Understanding Of Dental Material Triethylene Glycol Dimethacrylate (TEGDMA) Using Molecular Dynamics Method

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***Abstract*—Context: Molecular dynamics studies have been conducted to investigate the behavior, structure, and interactions of TEGDMA at the molecular level. These studies provide valuable insights into the properties and characteristics of TEGDMA, aiding in the understanding of its applications in dental materials.**
Method: To achieve this, we utilized Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for computing the degree of conversion, General Utility Lattice Program (GULP) for calculating physical parameters such as elastic constants, moduli, zero-point energy, heat capacity, p- and s-wave velocities, lattice energy, and WebMO for computing Raman, UV-Vis, FTIR, and NMR spectra of TEGDMA. These results have been compared with the reported experimental data. Our simulations reveal that TEGDMA exhibits high elastic moduli and lattice energy, suggesting its robustness and stability. Additionally, the spectral analysis from WebMO aligns well with experimental observations, confirming the accuracy of our computational methods. The calculated p- and s-wave velocities provide insights into the material's acoustic properties, further supporting its suitability for dental applications.

***Index Terms*—TEGDMA, Molecular dynamics, Bulk, youngs moduli and Poisson ratio**

I. INTRODUCTION

TEGDMA, short for Triethylene Glycol Dimethacrylate, is a key component found in various dental materials [1]. It is a versatile monomer commonly used in dental composites, adhesives, and sealants. TEGDMA helps to enhance the mechanical properties, durability and aesthetics of dental restorations [2-10]. One of the key advantages of TEGDMA is its ability to cross-link with other monomers, forming a strong and stable network. This cross-linking process helps improve the strength and longevity of dental materials, ensuring that restorations withstand the daily wear and tear in the oral cavity. Moreover, TEGDMA contributes to the excellent bonding properties of dental adhesives [11-17]. It promotes adhesion between the restoration and the natural tooth structure, creating a tight seal and preventing microleakage. This contributes to the overall success and longevity of dental restorations. It's worth noting that while TEGDMA offers many benefits, it has been associated with potential biocompatibility concerns in some studies. However, dental material manufacturers continuously work towards optimizing the formulation and reducing any potential risks associated with TEGDMA. Overall, TEGDMA plays a vital role in modern dental materials, improving their performance, strength, and aesthetics. Its versatility and bonding properties make it a valuable component in creating durable and aesthetically pleasing dental restorations.

Physical and chemical characterization plays a crucial role in understanding the properties and behavior of TEGDMA (Triethylene Glycol Dimethacrylate) material. Researchers have conducted extensive studies to explore various aspects of TEGDMA, shedding light on its structure, physical properties and reactions. TEGDMA has been the subject of several experimental spectral analysis studies aimed at understanding its molecular structure, vibrational characteristics and chemical interactions. These analyses provide valuable insights into the behavior and properties of TEGDMA.

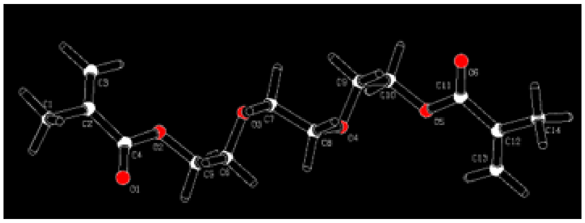
Molecular dynamics studies have been conducted to investigate the behavior, structure, and interactions of TEGDMA at the molecular level. These studies provide valuable insights into the properties and characteristics of TEGDMA, aiding in the understanding of its applications in dental materials.

At the molecular level, TEGDMA consists of two methacrylate groups connected by a chain of ethylene glycol units. These methacrylate groups have double bonds that can undergo a chemical reaction called polymerization when exposed to certain conditions, such as light or heat. When TEGDMA is mixed with other dental materials, such as resin-based composites, the methacrylate groups in TEGDMA can react with the monomers present in the composite material. This reaction is known as free radical polymerization.

Quantifying the polymerization aspect of TEGDMA can be done using various techniques, apart from absorption studies. Here are a few common methods used to measure the extent of polymerization:

1. Degree of Conversion: This method measures the percentage of monomer units that have converted into polymer chains. It can be determined using techniques such as Fourier-transform infrared spectroscopy (FTIR) or Raman spectroscopy. By comparing the peak intensities of specific functional groups before and after polymerization, the degree of conversion can be calculated.
2. Gel Permeation Chromatography (GPC): GPC is a technique used to determine the molecular weight distribution of polymers. By analyzing the elution times of the polymer chains, the average molecular weight and the degree of polymerization can be estimated. This method provides insights into the size and structure of the polymerized TEGDMA.
3. Differential Scanning Calorimetry (DSC): DSC measures the heat flow associated with thermal transitions in a material. By monitoring the heat released or absorbed during the polymerization process, important parameters such as the glass transition temperature and the enthalpy of polymerization can be determined.
4. Rheological Analysis: Rheological measurements, such as dynamic mechanical analysis (DMA) or viscoelasticity testing, can provide information about the mechanical properties and curing behavior of the polymerized TEGDMA. These tests assess the factors such as stiffness, elasticity and viscosity changes during the polymerization process.
5. Real-time Monitoring Techniques: Some advanced techniques allow for the in-situ monitoring of polymerization. For example, real-time FTIR or Raman spectroscopy can provide continuous analysis of the changing chemical bonds during polymerization, offering insights into reaction kinetics and the progress of the reaction over time.

These methods collectively provide a comprehensive understanding of the polymerization behavior, degree of conversion, molecular weight, thermal properties, and mechanical performance of TEGDMA. By employing these quantification techniques, researchers and dental professionals can assess the efficacy and quality of dental materials containing TEGDMA, ensuring optimal performance and patient safety. Chemical structure of TEGDMA is given below.



II. MOLECULAR DYNAMIC METHOD

In molecular dynamics simulations, the behavior of a system is described by tracking the positions and velocities of individual atoms or molecules over time. A step-by-step procedure for such simulations is provided below:

Step 1: Use LigParGen (LPG), an online program, to draw the chemical structure of TEGDMA and create various output files, including a *.pdb file [18-20].

Step 2: Utilize the Visual Molecular Dynamics (VMD) program and select TkConsole. Execute the following commands: 'topo retypbonds', 'topo guessangles', 'topo guessdihedrals', and 'topo writelammps data file.data' [21].

Step 3: Modify appropriate lines in the file.data for the proper format of the input file to be executed using LAMMPS [22].

Step 4: Create an input file for GULP by adjusting the Buckingham potential Aexp(-r/ρ)-C/r^6 with the three parameters so that the output contains 6x6 elastic constants corresponding to a stable crystal, which is verified by the online ELATE TENSOR PROGRAM [23].

Step 5: Use the versatile WebMO online program to compute (i) Raman Shift spectra, (ii) UV-Vis spectra, (iii) FTIR spectra, and (iv) NMR spectral of the material TEGDMA [24].

Step 6: Create a LAMMPS [22] input script file for computing (i) surface tension, (ii) viscosity, (iii) glass transition temperature, and (iv) radial distribution function.

2.1 Degree of conversion.

The input file for computing the degree of conversion includes the necessary commands and parameters. The calculation of the degree of conversion (DC) in terms of bond formation during a simulation can be approached by monitoring the number of reacted monomer units compared to the initial number of monomers. Equation in LAMMPS script is variable conversion equal "(v_init_mol - v_final_mol) / v_init_mol". Here is a basic outline of the same. For the sake of completeness, we provide the file details as follows

```
# Define simulation parameters
units real
dimension 3
boundary p p p
atom_style full

# Create atom data
read_data data.tegdma

# Define potential and settings
pair_style lj/cut 10.
pair_coeff * * .1 3.

# Set initial conditions
velocity all create 300.0 4928459 dist gaussian
fix 1 all npt temp 300.0 300.0 100.0 iso 0.0 0.0 100.0 drag 1.0

# Run minimization and equilibration steps
minimize 1.e-6 1.e-8 100 10000
run 10000

# Compute degree of conversion
Compute vconversion all property/atom mol
Variable init_mol equal count(all)
Group unreacted type 1
run 1000

# Output results
Variable final_mol equal count(unreacted)

# Calculate the degree of conversion
variable conversion equal "(v_init_mol - v_final_mol) / v_init_mol"

# Print the degree of conversion
```

Output of the above gave a value of 97 percent for the degree of conversion in the case of TEGDMA material.

2.2 Degree of polymerization

This refers to the number of monomer units in a polymer chain. It is often calculated as the ratio of the total number of monomers to the number of polymer chains. Equation used in the LAMMPS script is variable dp equal count(all)/c_avgchain print "Degree of Polymerization: ${dp}". To compute this, we need the following additional commands:

```
# Compute the degree of polymerization
compute chain all property/atom mol
compute chains all chunk/atom c_chain
compute avgchain all reduce ave c_chains
run 4468

# Output the degree of polymerization
variable dp equal count(all)/c_avgchain
print "Degree of Polymerization: ${dp}"
```

The degree of polymerization varies between 50 to 70 depeding on the parameters. We never got a unique value for the degree of polymerization of TEGDMA material.

2.3 Glass transition temperature (Tg) and Radial distribution function.

The glass transition temperature (Tg) of a polymer is the temperature at which an amorphous polymer transitions from a hard, glassy state to a softer, rubbery state. This transition is characterized by a change in the polymer's mechanical properties, such as stiffness and brittleness. The Tg is an important parameter in determining the processing and performance of polymers in various applications. The following commands are used to compute the glass transition temperature and radial distribution function.

```
# Calculate glass transition temperature (Tg)
variable Tg equal "temp +
0.5*step*dt*sqrt(c_msd[4])"
print "Glass Transition Temperature (Tg): ${Tg}"
```

Glass transition temperature computed value is 625K. Radial distribution function is calculated using “dump.lammps” file and Visual Molecular Dynamics (VMD) software.

2.4 Determination of Viscosity

Curing behaviour of TEGDMA can be understood by computing viscosity and we have used the following commands in lammps input script:

```
variable pxy equal pxy
variable pxz equal pxz
variable pyz equal pyz
fix SS all ave/correlate $s $p $d &
v_pxy v_pxz v_pyz type auto file S0St.dat ave running
variable scale equal
${convert}/(${kB}*$T)*$V*$s*${dt}
variable v11 equal trap(f_SS[3])*${scale}
variable v22 equal trap(f_SS[4])*${scale}
variable v33 equal trap(f_SS[5])*${scale}
thermo_style custom step temp press v_pxy v_pxz
v_pyz v_v11 v_v22 v_v33
run 100000
variable v equal (v_v11+v_v22+v_v33)/3.0
variable ndens equal count(all)/vol
print "average viscosity: $v [Pa.s] @ $T K, ${ndens}
atoms/A^3"
```

2.5 Determination of surface tension

This script includes a fix for time integration and a fix for computing the surface tension using the ave/spatial command. A few of the statements are given below.

```
variable xPress equal c_thermo_press[1]
variable yPress equal c_thermo_press[2]
variable zPress equal c_thermo_press[3]
# Evaluate and average surface tension in mN/m:
variable st equal 0.5*lz*(v_zPress-
0.5*(v_xPress+v_yPress))*${convFac}
#fix st all ave/time 10 100 1000 v_st
fix st all ave/time 1 2000 2000 v_st
#fix st all ave/time 10 100 100 v_st
#variable xyArea equal lx*ly
thermo_style custom step temp f_st press etotal
thermo_modify lost warn
#run 10000
#thermo 1000
dump trj all atom 1000 tegdma.trj
#timestep 10
#run_style verlet
run 22000
print "surface tension : $st[Pa.s] @ $T K"
```

2.6 Computation of Cohesive energy

Following commands were inserted into the input script for computing Cohesive energy at different temperatures for TEGDMA.

```
velocity all create 500 102486 mom yes rot yes dist
gaussian fix NVT all nvt temp 350 350 10 drag 0.2
run 8000
# ---------- Define Settings ---------------------
compute eng all pe/atom
compute eatoms all reduce sum c_eng
# ---------- Run Minimization ---------------------
reset_timestep 0
fix 1 all box/relax iso 0.0 vmax 0.001
thermo 10
thermo_style custom step temp pe lx ly lz press pxx
pyy pzz c_eatoms
min_style cg
minimize 1e-25 1e-25 5000 10000
variable natoms equal "count(all)"
variable teng equal "c_eatoms"
variable length equal "lx"
variable ecoh equal "v_teng/v_natoms"
variable T equal "temp"
print "Total energy (eV) = ${teng};"
print "Number of atoms = ${natoms};"
print "Lattice constant (Angstoms) = ${length};"
print "Cohesive energy (eV) = ${ecoh};"
print "Temperature = $T K;"
```

Brief description of molecular dynamic method:
Molecular Dynamics Simulation

In this study, molecular dynamics (MD) simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to investigate the behavior and interactions of TEGDMA at the molecular level. The MD simulations were crucial for understanding the degree of conversion (DC) during polymerization and the structural properties of TEGDMA.

Simulation Setup

- System Initialization: The initial configuration of TEGDMA molecules was prepared using a data file containing atomic coordinates and connectivity information. The system was modelled in a periodic cubic simulation box with dimensions sufficient to avoid spurious interactions due to periodic images.
- Force Field Parameters: The interactions between atoms were described using the following force field parameters:
- Pair Style: Lennard-Jones potential with a cutoff distance of 2.5 Å.
- Bond Style: FENE (finite extensible nonlinear elastic) potential to model the covalent bonds.
- Angle Style: Harmonic potential to model the angular interactions.
- Neighbor List: The neighbor list was updated every timestep with a binning algorithm to efficiently track atomic interactions, with a neighbor skin distance of 2.0 Å.

Equilibration

The system was equilibrated in two stages:

1. Initial Equilibration: A brief equilibration run of 1000 timesteps was performed under the NPT ensemble (constant number of particles, pressure, and temperature) to adjust the system to the target temperature of 300 K and pressure of 1 atm. The velocity command was used to initialize atomic velocities corresponding to the desired temperature.
2. Production Run: Following equilibration, a production run of 10,000 timesteps was conducted under the same NPT conditions to gather data for analysis

III. SIMULATION OF RAMAN, IR, UV-VIS, H-NMR AND C13-NMR SPECTRA

The WebMo method is a computational approach used to simulate Raman and IR spectra of TEGDMA (triethylene glycol dimethacrylate). This method involves utilizing web-based molecular modeling tools to calculate the vibrational frequencies and intensities of TEGDMA, which are then used to predict the Raman and IR spectra of the compound. By applying the WebMo method, researchers can gain valuable insights into the molecular structure and behavior of TEGDMA, aiding in the interpretation of experimental spectroscopic data[25]. For Raman and IR spectra, we have used the Hartree-Fock and STO-3G basis set. To simulate H-NMR and C13-NMR, we have employed the Hartree-Fock and 3-21G NMR basis set. For simulating UV-Vis spectra of TEGDMA, we have used CIS and STO-3G basis set. Here, CIS stands for Configuration Interaction Singles, a treatment similar to the Hartree-Fock method for excited states, and to optimize the geometry of selected states (both singlet and triplet).

IV. COMPUTATION OF PHYSICAL PARAMETERS OF TEGDMA

The Molecular Dynamics Simulation using the GULP program (General Utility Lattice Program) with input data in the format *.pdb [26] serves as the foundation for investigating the dependence of physical parameters on the chemical structure and its variations. In this study, predictions of elastic constants, shear modulus, bulk modulus, Young's modulus, and Poisson's ratio have been conducted. Additionally, the s-wave and p-wave velocities, as well as the static dielectric constant tensor, were evaluated using the molecular dynamics simulation method.

V. RESULTS AND DISCUSSION

The computational value of the degree of conversion for TEGDMA is determined to be 97%, which is the highest, and it broadly agrees with the conclusion of the experimental method reported earlier [27]. Here, MD simulation techniques provide valuable qualitative information, and when combined with experimental results, one can gain a comprehensive understanding of TEGDMA's properties.

The computation of the degree of polymerization of TEGDMA using LAMMPS depends on parameters, and we observe that this value varies between 50 to 70%. A simple formula involves dividing the molecular mass of the polymer by the molecular weight of the monomer. The program relies on the representation of the polymer chain to track the formation of chains by monitoring the creation of bonds between monomers and then determining the degree of polymerization by knowing the number of monomers. The temperature variation of cohesive energy for TEGDMA is illustrated in Figure 1.

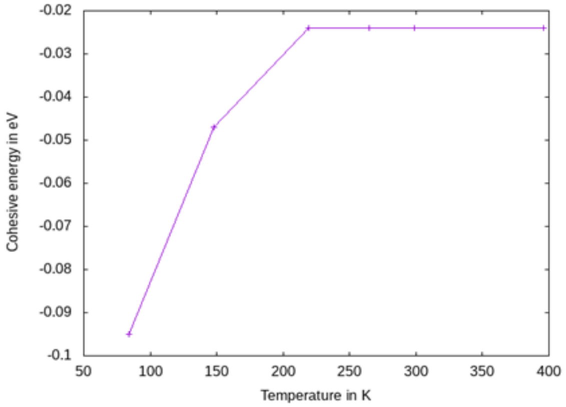


Figure 1. Temperature variation of Cohesive energy for TEGDMA

This study provides information on how materials behave at different temperatures. By analyzing the cohesive energy as a function of temperature, one can understand how the polymer's molecular structure and interactions change with heat, which can impact its chemical properties. This information can be crucial for polymer processing and understanding the behavior of polymers in different environments.

In the LAMMPS script, the glass transition temperature is computed by gradually increasing the temperature of the system, monitoring specific heat capacity, volume change/mean square displacement, and determining the slope of these properties as a function of temperature. In the same setup, the radial distribution function is computed by defining minimum and maximum distances, as well as the number of bins. For TEGDMA, the glass transition temperature is found to be 625K, and the radial distribution function is depicted in Figure 2. The experimental boiling point value is 428K [pubchem:7979].

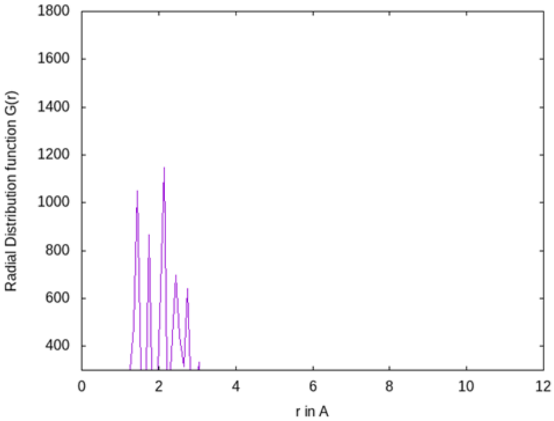


Figure 2. Simulated Radial distribution of TEGDMA with respect to Carbon atom

From Figure 2, we observe that from a reference point in a system of molecules, the intensity and peak position indicate the most probable distance and frequency of occurrence between TEGDMA monomers. This plays a role in the packing density and organization of TEGDMA in polymerization. Narrower peaks indicate an ordered structure.

Computing the viscosity of TEGDMA requires an input file containing the definition of the TEGDMA molecule and simulation parameters such as box size, temperature, and pressure conditions. An appropriate force field file and necessary parameters for TEGDMA are essential, and an equilibrium simulation is performed through a series of steps by relaxing the system towards the desired temperature and pressure conditions. This is achieved by introducing a velocity gradient to the equilibrated system using Non-Equilibrium Molecular Dynamics (NEMD), assigning different velocities to regions of the simulation box. This process yields multiple sets of shear stress values, and viscosity is computed for each set, with the average value estimated. Figure 3 illustrates the temperature variation of the viscosity of TEGDMA. Experimental values are 20°C, 0.0115 Pa•s; 25°C, 0.0062 Pa•s [28]. Molecular dynamics shows a significant variation with an increase in temperature.

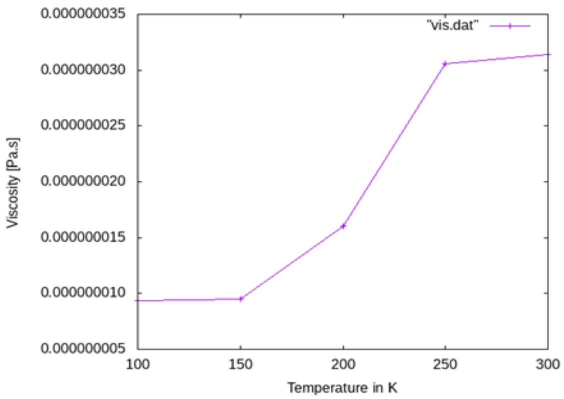


Figure 3. Temperature variation of viscosity for TEGDMA.

There is an inverse relation between viscosity and temperature, which is related to the mobility of the molecules. The simulated viscosity of TEGDMA is less than the experimental viscosity of water, which is 10^-3 Pa•s, a factor that may be important for dental resins.

In the computation of surface tension, along with some of the steps mentioned above, we need to heat up the system from an initial low temperature to the desired simulation temperature, and then use the pressure difference method with the command provided. The temperature variation of surface tension is depicted in Figure 4. The reported experimental value of surface tension is 0.033 N/m, which is significantly different from the computed values over a wide temperature range [http://www.chemspider.com/Chemical-Structure.7691.html #suppInfoTab]. The experimental value of polarizability is reported as 29.0x10^-24 cm^3. Molecular polarizability for each, which is a symmetric tensor, has been computed using the method of Wilkins et al. [29], resulting in a value of 194.3x10^-24 cm^3. The reported surface tension of TEGDMA at room temperature (around 25°C) is typically in the range of 33.7 mN/m (milliNewtons per meter)[30] .

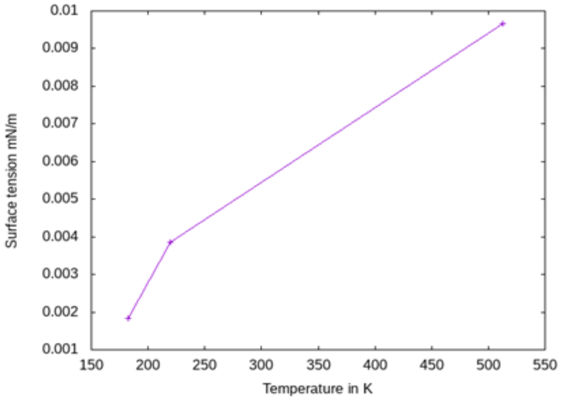
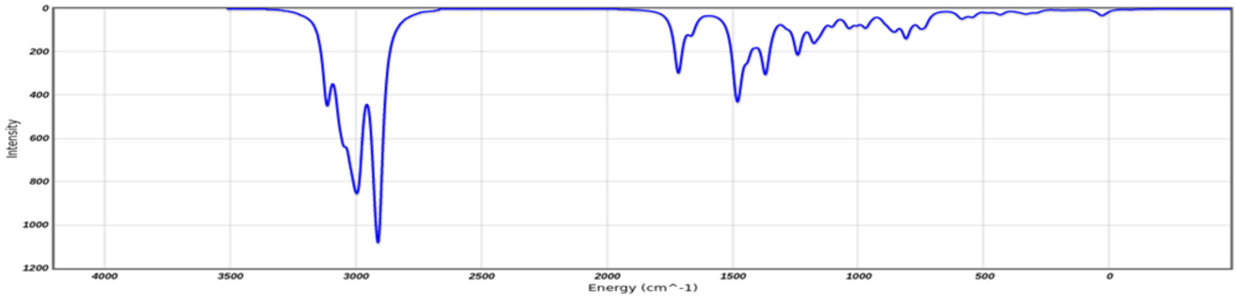
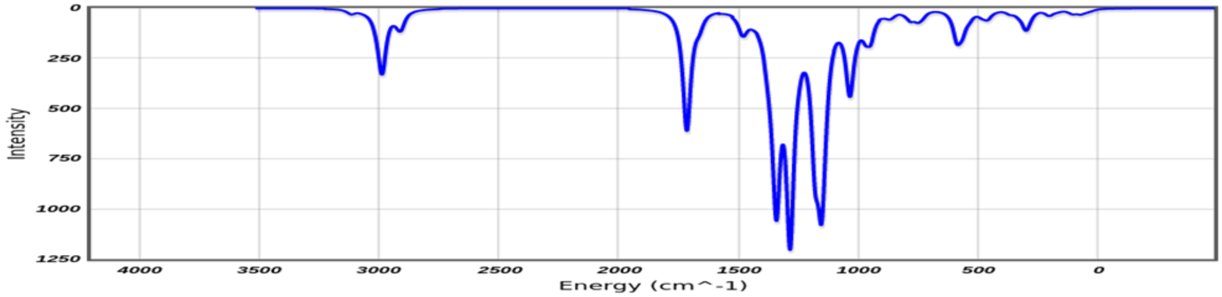


Figure 4.Temperature variation of surface tension in the case of TEGDMA

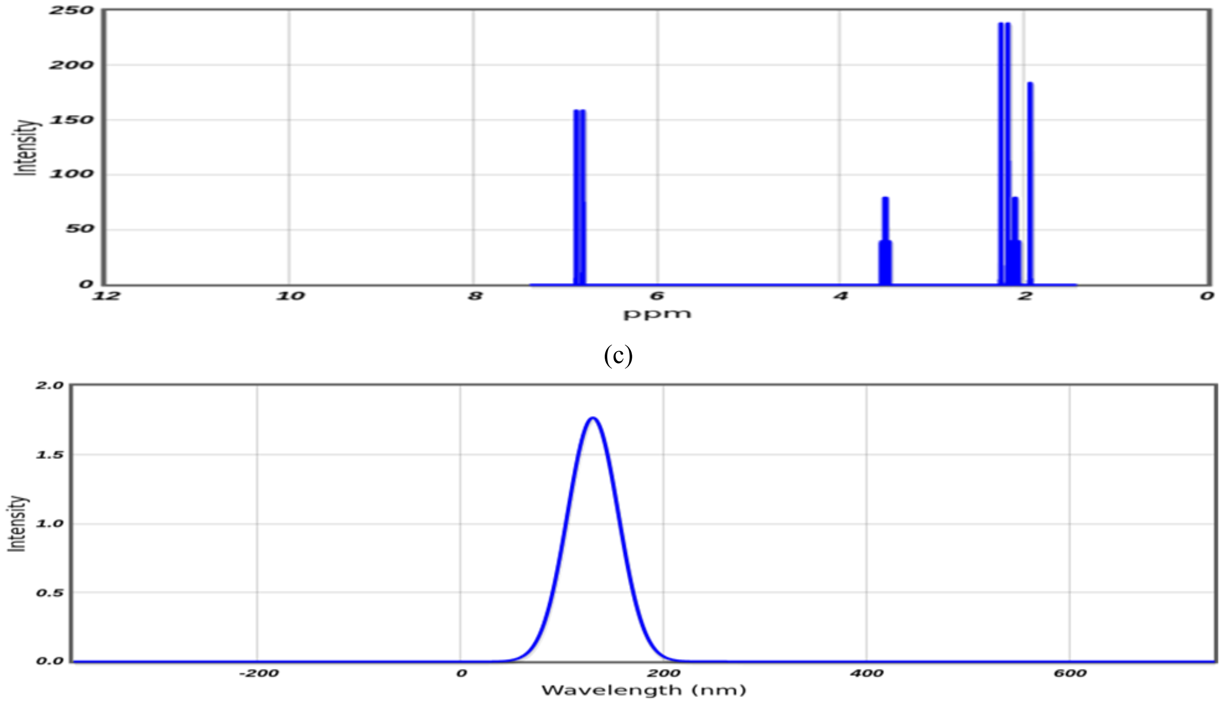
Spectral studies of TEGDMA has been carried out using LAMMPS with commands mentioned in the section “methods”. Figures 5(a-d) show Raman, IR and UV-Vis simulated spectra of TEGDMA.



(a)



(b)



(c)

(d)

Figure 5. (a) Raman ; (b) IR; (c) H-NMR and (d) UV-Vis simulated spectra of TEGDMA.

Experimentally, C=O stretching was observed at 1725 cm^-1 and C=C at 1640 cm^-1, whereas the simulated values were at 1500 cm^-1 and 1200 cm^-1, respectively, which may be attributed to the effect of temperature or a different kind of stretching mode [31]. In the IR spectrum, experimental absorbance occurs at 1715 cm^-1, whereas the simulated one occurs at 1250 cm^-1, corresponding to C=O stretching. C=C stretching was also observed in the simulated IR spectra at 1750 cm^-1, but it was less intense compared to the experimental data [pubchem: 7979]. Reported experimental data of the NMR spectra shows a peak at 6.2 ppm [pubchem: 7979], while the simulated peak is at 7.0 ppm. In the UV-Vis spectra, experimental data gives a broad absorption spectra at 200 nm, whereas the simulated spectra show an absorption peak at 120 nm, which is reasonable given the understanding that simulated dynamic motion may not exactly replicate the real system.

The computation of physical parameters of TEGDMA requires information about the lattice parameters, unit cell dimensions, and atomic positions. One also needs force field parameters for the interatomic interactions, such as bond lengths, angles, torsion, and dihedral angles. Calculation setting options include "opti, prop, conp, efg, pot, eem, bond, conq, simu, comp, phon, nofreq, regi, and thermal". The output will include electronegativity, self-energy, lattice energy, elastic constants, bulk and shear moduli, velocity of s- and p-waves, static refractive index, zero-point energy, and phonon density of states. These values are presented in Table 1. Figure 6 shows the frequency variation of the phonon density of states in the case of TEGDMA.

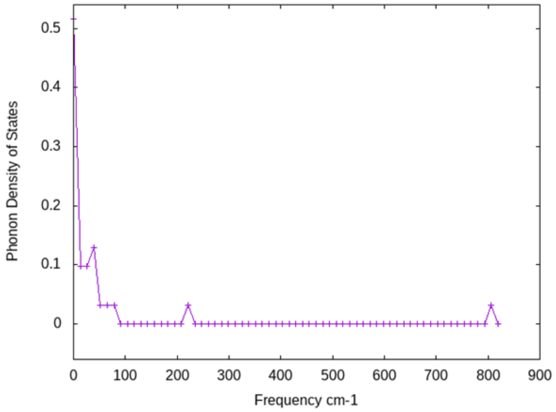


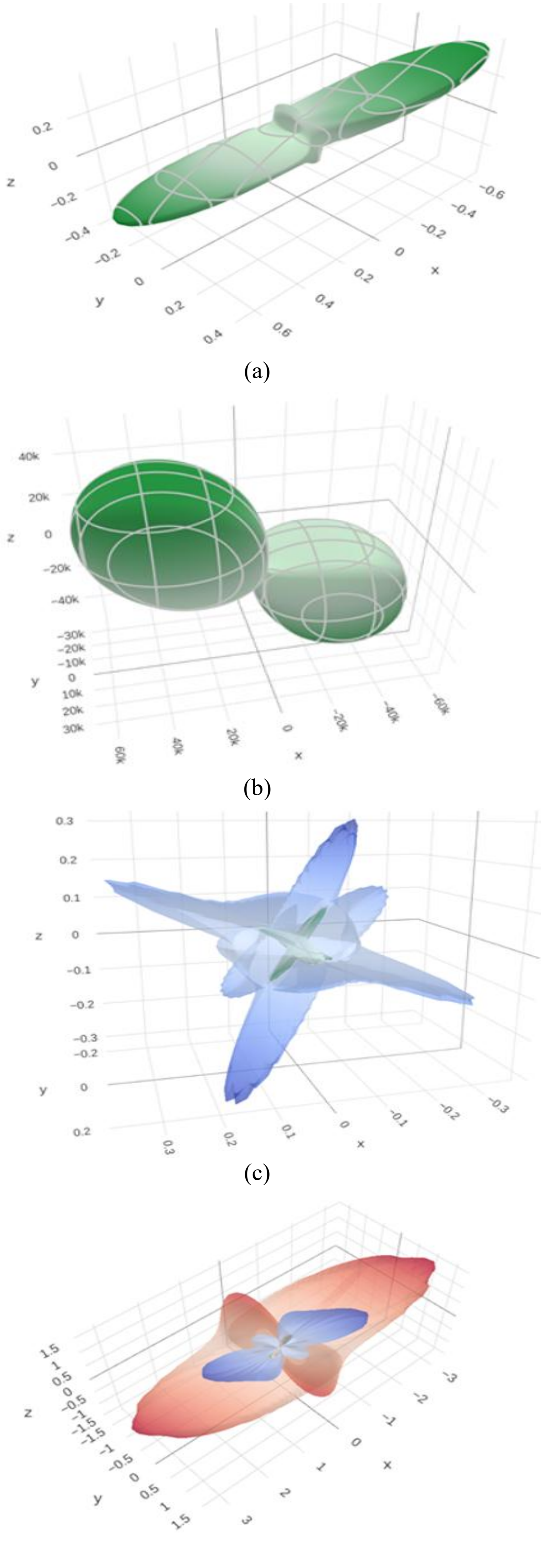
Figure 6. Variation of Phonon Density of states with frequency in the case of TEGDMA

Specifically, this observation may suggest that certain molecular bonds or interactions within the TEGDMA structure are vibrating at or near the 100 cm^-1 frequency. This could be related to the presence of specific chemical groups, such as C-H, C-C, or C=O bonds, that exhibit characteristic vibrational modes in this frequency range. Furthermore, the distribution of density of states at different frequencies can also reveal important information about the material's thermal conductivity, mechanical properties, and overall stability. Electronegativity is a fundamental concept in chemistry; however, it is an elusive quantity to evaluate experimentally. Experimental values for O-O surface atoms have been reported [32].

Table 1. Physical parameters of TEGDMA computed using GULP program using (Voigt) averaging procedure.

Physical parameter	Computed Value	Experimental value (pubchem:7979)
Electronegativity	6.6 eV	For O-O atoms value is 3.5[33]
Self-energy	-0.64 eV	
Total Lattice energy	-0.87 eV	
Elastic constants (GPa)	C11 0.942; C22 0.210 C33 0.191; C44 0.147 C55 0.306; C66 0.214 Young's Modulus: 0.133 Bulk Modulus: 0.105 Shear Modulus: 0.236	Young's Modulus is 2.37GPa [33]
Sound wave velocity (km/s)	S-wave 2.156 P-wave 2.876	
Refractive index	1.12	1.4595
Zero-point energy	0.105eV	

Spatial variation of Young's, Linear, Bulk, Shear moduli and Poisson ratio computed using ELATE program are given in Figure 7.



(a)

(b)

(c)

(d)

Figure 7. Spatial variation of Young's, Linear, Shear moduli and Poisson ration computed using ELATE program (https://progs.coudert.name/elate) and 21 elastic constants (Table 1) for TEGDMA.

VI. CONCLUSIONS

In the molecular dynamics study of TEGDMA, a dental material, the following observations emerge:

1. Changes in surface tension and viscosity can influence the properties of materials containing TEGDMA. For instance, in dental composites or adhesives, higher surface tension and viscosity can affect the wetting and bonding characteristics of the material to the tooth surface. These properties can significantly impact the overall performance and durability of dental restorations.
2. Spectral studies shed light on the possible chemical transformations and reaction kinetics of TEGDMA.
3. The physical properties of TEGDMA play an important role in dental composites. Research focused on parameters such as lattice energy, electronegativity, elastic constants, spatial dependence of moduli, refractive index, and molecular polarizability provide valuable information on how TEGDMA affects these properties.
4. The degree of conversion, degree of polarization, and glass transition temperature (Tg) values may indicate how TEGDMA behaves in composites.

Author contributions: B.N.A: Computation, writing and investigation.
H.S: resources, writing review.
M.M: investigation,
M.B.N: investigation.
S.G.J: investigation,
B.C.M: supervision, writing review.
R.S: supervision, resources, writing, conceptualization.

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