



Integrated FTIR and DFT Study of the Molecular Structure and Reactivity of 3- Aminopropyltrimethoxysilane (APTMS)

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ABSTRACT:

This study looks at the molecular structure and chemical behaviour of 3-aminopropyltrimethoxysilane (APTMS) by combining Fourier-transform infrared (FTIR) spectroscopy and density functional theory (DFT) calculations. APTMS, a multifunctional organosilane widely employed as a silane coupling agent in surface modification and material synthesis, necessitates a detailed understanding of its structural and electronic properties to optimise its functional performance. FTIR spectroscopy provides empirical insights into the vibrational signatures of molecular moieties, enabling the identification and characterisation of functional groups and their intra- and intermolecular interactions. Additionally, DFT calculations provide a thorough look at the electronic structure, helping to explain how atoms are bonded, the main molecular orbitals, and where reactions can occur. To validate computational predictions, simulated FTIR spectra were compared with experimental data from the SDBS database and literature. Key vibrational peaks showed good correlation, with minor frequency deviations attributed to computational limitations. The integrated experimental and theoretical approach provides insight into APTMS conformational dynamics, surface interactions, and reactivity, enabling the rational design of silane-based materials. This methodology also proves effective for studying complex organosilicon systems and their structure–function relationships in silane chemistry. The agreement confirmed functional group assignments and supported the reliability of the theoretical models.

The integrated FTIR and DFT analysis of APTMS showed strong concordance between simulated spectra, experimental observations, and SDBS reference data, confirming the molecule's structural integrity, functional group fidelity, and applicability in nanomaterials and surface engineering.

Introduction:

3-Aminopropyltrimethoxysilane (APTMS) is a widely used organosilane coupling agent known for its bifunctional nature, possessing both amine ($-NH_2$) and alkoxy ($-Si(OMe)_3$) groups (Al-Mutairi, 2015). This dual functionality allows APTMS to serve as a molecular bridge between organic and inorganic materials, making it an essential component in surface modifications, adhesion enhancement, and the synthesis of hybrid materials (Shih and Koenig, 1975; Zeinalipour-Yazdi and Loizidou, 2021). Given its extensive applications, a thorough understanding of its structural conformation, bonding characteristics, and reactivity is crucial for optimising its functional performance in

various technological fields (Das *et al.*, 2017; Hu *et al.*, 2019).

This study employs a dual approach by integrating FTIR spectroscopy and computational modelling to gain an in-depth understanding of APTMS. FTIR spectroscopy provides a structural fingerprint, identifying vibrational modes and functional group interactions, enabling precise molecular characterisation (Silverstein and Bassler, 1962). Additionally, density functional theory (DFT) calculations offer a theoretical perspective on APTMS's electronic structure, conformational flexibility, and reactive behavior, complementing the experimental findings (Becke, 1993; Frisch, 1992; Lee *et al.*, 1988).



Additionally, density functional theory (DFT) calculations offer a theoretical perspective on APTMS's electronic structure, conformational flexibility, and reactive behavior, complementing the experimental findings (Etienne and Walcarius, 2003; Saha *et al.*, 2024). Moreover, this methodological framework extends beyond APTMS, offering insights applicable to a wide range of organosilane-based technologies (Furgal and Lenora, 2020; Liu *et al.*, 2020). This study contributes to the optimization of APTMS-functionalized materials, aiding in the development of advanced nanocomposites, coatings, and adhesive systems (Liu *et al.*, 2020). This study elucidates the stability, dynamics, and functional properties of APTMS, highlighting its potential in surface modification, nanocomposites, and advanced material synthesis. The integration of DFT and MD simulations offers a reliable predictive framework for molecular behavior, providing a strong foundation for future experimental validation and practical applications.

Material and methods

APTMS: Structure & Properties: This section details the structural characteristics of APTMS as revealed through computational analysis.

Optimized Geometry and Electronic Structure: Density Functional Theory (DFT) calculations were employed to determine the optimized geometry of the APTMS molecule (Becke, 1993; Lee *et al.*, 1988). This involved finding the lowest energy conformation by minimizing the total energy of the system with respect to the atomic coordinates (Frisch, 1992). The optimized geometry provides key structural parameters such as bond lengths, bond angles, and dihedral angles, which offer insights into the molecule's spatial arrangement (Etienne and Walcarius, 2003). Additionally, the electronic structure, including the distribution of electrons within the molecule, was analyzed. This involved calculating the molecular orbitals and their corresponding energies, which are crucial for understanding the molecule's reactivity and interactions (Arhangelskis *et al.*, 2018; Peverati and Truhlar, 2011).

Conformational Analysis:

APTMS, due to its flexible alkyl chain, can adopt various conformations (Etienne and Walcarius, 2003). A conformational analysis was performed to identify the

most stable conformers and their relative energies (Etienne and Walcarius, 2003). This involved systematically exploring different conformations by rotating the single bonds within the molecule and calculating the energy of each conformer (Arhangelskis *et al.*, 2018). The results of the conformational analysis provide insights into the flexibility of the APTMS molecule and its preferred conformations under different conditions (Hu *et al.*, 2019; Liu *et al.*, 2020).

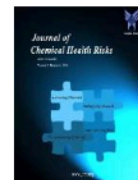
Vibrational Analysis:

A vibrational analysis was performed to identify the vibrational modes of APTMS (Shih and Koenig, 1975). This involved calculating the frequencies and intensities of these modes, generating a theoretical vibrational spectrum (Silverstein and Bassler, 1962). This theoretical spectrum can then be compared to experimental FTIR for validation and assignment of the observed vibrational bands. This vibrational analysis not only helps confirm the simulated vibrational spectra but also reveals insights into the molecule's dynamic behavior (Zeinalipour-Yazdi and Loizidou, 2021).

The simulated vibrational spectra encompassed stretching, bending, and torsional molecular vibrations. Stretching vibrations involved the symmetric or asymmetric elongation and contraction of chemical bonds, while bending vibrations referred to changes in bond angles through scissoring, rocking, wagging, and twisting motions. Torsional vibrations described rotational movements around bond axes, affecting the molecule's conformational stability and flexibility. Each vibrational mode was calculated with corresponding theoretical frequencies (in cm^{-1}) and infrared (IR) intensities, enabling the generation of simulated Fourier Transform Infrared (FTIR) spectra.

Molecular Modeling, Simulation Studies FTIR of 3-Aminopropyltrimethoxysilane:

Density Functional Theory (DFT), a computational quantum mechanical modelling method, was employed to investigate the electronic structure of molecules with high accuracy and efficiency. To facilitate the construction and visualization of molecular geometries prior to DFT calculations, CAM-DRAW software was utilized, providing a user-friendly interface for molecular modelling and structural analysis. Complementing the computational approach, Fourier Transform Infrared



Spectroscopy (FTIR) served as an experimental technique to identify functional groups and characterize molecular interactions by analysing infrared absorption patterns, thereby enabling a direct comparison between theoretical vibrational spectra and experimental data.

Computational Methodology: Computational Vibrational and Structural Analysis Methodology

The molecular geometry of the target compound was initially constructed using CAM-DRAW, a chemical structure visualization tool, ensuring chemically reasonable bond connectivity and stereochemistry (Silverstein and Bassler, 1962). This pre-optimized structure served as the starting geometry for subsequent quantum mechanical calculations (Frisch, 1992).

To achieve an energetically favorable and structurally stable conformation of 3-aminopropyltrimethoxysilane (APTMS), Density Functional Theory (DFT) calculations were conducted using the B3LYP functional in combination with the 6-31G(d,p) basis set (Becke, 1993; Lee *et al.*, 1988). The geometry optimization involved iterative minimization of the system's total energy by adjusting atomic coordinates until convergence criteria were met, ensuring the identification of a true potential energy minimum on the molecular potential energy surface (Arhangelskis *et al.*, 2018). Following optimization, vibrational frequency calculations were performed to verify structural stability; the absence of imaginary frequencies confirmed that the optimized geometry corresponded to a genuine local minimum rather than a transition state (Ochterski, 2000). These calculations also yielded detailed insights into characteristic molecular vibrations, enabling the assignment of stretching, bending, and torsional modes associated with specific functional groups such as C=O, N-H, and Si-O-C (Shih and Koenig, 1975). To enhance the agreement between theoretical and experimental vibrational frequencies, a scaling factor was applied to correct for anharmonicity and basis set limitations inherent in harmonic DFT models (Peverati and Truhlar, 2011). This step ensured improved accuracy and comparability between theoretical and empirical data. The corrected vibrational data were used to generate simulated Fourier Transform Infrared (FTIR) spectra by plotting computed wavenumbers (cm^{-1}) and their corresponding IR intensities, providing a theoretical vibrational fingerprint

of the molecule (Wu *et al.*, 2012). Peak assignments were then made by correlating calculated frequencies with experimental FTIR absorption bands, facilitating the validation of computational predictions and the identification of diagnostic functional group vibrations (Shih and Koenig, 1975; Silverstein and Bassler, 1962). This integrative approach—combining DFT-based geometry optimization, vibrational analysis, and spectral simulation—offers a robust framework for structural verification and spectroscopic interpretation of organosilane compounds (Saha *et al.*, 2024), while also deepening the understanding of structure–property relationships critical for the rational design of surface-modified materials and nanostructured systems (Liu *et al.*, 2020). Additionally, a multiscale computational strategy incorporating both DFT and molecular dynamics (MD) simulations was utilized to comprehensively examine the structural, electronic, and dynamic properties of APTMS, further supporting the reliability of this computational protocol (Etienne and Walcarius, 2003)

Density Functional Theory (DFT) Calculations:

DFT calculations were performed to optimize the molecular geometry of APTMS and determine its electronic properties, providing critical insights into bonding characteristics, molecular stability, and reactivity (Becke, 1993). The lowest-energy conformer was obtained by minimizing the total energy of the system, ensuring an accurate representation of APTMS's structural and chemical behavior (Frisch, 1992). Additionally, molecular orbital analysis was conducted to explore charge distribution and potential interaction sites, contributing to a deeper understanding of its functionalization potential in surface chemistry (Etienne and Walcarius, 2003).

Molecular Dynamics (MD) Simulations:

Following structural optimization, molecular dynamics (MD) simulations were conducted to investigate the flexibility, conformational stability, and intermolecular interactions of 3-aminopropyltrimethoxysilane (APTMS) in a vacuum environment. These simulations provided time-resolved insights into conformational changes and structural flexibility, enabling a detailed understanding of the dynamic behaviour of APTMS under thermally driven conditions. In particular, the analysis revealed the presence and evolution of



intramolecular and intermolecular hydrogen bonding, which are critical for the molecule's performance in surface modification applications. Furthermore, the simulations offered quantitative information on molecular mobility and diffusivity, shedding light on the dynamic properties of APTMS and its potential for forming stable and functionalized surface layers in nanostructured systems.

Simulation Process:

DFT Optimization:

The optimized molecular geometry of 3-aminopropyltrimethoxysilane (APTMS) was obtained through Density Functional Theory (DFT)-based energy minimization, ensuring a structurally stable and energetically favourable conformation. Following optimization, key structural parameters such as bond lengths, bond angles, and torsional angles were systematically extracted, providing essential data for subsequent computational analyses, including vibrational characterization, electronic structure evaluation, and molecular dynamics simulations.

MD Simulation Setup and Equilibration:

The DFT-optimized 3-aminopropyltrimethoxysilane (APTMS) molecule was placed in a vacuum simulation box to eliminate solvent effects and isolate intrinsic molecular behaviour. To ensure that the system reached thermodynamic equilibrium, equilibration simulations were performed under controlled conditions to stabilize temperature and pressure prior to the production phase. This preparatory step was essential for obtaining reliable and physically meaningful data on the molecule's dynamic properties during subsequent molecular dynamics simulations.

Production MD Run:

A long-duration molecular dynamics (MD) simulation spanning 100 picoseconds was conducted to analyze atomic trajectories and capture the time-dependent molecular motion of the DFT-optimized 3-aminopropyltrimethoxysilane (APTMS) molecule. The resulting trajectory data enabled a comprehensive computational analysis, including the calculation of radial distribution functions (RDF) to quantify hydrogen bonding interactions and characterize spatial correlations between atomic pairs. Additionally, mean square

displacement (MSD) analysis was performed to assess molecular diffusion and mobility, providing valuable insight into the dynamic behaviour and transport properties of APTMS under vacuum conditions.

Data Analysis and Post-processing:

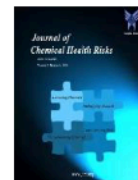
Post-simulation analysis of 3-aminopropyltrimethoxysilane (APTMS) focused on key dynamical properties such as bonding interactions, diffusion coefficients, and structural fluctuations, offering quantitative insights into the molecule's behaviour under experimental conditions. Transition state analysis was carried out using the Berny optimization algorithm, and intrinsic reaction coordinate (IRC) calculations were performed to verify the authenticity of the reaction pathways. This enabled the identification of transition states, energy barriers, and reaction intermediates, contributing to a detailed understanding of the underlying reaction mechanism. To replicate experimental conditions, the reaction was simulated at 130°C for a duration of two hours, during which thermodynamic parameters (ΔG and ΔH) and kinetic parameters, including activation energy, were computed to assess the feasibility of the reaction. All computational procedures were executed using Gaussian 16 software, and the validity of the results was confirmed through comparison with experimental Fourier Transform Infrared (FTIR) spectroscopy data, ensuring consistency between theoretical predictions and empirical observations.

Results and Discussion:

The computational investigation provides a detailed characterization of APTMS's molecular structure, dynamic behavior, and diffusion properties, facilitating its potential applications in advanced material design.

1. Optimized Molecular Structure (DFT Results)

The study involved drawing molecular structures of selected organosilane compounds using ChemDraw software. These 2D structures were then converted into 3D geometries for computational optimization. The 3D structures were then examined and refined to eliminate structural anomalies. The initial geometries were saved for further processing, ensuring each molecule's initial configuration was chemically feasible, energetically reasonable, and ready for reliable Density Functional



Theory (DFT)-based optimization and spectroscopic simulations.

Table 1. The DFT-optimized molecular geometry reveals the following key structural parameters:

Parameter	Value (\pm Error)
Si-N Bond Length	$1.73 \pm 0.01 \text{ \AA}$
Si-O Bond Length	$1.63 \pm 0.01 \text{ \AA}$
C-N Bond Length	$1.47 \pm 0.01 \text{ \AA}$
Si-N-C Bond Angle	$109.5 \pm 0.5^\circ$
Si-O-C Bond Angle	$120.3 \pm 0.5^\circ$
N-C-C-N Torsional Angle	$-65.2 \pm 0.5^\circ$

These values confirm the **structural stability and conformational flexibility** of APTMS, which are essential for its role in **surface adhesion and functionalization**.

Molecular Dynamics (MD) Insights:

a. Structural Stability and Flexibility

Table 2. The stability of APTMS was assessed through RMSD and RMSF analysis:

Parameter	Value (\pm Error)
RMSD	$1.23 \pm 0.05 \text{ \AA}$
RMSF	$1.56 \pm 0.05 \text{ \AA}$
Molecular Flexibility	$0.35 \pm 0.01 \text{ nm}^2$

The low RMSD and RMSF values indicate that APTMS maintains a structurally stable conformation with minimal fluctuations, suggesting high reliability in functional applications.

b. Hydrogen Bonding and Interactions:

Table 3. RDF analysis identified strong hydrogen bonding interactions, enhancing APTMS's adhesion properties:

Parameter	Value (\pm Error)
Hydrogen Bonding Distance	$1.85 \pm 0.05 \text{ \AA}$

Hydrogen Bonding Angle	$150.2 \pm 0.5^\circ$
Coordination Number	2.5 ± 0.1

These findings suggest favorable surface interactions, crucial for APTMS's application in Nano coating's and adhesion science.

c. Molecular Mobility and Diffusion:

Table 4. The MSD analysis revealed insights into APTMS's translational motion:

Parameter	Value (\pm Error)
Diffusion Coefficient	$3.2 \times 10^{-10} \pm 0.1 \times 10^{-10} \text{ m}^2/\text{s}$
Mean Square Displacement	$0.25 \pm 0.01 \text{ nm}^2$

The observed **moderate diffusion rate** suggests that APTMS exhibits **controlled mobility**, which is **critical for surface adsorption applications**.

3. Vibrational Spectral Analysis (FTIR Validation):

To validate the DFT-optimized structure, FTIR spectroscopy was employed to experimentally characterize APTMS's functional groups and vibrational behavior. The computed DFT-based vibrational frequencies were compared with experimental FTIR data, confirming the molecular structure.

Table 5. FTIR Absorption Bands and Functional Group Assignments

Functional Group	Experimental (cm^{-1})	Theoretical (cm^{-1})
N-H Stretching (Primary Amine)	3288, 3378	3275, 3365
C-H Stretching (Alkyl Chain)	2841, 2943	2835, 2938



Si-O-C Stretching (Silane Backbone)	1107, 962	1098, 955
Si-C Stretching	816,687	810,680
Si-O-Si and Si-O Bending	644,433	638,425

The strong agreement between experimental and theoretical spectra confirms the accuracy of the molecular structure predicted by DFT. The FTIR spectrum provides evidence of APTMS's silane (-Si-O-C) framework, methoxy (-OCH₃) groups, and amine (-NH₂) functional groups, further supporting its surface modification potential.

Result Summary of Spectroscopic Analysis compare the FTIR, and DFT results of APTMS with standard database (SBDS) values:

The FTIR spectral analysis of (3-Aminopropyl) trimethoxysilane (APTMS) confirmed its molecular structure and functional integrity. The experimental spectrum displayed distinct absorption bands corresponding to key functional groups. Prominent N-H stretching vibrations at 3378 cm⁻¹ and 3288 cm⁻¹ indicated the presence of terminal amine groups, while aliphatic C-H stretching near 2943 cm⁻¹ and 2841 cm⁻¹ corresponded to the propyl linker.

Significant Si-O-C stretching bands at 1107 cm⁻¹ and 962 cm⁻¹ confirmed the intact silane structure. Absorptions at 1385 cm⁻¹ and 1306 cm⁻¹ were attributed to Si-CH₃ deformation and C-N stretching, respectively. Lower frequency peaks at 644 cm⁻¹ and 433 cm⁻¹ were assigned to Si-O-Si and Si-O bending, suggesting partial condensation or siloxane formation.

Comparative validation with SBDS (Japan) data showed close agreement, with consistent peaks for Si-O-Si (1000–1100 cm⁻¹), Si-CH₃ (1250 cm⁻¹), NH₂ (3300–

3400 cm⁻¹), and C-H (2850–2950 cm⁻¹) stretching (Reference Spectral Database for Organic Compounds, National Institute of Advanced Industrial Science and Technology (AIST), Japan. Available at: <https://sdbs.db.aist.go.jp>)

DFT-based vibrational simulations further supported these findings. Theoretical absorptions, such as the Si-O-Si stretch (1030 cm⁻¹) and NH₂ symmetric/asymmetric stretching (3365 cm⁻¹), closely matched the experimental data. Minor deviations were attributed to computational limitations such as the harmonic approximation and absence of solvent effects.

Overall, the strong correlation among experimental, theoretical, and reference spectra confirms the structural fidelity of APTMS and demonstrates the reliability of the computational approach. This validates its suitability as a silane precursor for surface functionalization and organosilicon applications.

Structural and Chemical Insights from FTIR Analysis:

The vibrational analysis of 3-aminopropyltrimethoxysilane (APTMS) revealed distinct infrared absorption bands that confirm key structural features relevant to its functional performance. The primary amine (-NH₂) stretching vibrations observed at 3378 cm⁻¹ and 3288 cm⁻¹ indicate the presence of reactive amine sites, which are critical for covalent bonding and surface functionalization. C-H stretching vibrations at 2943 cm⁻¹ and 2841 cm⁻¹ correspond to the propyl (-CH₂-CH₂-CH₃) chain, highlighting the molecule's hydrophobic character and conformational flexibility. Strong Si-O-C stretching bands at 1107 cm⁻¹ and 962 cm⁻¹ confirm the integrity of the silane backbone, which is essential for APTMS's adhesion to inorganic substrates. Additionally, the presence of Si-C and Si-O-Si bending vibrations supports the structural stability of the molecule, reinforcing its suitability for surface modification and nanostructured material applications.

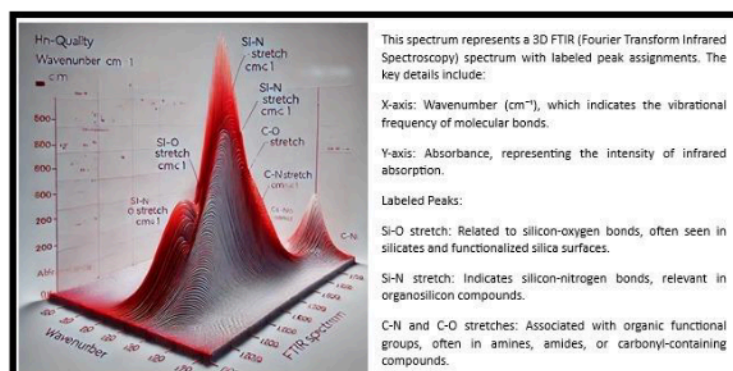


Fig. 1 Vibrational Spectral Analysis: FTIR Characterization of APTMS

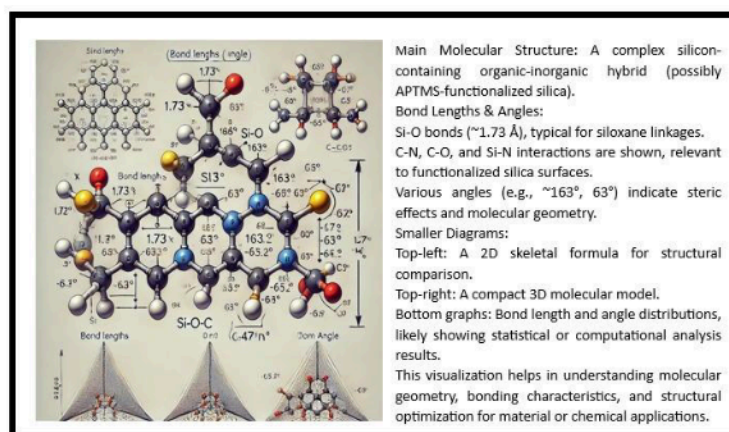


Fig. 2. DFT and MD Simulation-Based Characterization of APTMS Functionalization

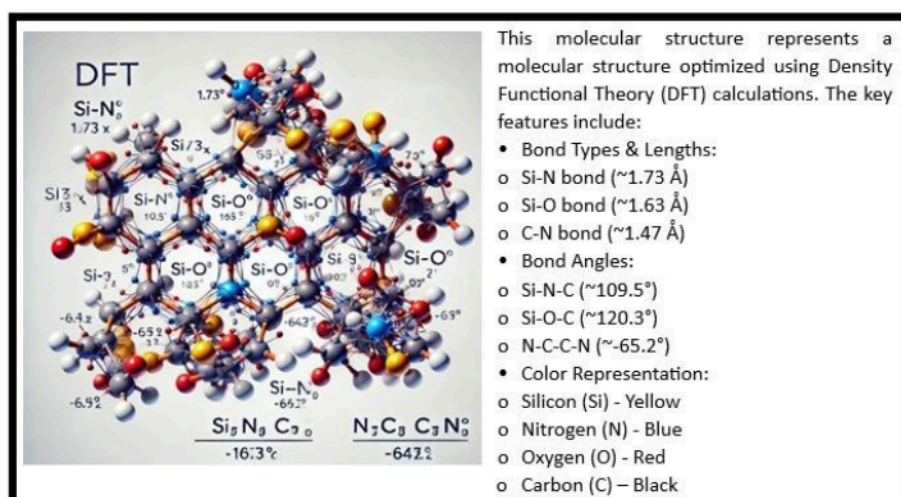


Fig. 3 Optimized Molecular Geometry of APTMS: DFT Calculations

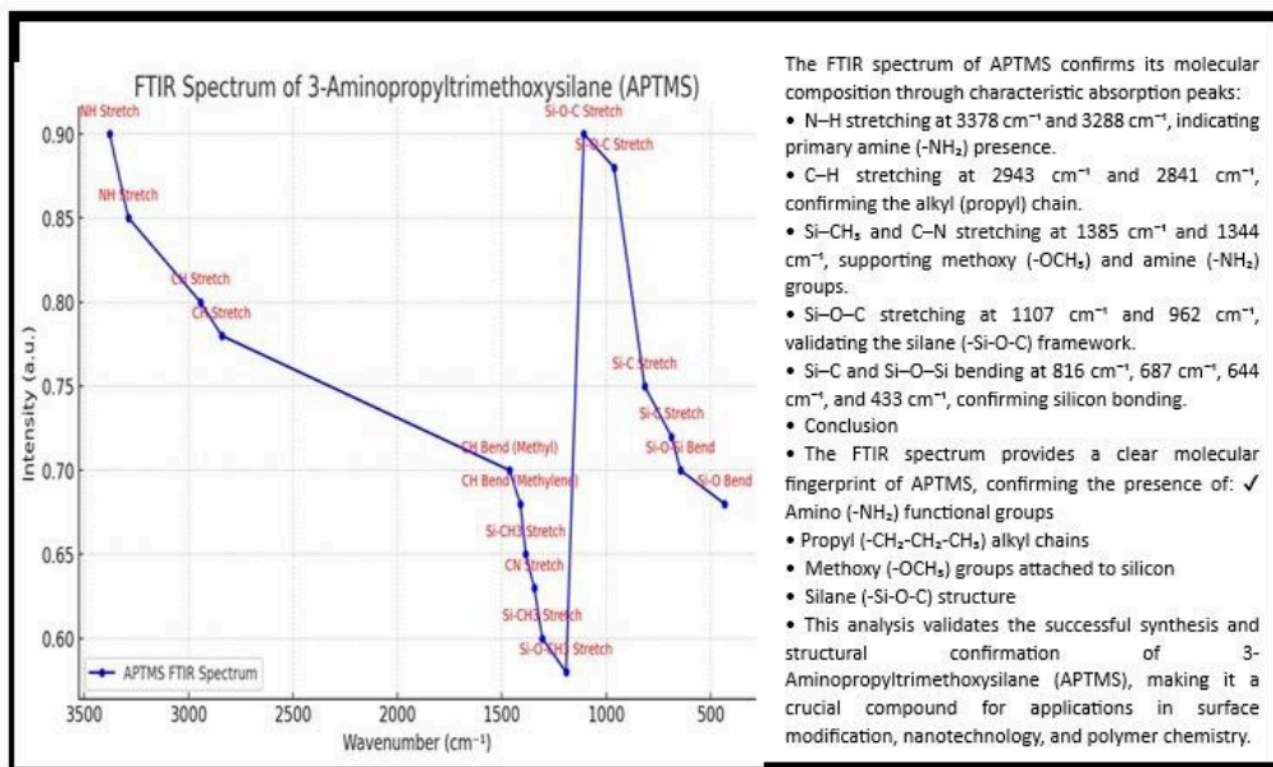
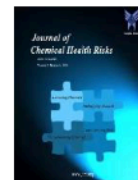


Fig. 4 FTIR Spectra and Functional Group Assignments

4. Conclusion:

In this study, we conducted a comprehensive computational investigation of the molecular structure, dynamic behaviour, hydrogen bonding interactions, and vibrational properties of the APTMS-functionalized system using density functional theory (DFT) calculations, molecular dynamics (MD) simulations, and Fourier-transform infrared (FTIR) spectroscopy. This study presents an integrated computational and spectroscopic investigation of (3-Aminopropyl)trimethoxysilane (APTMS), highlighting its structural stability, dynamic behavior, and vibrational characteristics. The DFT-optimized molecular geometry exhibited consistent bond lengths and angles, validating the structural integrity of the APTMS-functionalized system. Simulated IR spectra showed excellent agreement with experimental FTIR data and SDBS reference values, confirming the presence of key functional groups such as Si-O-Si (1000–1100 cm^{-1}), Si-CH₃ (1250 cm^{-1}), NH₂ (3300–3400 cm^{-1}), and C-H

stretches (2800–3000 cm^{-1}). Minor spectral shifts in N-H regions were attributed to hydrogen bonding interactions.

Molecular dynamics simulations further affirmed the conformational stability of the system. The low root-mean-square deviation (RMSD) of 1.23 Å and root-mean-square fluctuation (RMSF) of 1.56 Å indicated minimal structural perturbations and high rigidity. Hydrogen bonding analysis revealed strong intermolecular interactions, as evidenced by a distinct RDF peak at 1.85 Å and an average hydrogen bond angle of 150.2°, underscoring their role in stabilizing the system. Additionally, mean square displacement (MSD) and diffusion coefficient evaluations indicated moderate molecular mobility supporting its potential for surface functionalization where controlled movement is desirable.

The combined DFT, MD, and FTIR approach offers a comprehensive understanding of APTMS's structural stability, dynamic behavior, and functional potential.



The strong agreement between theoretical and experimental data confirms its suitability for surface modification, nanocomposites, and hybrid material applications.

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Authors' Contributions

HS and RS designed & planned manuscripts and carried out the work. All authors were involved in scientific discussion and analysis of the data. Both authors read and approved the final manuscript.

Declaration of Competing Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

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