilizing the B3LYP/6-311++G(d,p) level of theory, we fully optimized the intermolecular interactions of the graphene oxide/epoxy resin composite system, analyzing its structural and electronic properties in the water phase.

Quantum chemical features were acquired after optimization in the water phase to better understand the intermolecular interactions within the composite. Analytical computation of the second energy derivatives confirmed all stationary points as authentic minima on their respective potential energy surfaces. Gaussian16 was utilized for DFT calculations to compute electronic ground state geometries.^[48] This comprehensive computational approach provides valuable insights into the structural and electronic characteristics of graphene oxide/epoxy resin composites, offering a foundation for advancing their applications in

material science.

3. Results and discussion

3.1 Classical all-atom MD simulation results

The interaction energies derived from classical all-atom Molecular Dynamics simulations offer valuable insights into the enhancement of graphene oxide-epoxy composite materials for structural applications.

Fig. 2 presents snapshots from classical all-atom MD simulations, illustrating the graphene oxide-epoxy matrix within the composite under two different conditions: (A) in the absence of a protective layer and (B) in the presence of a protective layer. In panel A, the absence of a protective layer allows for direct exposure of the epoxy matrix and graphene oxide layers to external environmental factors, potentially leading to material degradation. Without protection, external agents can interact with the matrix, weakening the bonding interface between the graphene oxide and epoxy.

In contrast, panel B demonstrates the reinforcing effect of a protective layer. In this case, the protective layer forms a barrier around the matrix, reducing the interaction between external factors and the epoxy-graphene oxide interface. This protection helps preserve the composite's structural integrity and enhances its overall durability, ensuring greater stability over extended

periods in harsh conditions. These simulations underscore the significance of protective layers in enhancing the longevity and performance of graphene oxide-epoxy composites in challenging environments.

Table 2 presents the interaction energies for the graphene oxide-epoxy composite, focusing on the interactions between GO, epoxy matrix components (EPON-828 and DETA), and the inclusion of a bis-phosphonic acid. In the absence of chloride media, the interaction energies within the composite components exhibit distinct patterns. The interaction energy between GO and GO within the composite is positive at 734.32 kJ/mol, indicating a favorable interaction between GO layers, suggesting a cohesive arrangement of GO sheets within the epoxy matrix.

The interactions between GO and the epoxy matrix components EPON-828 and DETA show negative energies of -1255 kJ/mol and -134.88 kJ/mol, respectively. These negative energies suggest strong interactions between GO and the epoxy matrix, indicating good compatibility and adhesion between the GO and epoxy matrix components. The interaction energy between EPON-828 and DETA within the composite is significantly negative at -6322.338 kJ/mol, highlighting the strong bonding and interaction between these epoxy resin components within the matrix. When exposed to

Table 2: Interaction energy for the graphene oxide-epoxy composite in the absence and presence of chloride environments.

Interactions	Energy (kJ/mol, SE)
GO and GO (Composite)	734.32 (± 22.65)
GO and EPON-828 (Composite)	-1255 (± 36.31)
GO and DETA (Composite)	-134.88 (± 3.07)
EPON-828 and DETA (Composite)	-6322.338 (± 165.82)
GO and GO (Composite + Chlorine ion)	735.45 (± 20.94)
GO and EPON-828 (Composite + Chlorine ion)	-749.44 (± 18.43)
GO and DETA (Composite + Chlorine ion)	-131.43 (± 2.69)
EPON-828 and DETA (Composite + Chlorine ion)	-6423.06 (± 173.58)

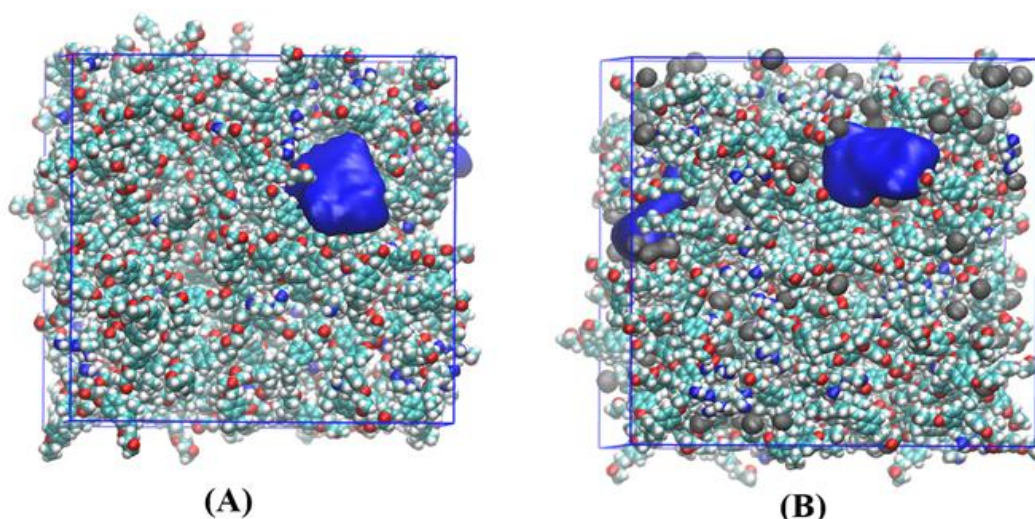


Fig. 2: Snapshot of the graphene oxide-epoxy matrix materials from classical all-atom MD simulations, showing (A) the matrix in the absence of a bis-phosphonic acid and chlorine environment, and (B) the matrix in the presence of a bis-phosphonic acid and chlorine environment. Color key: white (hydrogen); orange (phosphorus); grey (carbon); blue (nitrogen); and red (oxygen). The blue isosurface in the MD simulation box illustrates the graphene oxide sheet.

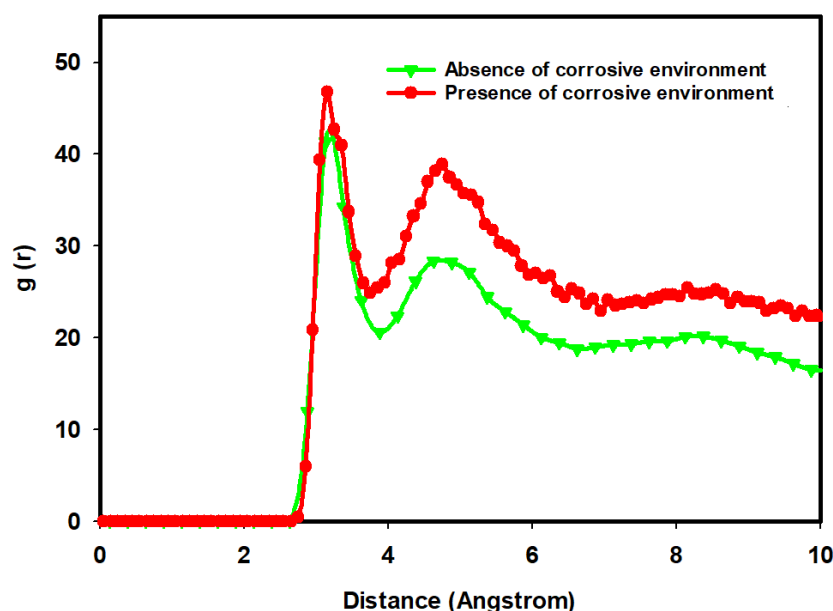


Fig. 3: Radial distribution function between EPON-828 and DETA before and after the addition of a corrosive environment.

specific environmental conditions, the interaction energies show slight variations compared to the baseline setup.

The interaction energies for GO and GO within the composite remain similar in the presence of chloride media, indicating a stable arrangement of GO layers even under chloride conditions. Similarly, the interactions between GO and the epoxy matrix components, as well as between EPON-828 and DETA, show resilience to the corrosive (chloride) environment with minimal changes in interaction energies.

These results suggest that the inclusion of an anticorrosive agent effectively mitigates the effects of the chloride media on the interactions within the composite, maintaining the structural integrity and stability of the composite material. The strong interactions between GO and the epoxy matrix components, both in the absence and presence of chloride, indicate the potential of GO-based composites with protective coatings for applications in environments with corrosive challenges, such as wind turbine applications.

The interaction energy analysis provides valuable insights into the stability and performance of GO-based composites in chloride environments, supporting the optimization of protective coatings and enhancing the durability of composite materials for wind turbine applications.

Fig. 3 illustrates the Radial distribution function (RDF) between EPON-828 and DETA before and after the addition of a corrosive (chloride) environment, specifically focusing on the changes in molecular interactions within the epoxy matrix components under different conditions. In the absence of a chloride environment, the RDF peak between EPON-828 and DETA is observed around 40 at 3 Angstrom, indicating a strong correlation and proximity between these molecules within the epoxy matrix. This peak suggests a well-defined spatial arrangement and interactions between EPON-828 and DETA molecules, characteristic of a stable and cohesive polymer matrix.

Upon the addition of a chloride ion environment, the RDF peak shifts to around 50 4 angstroms for EPON-828 and DETA. This shift in the RDF peak position reflects changes in the molecular interactions within the epoxy matrix components in response to this environment. The increase in the RDF peak position and intensity suggests a broader spatial distribution and slightly weakened interactions between EPON-828 and DETA molecules when exposed to chloride ion. This can be attributed to the influence of the chloride ion on the molecular dynamics and arrangement of the epoxy matrix components.

The observed changes in the RDF peak position and shape indicate a moderate disruption or alteration in the intermolecular interactions within the epoxy matrix due to the presence of corrosive media. However, it's noteworthy that the peak remains prominent, indicating that despite the influence of the corrosive environment, the interactions between EPON-828 and DETA molecules within the epoxy matrix are still significant and structurally meaningful.

These findings suggest that while environmental conditions can lead to slight modifications in the molecular interactions within the epoxy matrix components, the overall structural integrity and stability of the matrix are maintained to a considerable extent. This resilience is crucial for ensuring the effectiveness of protective materials, such as Graphene Oxide (GO)-based composites, in challenging environments. Fig. 3 provides valuable insights into the impact of these conditions on the molecular interactions within the epoxy matrix components, highlighting the adaptive nature of these materials and emphasizing the importance of optimizing protective coatings for enhanced durability and performance. Table 3 presents the interaction energies for the graphene oxide-epoxy composite, focusing on the interactions between GO, epoxy matrix components (EPON-828 and DETA), and bisphosphonic acid (BPA). The interaction energies reveal

important insights into the effectiveness of bisphosphonic acid (BPA) and its impact on the molecular interactions within the graphene oxide-epoxy composite material.

The interaction energy between GO and BPA within the composite is -197.12 kJ/mol, indicating a favorable interaction between GO and the bisphosphonic acid. This suggests that BPA can effectively bind to GO within the composite material, potentially forming a protective layer or modifying the surface properties. The interaction energies between EPON-828 and BPA, as well as between DETA and BPA, show values of -1824.64 kJ/mol and -277.34 kJ/mol, respectively. These negative energies signify strong interactions between the epoxy matrix components and BPA, highlighting the ability of BPA to bond with the polymer matrix, potentially enhancing its structural integrity.

Table 3: Interaction energy for CFRP with bisphosphonic acid (BPA) in the presence of various environments.

Interactions	Energy (kJ/mol, SE)
GO and BPA (Composite + Chloride)	-197.12 (± 4.25)
EPON-828 and BPA (Composite + Chloride)	-1824.64 (± 24.63)
DETA and BPA (Composite + Chloride)	-277.34 (± 8.67)

The presence of bisphosphonic acid (BPA) in the composite material leads to favorable interactions between GO, epoxy matrix components, and BPA. This suggests that BPA effectively contributes to the stability and protection of the composite material under challenging conditions. The negative interaction energies between BPA and the components of the composite indicate the potential of BPA to enhance the durability and performance of the material. By forming strong bonds with GO and the epoxy matrix components, BPA may help reinforce the material's structure and reduce the risk of degradation.

Table 3 underscores the role of BPA in enhancing the performance and longevity of the composite. The favorable interaction energies between BPA, GO, and epoxy matrix components highlight the potential of BPA-based treatments or coatings to improve the overall stability and effectiveness of the composite material in various applications.

3.2 DFT calculation results

The integration of atomistic modeling techniques in the development of GO-enhanced epoxy resin composites marks a significant step forward in understanding the interaction mechanisms within these advanced materials. This study employs DFT calculations to optimize the structural and electronic properties of the epoxy resin components, EPON-828 and DETA, in combination with bisphosphonic acid as an additive, under varying conditions.

Fig. 4 presents the optimized molecular structures of bisphosphonic acid, epoxy resin supported by bisphosphonic

acid, and the epoxy resin-bisphosphonic acid complex in the presence of graphene oxide. The optimization reveals that the components of the epoxy resin preferentially orient themselves around the phosphorus atoms of bisphosphonic acid. This alignment suggests a strong interaction between the resin and bisphosphonic acid, highlighting the role of phosphorus-centered bonding as a key factor in stabilizing the composite structure.

These interactions are crucial for enhancing the integration of graphene oxide within the epoxy resin matrix. By promoting a uniform distribution and robust binding of graphene oxide to the resin, bisphosphonic acid effectively bridges the gap between organic and inorganic components of the composite. This enhanced integration can lead to notable improvements in the material's structural integrity and electronic properties.

The presence of bisphosphonic acid appears to create an environment conducive to better dispersion and adhesion of graphene oxide. This is particularly important in applications where mechanical strength, thermal stability, or electrical conductivity are critical. The phosphorus atoms may also facilitate additional electrostatic or covalent interactions with graphene oxide, further solidifying the composite's network structure.

These findings underscore the significance of molecular-level interactions in designing advanced composite materials. By leveraging the affinity of epoxy resin components for bisphosphonic acid, and subsequently for graphene oxide, this approach offers a pathway to developing materials with superior performance. Future studies could explore how modifications to bisphosphonic acid, such as functionalization or doping, might further enhance these interactions and expand the utility of such composites in fields ranging from aerospace to electronics.

The presence of chloride ions introduces a new dynamic, where the chloride ions are situated between the nitrogen atoms of the epoxy resin and the oxygen atoms of the graphene oxide. This positioning indicates a potential vulnerability in the resin-GO complex, where chloride ions could disrupt the interaction between the resin and graphene oxide, potentially compromising the stability of the composite. However, the structural integrity observed in the complex suggests that the material remains relatively stable, indicating the resilience of the graphene oxide-epoxy resin system even in challenging environments.

The molecular electrostatic potential (MEP) maps presented in Fig. 5 offer further insights into the charge distribution within the graphene oxide, the epoxy resin-graphene oxide complex, and their interaction in the presence of chloride ions. The MEP maps highlight areas of electron density and potential sites for nucleophilic and electrophilic attack, which are crucial for understanding the interaction mechanisms at the atomic level.

In the graphene oxide (Fig. 5A), the MEP map indicates a significant electron density around the oxygen atoms, making

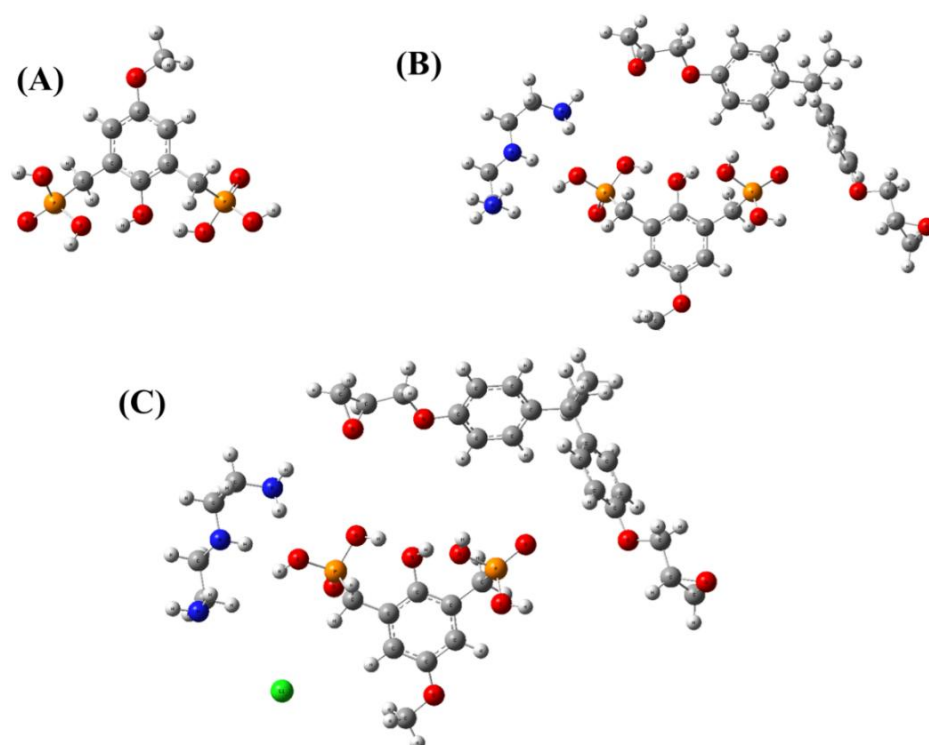


Fig. 4: Optimized structures of (A) bis-phosphonic acid, (B) epoxy resin supported by bis-phosphonic acid, and (C) epoxy resin supported by bis-phosphonic acid in the presence of chloride. Color key: white (hydrogen); orange (phosphorus); grey (carbon); green (chloride); blue (nitrogen); and red (oxygen).

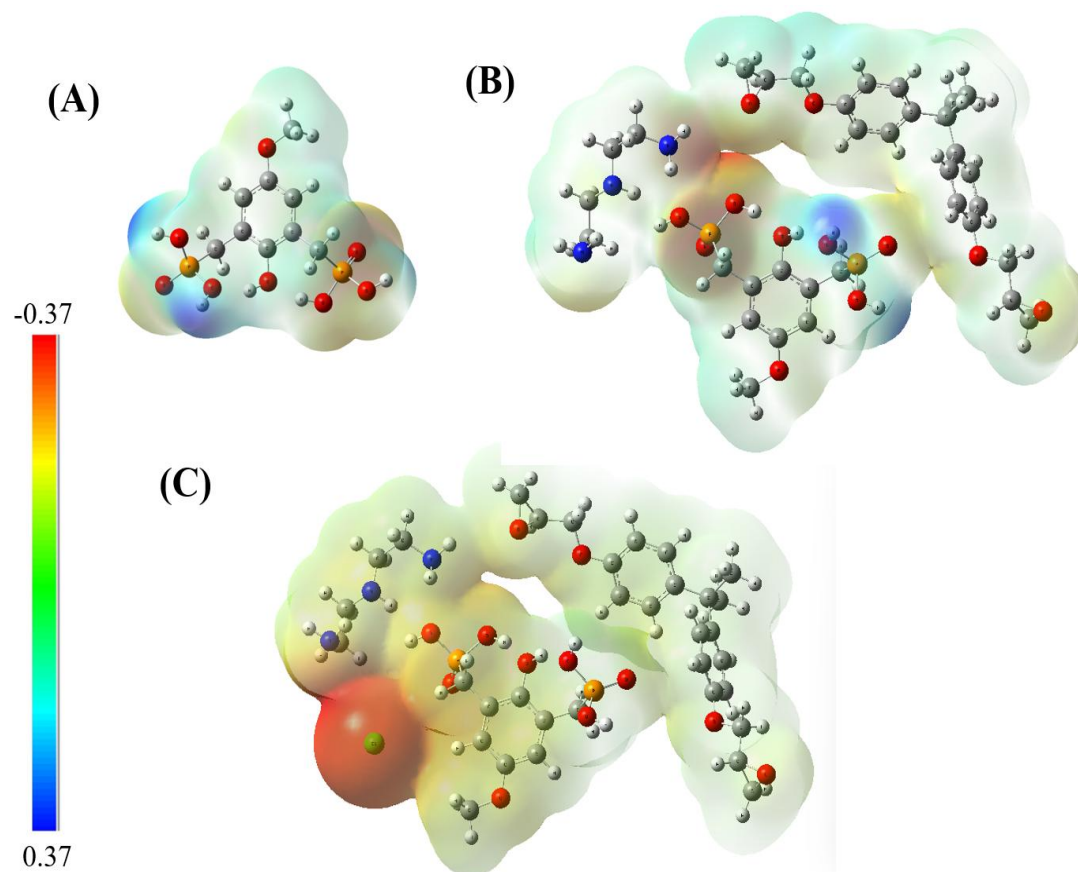


Fig. 5: Molecular electrostatic potential maps of (A) bis-phosphonic acid, (B) epoxy resin supported by bis-phosphonic acid, and (C) epoxy resin supported by bis-phosphonic acid in the presence of chloride. Color key: white (hydrogen); orange (phosphorus); grey (carbon); green (chloride); blue (nitrogen); and red (oxygen).

these sites potential interaction points with the epoxy resin. When the epoxy resin is supported by graphene oxide (Fig. 5B), the electron density is distributed more evenly across the complex, particularly around the oxygen and nitrogen atoms. This distribution suggests a synergistic interaction where the electron-donating and electron-withdrawing groups of the epoxy resin and graphene oxide, respectively, stabilize the complex.

The addition of chloride ions (as shown in Fig. 5C) induces a significant delocalization of charge around both the chloride ions and the oxygen atoms of graphene oxide. This observation highlights an active interaction between chloride ions and the epoxy resin-graphene oxide complex, suggesting their potential to influence the system's electronic environment. The redistribution of charge indicates that chloride ions are not merely passive entities in the mixture but actively engage with the functional groups of the complex. This interaction could lead to localized variations in the electrostatic potential of the system. Such variations might play a critical role in modulating the binding affinity between the epoxy resin and graphene oxide. Depending on the surrounding environmental conditions, these electrostatic effects may either strengthen or weaken the adhesion between these components.

The ability of chloride ions to influence the electronic properties of the epoxy resin-graphene oxide system opens

new possibilities for tailoring material behavior in applications where specific adhesion or conductivity properties are required. For instance, in anti-corrosion coatings or composite material development, manipulating the concentration of chloride ions might enable precise control over the system's performance.

Moreover, understanding this interaction at a molecular level provides insights into the broader implications of charge redistribution in multi-component systems. It underscores the importance of considering ionic contributions in designing materials with desired structural and electronic characteristics. Future studies could explore how variations in chloride ion concentration, temperature, or solvent conditions further impact these interactions, potentially unlocking new functionalities in advanced material systems.

The frontier molecular orbitals, specifically the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), provide critical insights into the electronic properties and stability of the molecular systems studied. Fig. 6 presents the HOMO-LUMO orbitals for graphene oxide, the epoxy resin supported by graphene oxide, and the epoxy resin-graphene oxide complex in the presence of chloride ions.

For graphene oxide, the HOMO is localized around the oxygen atoms, with a value of -6.30 eV, while the LUMO is distributed across the entire molecule with a value of -1.04 eV.

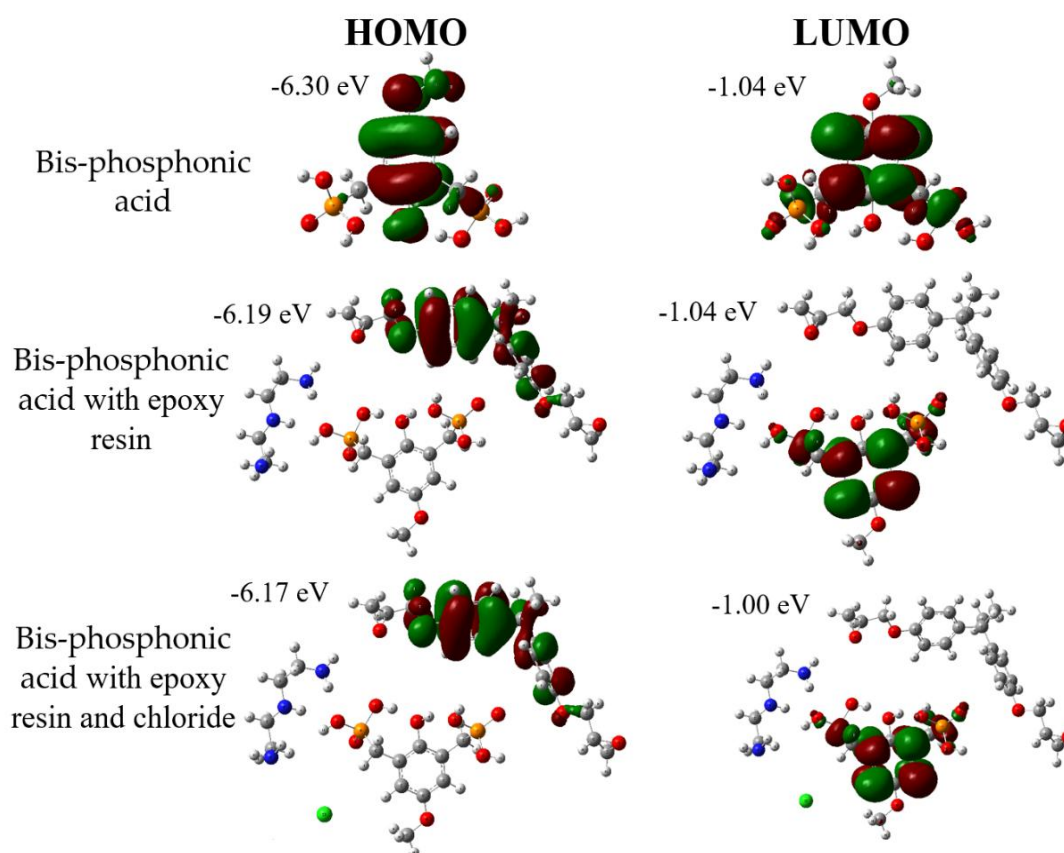


Fig. 6: HOMO-LUMO orbitals of bis-phosphonic acid, epoxy resin supported by bis-phosphonic acid, and epoxy resin supported by bis-phosphonic acid in the presence of chloride. Color key: white (hydrogen); orange (phosphorus); grey (carbon); green (chloride); blue (nitrogen); and red (oxygen).

This distribution suggests that graphene oxide has a strong potential for electron donation, particularly in interactions involving aromatic systems.

In the graphene oxide-epoxy resin complex, the HOMO value slightly increases to -6.19 eV, indicating a slight reduction in electron-donating capability, which is expected due to the interaction with the epoxy resin. The LUMO remains unchanged at -1.04 eV, but its distribution shifts to be more localized around the oxygen atoms of graphene oxide, suggesting that the epoxy resin modifies the electronic environment of the graphene oxide, possibly enhancing its ability to accept electrons from potential external agents.

When chloride ions are introduced, the HOMO value further increases to -6.17 eV, and the LUMO decreases slightly to -1.00 eV. The HOMO remains localized around the epoxy resin, while the LUMO remains around the graphene oxide. This shift in electronic properties indicates that chloride ions influence the electron distribution within the complex, potentially enhancing the complex's reactivity and its ability to interact with external corrosive agents.

The findings from this study have significant implications for the development of advanced composites for structural applications, particularly in environments exposed to chloride ions. The interaction between the epoxy resin and graphene oxide demonstrates that graphene oxide can serve as an effective reinforcing agent, enhancing the overall stability and mechanical properties of the composite material.

While the resin-graphene oxide complex shows resilience in the presence of chloride ions, the potential for charge delocalization and alterations in electronic properties could impact the long-term stability and effectiveness of the composite material. These findings suggest that graphene oxide is a promising reinforcing material, but further optimization may be needed to enhance its performance in chloride-rich environments.

Future research could focus on modifying the chemical structure of graphene oxide or the epoxy resin to improve the stability and durability of the composite. Additionally, experimental validation of these findings would provide valuable insights into the practical applications of these composites in demanding environmental conditions.

This study offers a detailed atomistic understanding of the interactions between epoxy resins and graphene oxide, which are critical for developing advanced composite materials. The DFT calculations reveal the strong interaction between the epoxy resin components and graphene oxide, highlighting the resilience of this interaction. However, the potential impact of charge delocalization on the electronic properties suggests that further optimization is needed to ensure long-term performance. These insights provide a foundation for future advancements in composite materials, contributing to their reliability and efficiency in challenging environments.

In line of the computational findings presented in this study, it is imperative to contextualize these results within the framework of existing experimental research. Recent studies

have demonstrated significant improvements in the mechanical properties of GO/epoxy resin composites, aligning with our simulation results. For instance, recent works reported that incorporating functionalized graphene into epoxy matrices resulted in a 77% increase in tensile strength and a 56% enhancement in flexural strength compared to pure epoxy resin.^[49-52] These experimental observations corroborate our MD simulations, which indicated favorable interaction energies between bisphosphate and composite components, suggesting enhanced interfacial bonding that contributes to improved mechanical performance. Furthermore, the findings from other research groups highlight graphene's role in reinforcing wind turbine blades by significantly enhancing their strength and durability under harsh operational conditions.^[53-56] This synergy between computational predictions and experimental validations not only reinforces the potential of bisphosphate-enhanced GO/epoxy composites but also underscores their applicability in advancing wind energy technologies. By bridging these computational insights with empirical data, we strengthen the argument for further exploration and optimization of graphene-based materials for wind turbine applications.

4. Conclusion

In conclusion, the combined use of classical all-atom MD simulations and DFT calculations provides valuable insights into the role of bisphosphate in GO/epoxy resin composites for wind turbine applications. MD simulations reveal favorable interaction energies between bisphosphate and the composite components, suggesting its ability to enhance interfacial interactions and maintain structural integrity. Detailed analysis through RDF profiles and simulation snapshots further illustrates the molecular arrangements and stability of bisphosphate within the composite matrix.

Additionally, DFT calculations highlight the optimized energies and electronic structures of bisphosphate, emphasizing its dual electron-donating and accepting capabilities. These electronic properties are crucial for improving the mechanical, thermal, and electrical performance of GO/epoxy resin composites. Together, the MD and DFT results underline the potential of bisphosphate to enhance the durability and reliability of these composites, making them suitable for the harsh operational conditions of wind turbine components.

This study underscores the significance of bisphosphate-based treatments in advancing the performance of GO/epoxy composites, contributing to the sustainability and efficiency of wind energy technologies. The findings provide a foundation for optimizing composite materials to meet the demands of renewable energy infrastructure. Further experimental validation and material optimization are recommended to bridge the gap between computational predictions and practical applications, ultimately promoting the adoption of bisphosphate-enhanced materials in next-generation wind turbine systems.

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Conflict of Interest

There is no conflict of interest.

Supporting Information

Not applicable.

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