

DENSITY FUNCTIONAL THEORY STUDY OF THE MOLECULAR INTERACTIONS IN POLYETHYLENE–GELATIN–WATER BIOCOMPOSITES

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Abstract.

This study investigates the molecular interactions within polyethylene–gelatin–glycerol biocomposites using density functional theory (DFT) calculations. The research focuses on intermolecular interactions, adsorption behavior, and electronic properties to evaluate the compatibility and stability of the composite system. FTIR spectral analysis identifies characteristic peaks for gelatin, glycerol, and maleic anhydride-grafted polyethylene (MPE), confirming the formation of hydrogen bonds and interfacial crosslinking. Calculated interaction energies and electronic structure analysis indicate strong molecular interactions, particularly between gelatin's amide groups and MPE's maleic anhydride moieties. The role of glycerol and triglycerides as plasticizers is also examined, revealing their impact on composite morphology and mechanical properties. These findings contribute to a deeper understanding of biopolymer–synthetic polymer interactions, supporting the development of biodegradable materials with enhanced mechanical performance and environmental sustainability.

Keywords: polyethylene, gelatin, glycerol, biocomposite, DFT modeling, molecular interactions, hydrogen bonding, biodegradable materials.

Introduction

The combination of synthetic and natural polymers has gained increasing attention in material science, particularly for packaging applications, due to the unique properties that cannot be achieved with individual components. Synthetic polymers, such as polyethylene (PE) and polypropylene, provide mechanical strength, water resistance, and thermal stability. In contrast, natural polymers, including starch, gelatin, and cellulose, contribute to biodegradability, environmental safety, and the potential for modification to meet specific requirements. These hybrid systems enable the development of materials with tailored properties, such as high-barrier films that protect food products from oxygen, moisture, and light. Additionally, blending synthetic and natural polymers reduces the overall synthetic polymer content, making the material more environmentally friendly without significantly compromising functionality [1-3].

One of the main motivations for developing such composite materials is addressing the environmental challenges associated with plastic waste pollution. Conventional packaging materials based solely on synthetic polymers accumulate in the environment due to their low biodegradability, leading to long-term soil and water contamination. Incorporating natural polymers into composite formulations accelerates degradation after disposal, significantly reducing environmental impact. For example, gelatin and starch, when combined with maleated polyolefins, enable the development of materials that degrade under microbial activity or composting conditions. Thus, such composites contribute to the transition toward a "green" economy by minimizing waste and decreasing dependence on non-renewable resources [6,7].

A particularly promising system consists of maleic anhydride-grafted polyethylene (MPE), gelatin, and glycerol. MPE is a modified synthetic polymer obtained through the grafting of maleic anhydride onto polyethylene. This modification enhances the polymer's polarity and hydrogen-bonding ability, improving compatibility with polar substances. Gela-

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tin, a protein-based biopolymer, is widely used due to its biocompatibility, biodegradability, and gel-forming properties, making it a key component in sustainable material design. Glycerol acts as a plasticizer, improving the flexibility and processability of gelatin-based composites [8-10].

Theoretical investigations of interactions within such polymeric systems are essential to understanding intermolecular forces, thermodynamic stability, and the influence of structural factors on composite properties. A deeper insight into these mechanisms will facilitate the optimization of processing conditions and the development of new materials with improved mechanical strength, flexibility, thermal stability, and barrier properties.

This study aims to conduct a theoretical investigation of the MPE–gelatin–glycerol system using computational modeling and physicochemical interaction analysis. Special attention is given to the effects of component concentration, mixing conditions, and external factors (e.g., temperature and pressure) on composite structure and properties. The results of this research could be applied in the development of biocompatible materials for food packaging, medical devices, and other applications where environmental sustainability and material performance are critical.

Thus, this work provides fundamental insights into the formation and behavior of MPE–gelatin–glycerol composites, supporting their potential applications across various industrial sectors.

Computational Study

To investigate the molecular interactions within the MPE–gelatin–glycerol system, density functional theory (DFT) calculations were performed. The electronic structure, intermolecular interactions, and thermodynamic stability of the composite were analyzed using quantum mechanical modeling.

Polyethylene was modeled as a linear hydrocarbon chain, gelatin as a polypeptide containing amino acid residues (glycine, proline, and hydroxyproline), and glycerol as a small molecule with three hydroxyl groups capable of forming hydrogen bonds. Molecular dynamics (MD) simulations were employed to evaluate the impact of temperature and pressure on the structural and mechanical properties of the composite.

DFT calculations were carried out using Quantum ESPRESSO, applying the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional and ultrasoft pseudopotentials [11]. A plane-wave basis set with a cutoff energy of 40 Ry was used. Geometry optimization was performed, ensuring that all atomic forces were minimized below 0.01 eV/Å. To prevent interactions between adjacent periodic images, a vacuum layer of 30 Å was introduced above the molecular system. Gaussian software was used for molecular-level energy and geometry optimizations employing the B3LYP/6-31++G(d,p) basis set [12,13].

Binding energies, charge distributions, and vibrational spectra were analyzed to assess the compatibility and stability of the composite. Additionally, the adsorption behavior of gelatin on the MPE surface was examined to quantify interaction strength. The natural bond orbital (NBO) method was used to evaluate charge transfer effects and electronic interactions between gelatin functional groups and maleic anhydride-modified polyethylene.

Results and discussion

The optimized molecular geometry of the gelatin biopolymer (Figure 1) and MPE was determined using DFT calculations. Structural relaxation ensured convergence to the lowest energy state, accounting for steric effects and possible conformational rearrangements.

The adsorption behavior of gelatin on the MPE surface was analyzed to quantify intermolecular interaction strength. The calculated binding energy ($E_{interaction}$) confirmed the stability of the gelatin–MPE complex. Charge distribution analysis using the NBO method revealed significant charge transfer between gelatin’s amide groups and MPE’s maleic anhydride moieties, which contributed to strong hydrogen bonding and interfacial adhesion.

Additionally, non-covalent interactions were examined through electrostatic potential mapping and weak interaction analysis (such as hydrogen bonding and van der Waals forces) to provide a comprehensive understanding of the physicochemical compatibility of the system. The obtained results contribute to elucidating the fundamental mechanisms governing gelatin–MPE interactions, which are crucial for optimizing composite material properties, such as adhesion, mechanical strength, and biodegradability.

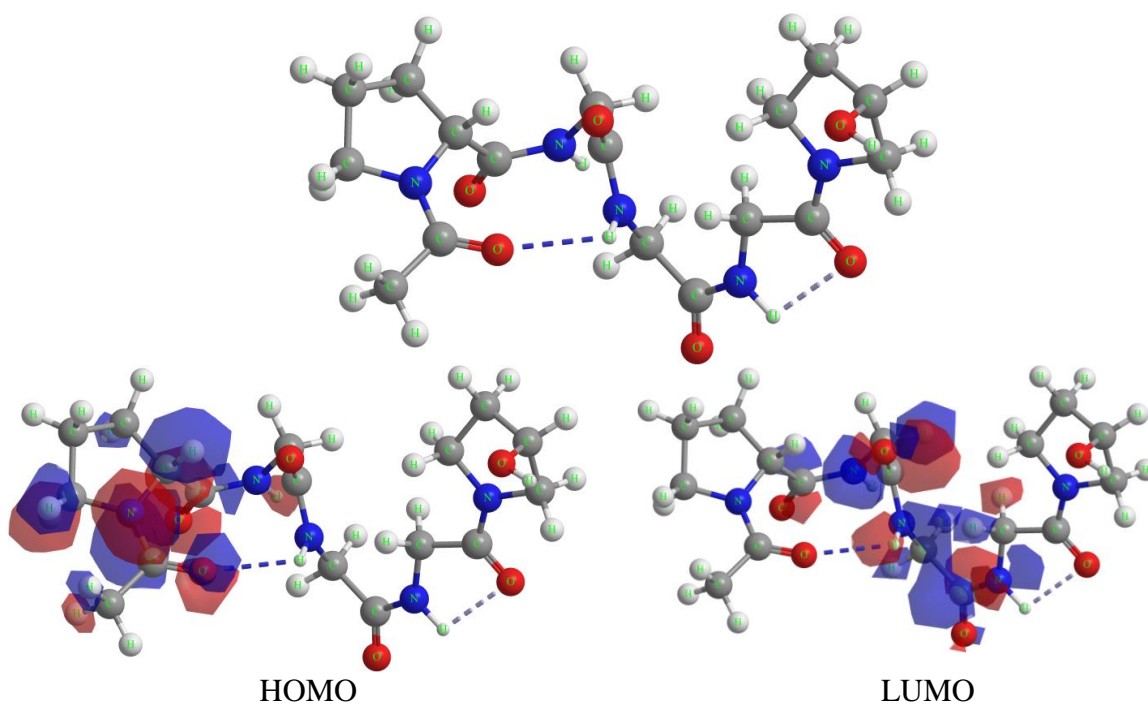


Figure 1. Optimized geometry of the gelatin molecule and representation of its frontier molecular orbitals.

Figure 1 clearly illustrates that the gelatin unit is stabilized by a specific type of intramolecular hydrogen bonding, namely $-N-H \cdots C=O$ interactions. The calculated hydrogen bond lengths range from 2.4 \AA to 2.2 \AA , indicating a moderate interaction strength that contributes to the structural stability of the molecule.

In experimental studies, **glycerol** is commonly used as a plasticizer to disrupt interchain hydrogen bonding, thereby enhancing the flexibility and processability of gelatin-based materials [3]. The presence of glycerol molecules interferes with the hydrogen bond network, leading to increased molecular mobility and reduced brittleness. This effect plays a crucial role in tailoring the mechanical and physicochemical properties of gelatin-containing biocomposites, making them suitable for applications in biodegradable packaging, biomedical materials, and controlled-release systems.

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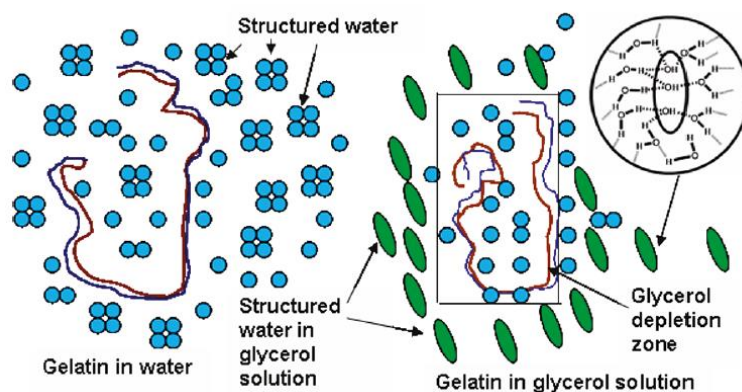


Figure 2. Graphical representation of the solvation of the gelatin molecule in aqueous and glycerol solutions [3].

In the glycerol solution, the hydration shell primarily consists of **amorphous water**, which forms a dynamic network around the biopolymer. However, a noticeable **depletion of glycerol density** is observed in the immediate vicinity of the gelatin molecule. This phenomenon suggests that water molecules preferentially interact with gelatin's hydrophilic functional groups, while glycerol tends to aggregate in regions farther from the biopolymer surface.

Such solvation behavior significantly influences the physicochemical properties of gelatin-based materials. In aqueous environments, **strong hydrogen bonding with water molecules** enhances gelatin's swelling and gel-forming ability, whereas in glycerol-rich systems, the reduced hydration leads to structural compaction and altered mechanical properties. Understanding the molecular-level interactions in these systems is essential for optimizing gelatin-based biomaterials for applications in **biodegradable films, drug delivery systems, and tissue engineering scaffolds** [3].

Figure 3 presents the optimized geometry of the interaction between a structural unit of gelatin and two glycerol molecules. The analysis reveals that the system is stabilized through the formation of multiple intermolecular hydrogen bonds, specifically: gelatin ($-C=O$) – glycerol ($-OH$), gelatin ($-NH$) – glycerol ($-OH$), and gelatin ($-OH$) – gelatin ($-OH$).

The presence of these hydrogen bonds plays a crucial role in determining the thermodynamic stability and structural organization of the gelatin–glycerol system. The hydrogen bonding network contributes to the modulation of gelatin's flexibility, plasticization effects, and water retention capacity, which are essential for controlling the mechanical and rheological properties of gelatin-based materials.

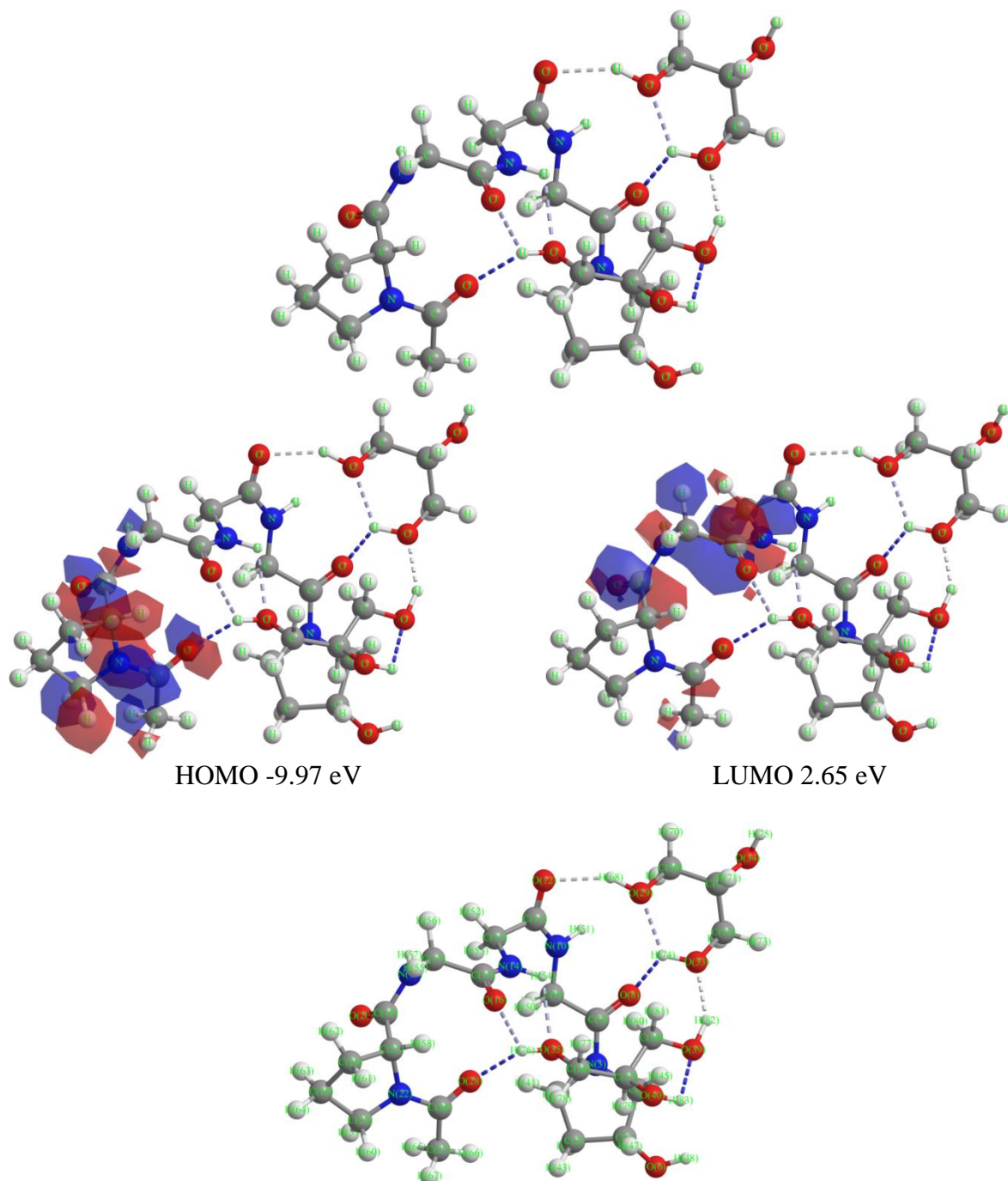


Figure 3. Optimized geometry of the interaction between a structural unit of gelatin and two glycerol molecules.

Table 1.

Interaction parameters of the gelatin–glycerol system.

Gelatin	Glycerol	Hydrogen Bond Length, Å
O (28)	H(76)	2.23
O(16)	H(76)	2.05
O(12)	H(68)	2.07
O(8)	H(74)	2.27
H(54)	O(35)	2.22

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The next stage of the study focused on analyzing the interactions within the gelatin-glycerol-MPE system. A comparative analysis of the optimized output structures revealed that the most stable configuration of the complex is characterized by the adsorption of a polyethylene monomer unit onto the gelatin molecule through the formation of hydrogen bonds between the –NH group of gelatin and the oxygen of the maleinized group (Figure 4).

Based on adsorption energy calculations, the most thermodynamically favorable structure was selected for further analysis. These findings indicate that the interaction between gelatin and maleinized polyethylene is primarily governed by hydrogen bonding, specifically through the interaction of the imine (-NH) group of gelatin with the oxygen of the maleinized functional group.

The interaction energy was calculated to be **-121.3 kJ/mol** using the following equation:

$$E_{interaction} = E_{complex} - (E_{gelatin} - E_{MPE})$$

where: $E_{interaction}$ is the adsorption energy, $E_{complex}$ represents the total energy of the gelatin-MPE complex, $E_{gelatin}$ and $E_{MA-p-PE}$ denote the individual energies of gelatin and MPE, respectively.

This calculation confirms the MPE, suggesting its potential for the development of biodegradable composite materials with enhanced interfacial interactions.

The moderate adsorption energy value indicates that the interaction lies between the regions of physisorption and chemisorption. This conclusion is further supported by the short bond length of 2.02 Å, suggesting a strong yet non-covalent interaction.

Additionally, the electronic characteristics of the system were analyzed by calculating the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy distributions (Figures 3 and 4). Figure 3 illustrates the HOMO electron distribution, which is primarily localized on the gelatin molecule, indicating its role as an electron donor. The LUMO orbitals, on the other hand, are preferentially located on the glycerol molecule, highlighting its electron-accepting nature. Figure 4 presents the HOMO electron distribution localized on the gelatin molecule, whereas the LUMO orbitals are predominantly situated on the MPE molecule. This spatial distribution suggests electronic interactions between the molecules, facilitating charge transfer.

The presence of nitrogen atoms in the gelatin structure contributes to its role as an electron donor. Notably, the most significant charge redistribution is observed at the interacting oxygen atom of the maleinized group and the nitrogen of the gelatin structure, aligning with the optimized geometric configuration of the system.

Summing up the charge distribution in the system, the calculated natural bond orbital (NBO) charge transfer value (QNBO) is $-0.41 e$, which confirms that charge is transferred from the gelatin molecule to MPE. This result provides further insight into the nature of interactions governing the stability and electronic behavior of the biodegradable composite.

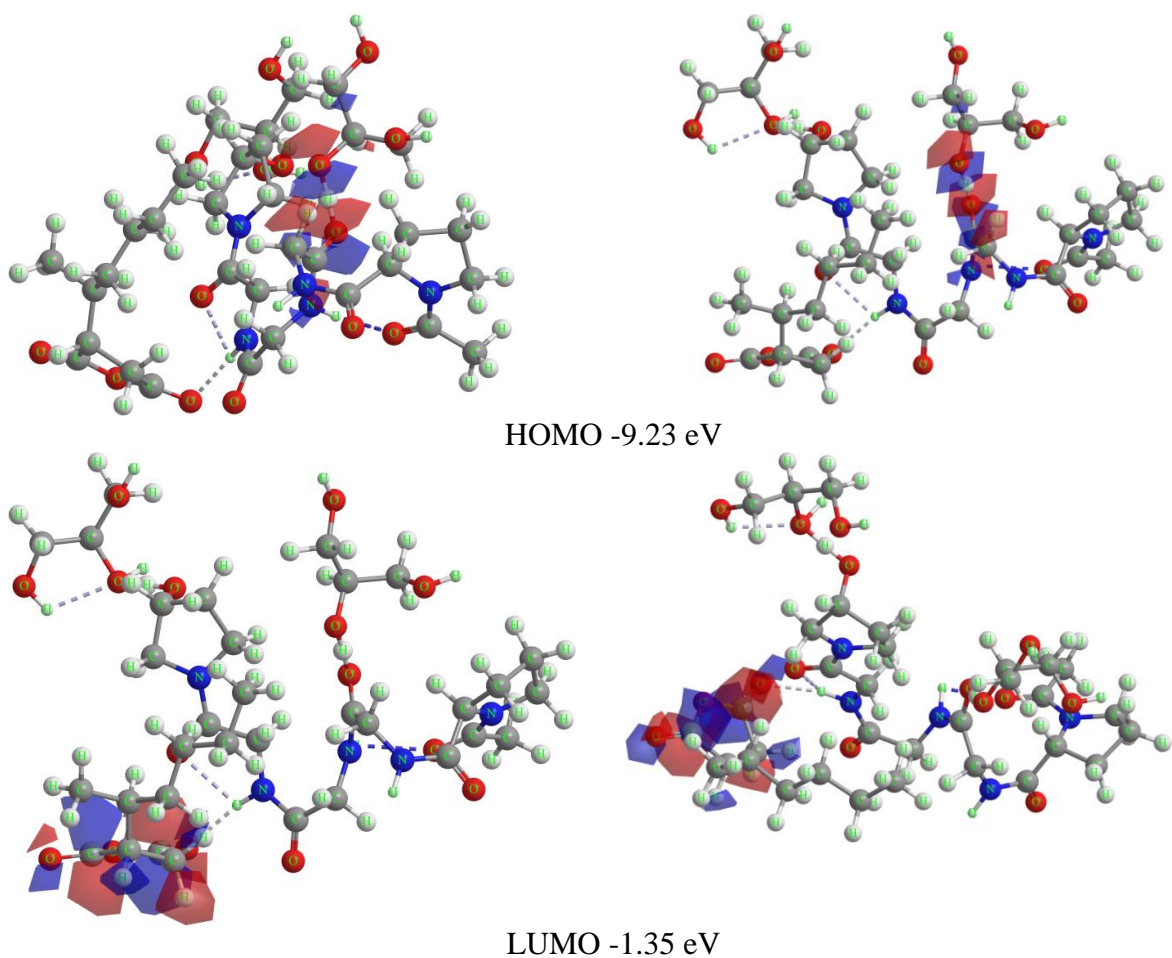
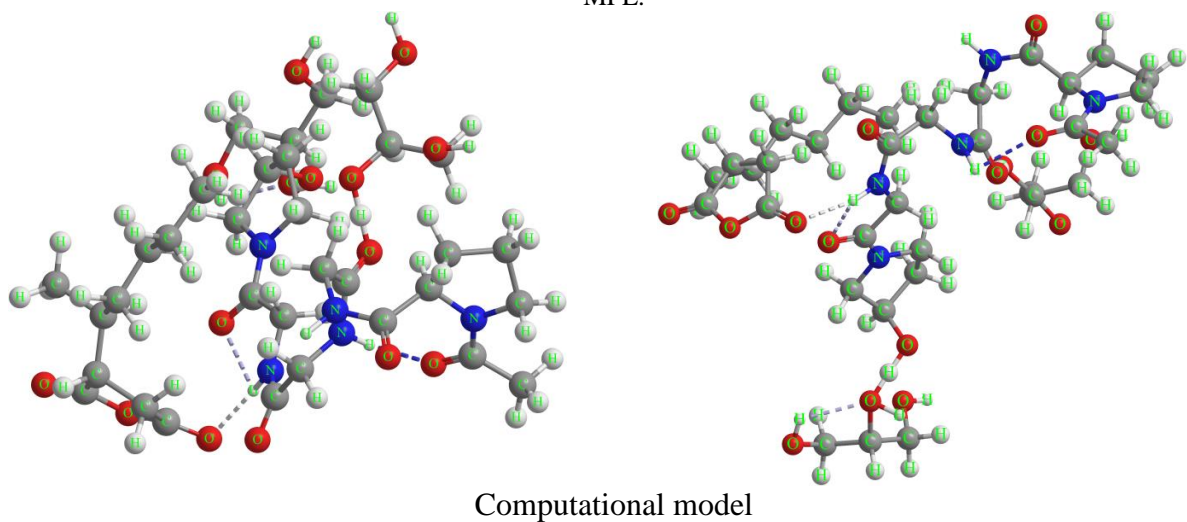


Figure 4. Optimized geometry of the interaction of a gelatin structural unit with two molecules of glycerol and MPE.



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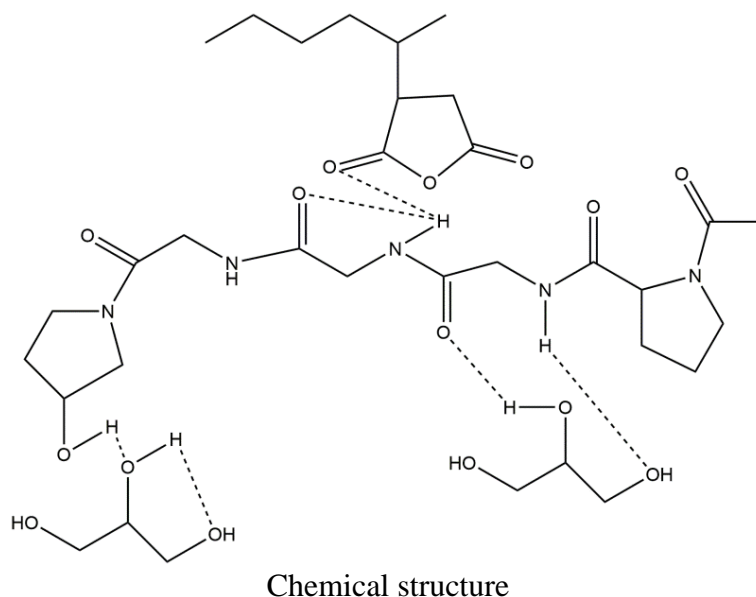


Figure 5. Computational model and chemical structure of Gelatin-Glycerol-MPE system

The computational model of the Gelatin-Glycerol- MPE system (Fig.5) was developed to analyze the molecular interactions between these components, providing insights into their structural and energetic properties. This model allows for the examination of hydrogen bonding, charge transfer, and adsorption behavior, which are critical for understanding the formation and stability of biodegradable polymeric composites.

It is well known that fats (triglycerides) act as plasticizers in polymer systems while simultaneously providing a lubricating function. In [15, 16], it was demonstrated that during the formation of the graft copolymer MPE with gelatin, the Melt Flow Index (MFI) remains almost unchanged. However, as the gelatin content increases, the MFI gradually decreases. Interestingly, the introduction of 30% vegetable oil triglyceride restores the MFI almost to the level of the original polyethylene. This trend is observed for all compositions of the graft copolymer.

Table 2.

Calculated interaction energies of various molecular systems

System	Energy, kcal/mol
MPE	27.56
Gelatin - 2 molecules of Glycerol - MPE	2983.69
Gelatin-2 molecules of Glycerol	3835.03
Gelatin-8 molecules of water	-69.26
8 molecules of water	-55.81
Gelatin	0.1379
2 molecule of Glycerol	-3.5405
Glycerol - Triglyceride- MPE	3592.04
Triglyceride	41.72

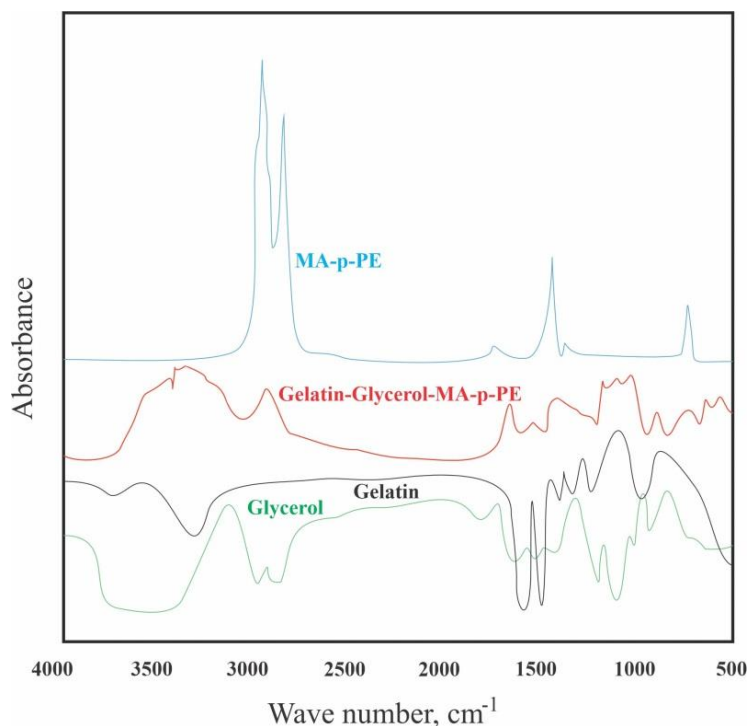


Figure 6. Calculated infrared spectrum of investigated systems

Calculated FTIR spectra of gelatin, glycerol, MPE, and their interactions are presented in Figure 6. Glycerol exhibited a broad band in the range of 600–3000 cm^{-1} , attributed to the stretching of O–H bonds involved in inter- and intramolecular hydrogen bonding. The FTIR analysis revealed distinct spectral peaks for gelatin showed characteristic peaks at 3433 cm^{-1} for –OH groups and amide-A, 1650 cm^{-1} for amide-I, 1540 cm^{-1} for amide-II, and 1240 cm^{-1} for amide-III. Symmetric and asymmetric bending vibrations of methyl groups were observed in the range of 1460–1380 cm^{-1} [17]. MPE exhibited peaks at 1715 cm^{-1} and 1792 cm^{-1} , corresponding to carboxylic acid and symmetric stretching of cyclic anhydride, respectively [18].

Gelatin displayed a band at 1328 cm^{-1} , primarily associated with the wagging vibrations of proline side chains. However, this band does not solely represent the carboxyl group but is part of a series of bands in the range of 1400–1260 cm^{-1} , indicative of type-I gelatin. In the MA-p-PE/gelatin/glycerol system, a gelatin peak was observed at 1540 cm^{-1} , whereas the characteristic maleic anhydride shoulder peak at 1715 cm^{-1} disappeared. The absence of this peak likely resulted from the ring opening of maleic anhydride, which then reacted with the –NH groups of gelatin. Given that gelatin contains a high number of –NH groups in its structure [19], this led to a high reaction rate with the maleic anhydride groups of MPE. This reaction facilitated interfacial crosslinking between gelatin and MPE, leading to the dispersion of MPE nanoparticles within the gelatin matrix and an improvement in tensile properties.

The formation of a core-shell structure was driven by several factors, including the partial miscibility of gelatin and MPE [20], the interaction between gelatin and glycerol [21] (Fig. 5), and the reaction between the –NH groups of gelatin and the maleic anhydride groups of MPE [22] (Fig. 5). These core-shell nanoparticles with high interfacial reactivity contributed to the enhancement of the mechanical properties of the MPE blend.

The addition of triglycerides at the component mixing stage and an increase in mixing speed within the range of 50–150 rpm lead to the formation of a fine-dispersed morphology in the blend. As a result, the tensile strength (σ) increases by more than 25%, the elongation at break (ϵ) decreases significantly from 655% to 85%, and the elastic modulus (E) nearly doubles. The underlying mechanisms of this behavior remain unclear. However, it is evident that

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the additional plasticization effect of the triglyceride restores the thermoplasticity of gelatin, which in turn facilitates the formation of the fine-dispersed morphology in the blends.

Given these observations, we also investigated the molecular interactions between gelatin and triglyceride to better understand their impact on the composite's structure and properties.

The calculated interaction energies for different molecular systems, presented in Table 2, provide insights into the stability and strength of interactions among gelatin, glycerol, water, triglycerides, and MPE. The purpose of these calculations was to assess the energetic stability of various molecular complexes and determine the most favorable configurations for further investigation. The computed interaction energies provide insights into the strength and nature of intermolecular interactions within the studied systems.

MPE (27.56 kcal/mol): This value corresponds to the intrinsic energy of the MPE monomer, serving as a reference point for evaluating its interactions with other molecular components.

Gelatin – 2 molecules of glycerol-MPE (2983.69 kcal/mol) and Gelatin - 2 molecules of glycerol (3835.03 kcal/mol): The significantly high interaction energies suggest strong molecular binding between gelatin, glycerol, and MPE. A comparison of these values indicates that the inclusion of MPE influences the overall system stability, potentially contributing to the structural reinforcement of the composite.

Gelatin – 8 molecules of water (-69.26 kcal/mol) and 8 Water (-55.81 kcal/mol): These negative interaction energy values reflect the solvation effects of gelatin in water, suggesting that hydration stabilizes the system. The stronger stabilization observed in the gelatin–water system compared to bulk water (-69.26 kcal/mol vs. -55.81 kcal/mol) indicates that gelatin interacts favorably with water molecules, likely through hydrogen bonding.

Gelatin (0.13 kcal/mol) and 2 molecules of glycerol (-3.540kcal/mol): The near-zero energy value for gelatin suggests that it is inherently stable as an isolated molecule. The slightly negative energy for the glycerol dimer indicates weak stabilization, most likely due to the formation of intermolecular hydrogen bonds between glycerol molecules.

Gelatin-Triglyceride-MPE (3592.04 kcal/mol) and triglyceride (41.77 kcal/mol): The high interaction energy of the gelatin-triglyceride complex suggests strong molecular interactions, which could significantly impact the structural integrity and functional properties of the composite material.

The calculated interaction energies provide valuable insights into the stability and compatibility of different molecular systems. Among the studied complexes, the gelatin–2 molecules of glycerol system exhibits the highest interaction energy (3838.44 kcal/mol), indicating the strongest molecular interactions. This suggests that the presence of glycerol significantly enhances gelatin's ability to form stable hydrogen-bonding networks, likely due to the strong affinity of glycerol hydroxyl groups for gelatin's functional sites.

In comparison, the gelatin–triglyceride system demonstrates a slightly lower interaction energy (3550.14 kcal/mol). This still suggests a strong interaction, which aligns with the known role of triglycerides as plasticizers in polymeric systems. The moderate interaction strength implies that triglycerides contribute to the flexibility of the gelatin matrix while maintaining overall structural integrity.

The gelatin–2 glycerol–MPE system exhibits a lower interaction energy (2959.54 kcal/mol) compared to the gelatin–glycerol system. The presence of MPE alters the hydrogen bonding network, likely leading to competition between polymer interactions and gelatin–

glycerol interactions. Although the interaction energy is lower, the inclusion of MPE contributes to improved polymer compatibility, facilitating the formation of composite materials with tailored mechanical properties.

Finally, the gelatin–8 water system exhibits the lowest interaction energy (-13.59 kcal/mol), suggesting weak solvation effects. The negative interaction energy value indicates that hydration leads to molecular destabilization rather than stabilization. This result is consistent with the fact that water weakens intermolecular forces by disrupting hydrogen bonds between gelatin and other components.

Conclusions

This study provides a theoretical analysis of the molecular interactions in MPE–gelatin–glycerol composites using density functional theory (DFT) modeling. The results highlight the key mechanisms governing interfacial bonding, plasticization, and structural stability in these hybrid materials. FTIR spectral analysis confirms the formation of hydrogen bonds between gelatin's amide groups and MPE's maleic anhydride moieties, leading to interfacial crosslinking. The calculated interaction energies demonstrate strong molecular interactions, supporting the formation of stable polymeric structures.

Furthermore, the presence of glycerol and triglycerides as plasticizers significantly influences composite morphology, enhancing flexibility while maintaining mechanical integrity. The introduction of triglycerides reduces brittleness and facilitates the development of finely dispersed morphologies, which, in turn, improve the material's mechanical performance.

The findings of this study contribute to the broader understanding of biopolymer–synthetic polymer interactions, offering valuable insights for the development of biodegradable composites with tailored properties. These materials hold great potential for applications in sustainable packaging, biomedical devices, and other fields requiring environmentally friendly and high-performance polymer systems. Future research should focus on experimental validation of the computational results and further optimization of processing conditions to enhance the practical applicability of these biocomposites.

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