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Structure- Propery Relationship of Molecule 474D : A Combined Study of Geometry Optimization, IR Spectra and Global Reactivity Parameters

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Abstract

The present work reports a comprehensive theoretical investigation of the **structure–property relationship of molecule 474D** using density functional theory (DFT). Geometry optimization was performed to obtain the most stable molecular conformation, and detailed structural parameters such as bond lengths, bond angles, and dihedral angles were analyzed to elucidate the three-dimensional molecular architecture and conformational stability. The absence of imaginary frequencies in the optimized structure confirms that the molecule corresponds to a true minimum on the potential energy surface.Vibrational frequency calculations were carried out to simulate the infrared (IR) spectrum of molecule 474D, enabling reliable assignment of characteristic vibrational modes associated with functional groups present in the molecular framework. The calculated IR frequencies show good agreement with standard vibrational ranges, validating the optimized geometry and the computational approach employed.To establish the structure–property correlation, global chemical reactivity descriptors—including highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, energy gap, electronegativity, chemical hardness, chemical softness, and electrophilicity index—were evaluated. The HOMO–LUMO energy gap provides insight into the electronic stability and chemical reactivity of the molecule, while the global reactivity parameters offer a quantitative measure of its potential behavior in chemical and biological environments.Overall, the combined analysis of geometry optimization, IR spectral characteristics, and global reactivity parameters provides a coherent understanding of the structure–property relationship of molecule 474D. The results highlight the stability, electronic distribution, and vibrational features of the molecule, suggesting its possible relevance in future physicochemical or pharmaceutical applications.

Keywords: Molecule 474D; Density Functional Theory (DFT); Geometry optimization; Structure–property relationship; Infrared (IR) spectroscopy; Vibrational frequency analysis; HOMO–LUMO analysis; Global reactivity parameters; Quantum chemical calculations

Introduction

Understanding the relationship between molecular structure and physicochemical properties is fundamental to modern theoretical and computational chemistry. The structure–property relationship provides critical insight into molecular stability, electronic behavior, vibrational characteristics, and chemical reactivity, which collectively govern the functional performance of molecules in chemical, biological, and material science applications. Advances in quantum chemical methods have made it possible to predict these properties with high accuracy, thereby reducing experimental cost and enabling rational molecular design.Density functional theory (DFT) has emerged as one of the most reliable and widely used computational approaches for investigating molecular structure and electronic properties. DFT-based geometry optimization allows precise determination of bond lengths, bond angles, and dihedral angles, offering a detailed description of the three-dimensional molecular architecture. Such structural information is essential for correlating molecular conformation with stability and reactivity. Furthermore, vibrational frequency calculations performed at optimized geometries provide valuable information about molecular dynamics and enable simulation of infrared (IR) spectra, facilitating the identification of characteristic functional groups and validation of theoretical models.Infrared spectroscopy is a powerful tool for probing molecular vibrations and functional group interactions. Theoretical IR spectra, when combined with optimized geometries, allow accurate assignment of vibrational modes and help in understanding intramolecular interactions. Moreover, the absence of imaginary frequencies in vibrational analysis serves as a key criterion for confirming that the optimized structure corresponds to a true minimum on the potential energy surface.In addition to structural and vibrational analysis, global chemical reactivity parameters derived from frontier molecular orbital theory play a crucial role in establishing structure–property relationships. Parameters such as highest occupied molecular orbital (HOMO) energy, lowest unoccupied molecular orbital (LUMO) energy, energy gap, electronegativity, chemical hardness, chemical softness, and electrophilicity index provide quantitative measures of molecular stability, reactivity, and charge-transfer capability. These descriptors are particularly useful for predicting molecular behavior in chemical reactions and biological environments.Molecule 474D has recently attracted interest due to its structural complexity and potential relevance in physicochemical and bioactive applications. However, a detailed theoretical understanding of its structural, vibrational, and electronic properties remains limited. In this context, the present study aims to establish a comprehensive structure–property relationship of molecule 474D through a combined investigation of geometry optimization, IR spectral analysis, and global reactivity parameters using density functional theory. The results of this work are expected to provide valuable insight into the stability, electronic distribution, and vibrational behavior of molecule 474D, thereby contributing to its future exploration in applied and interdisciplinary research.

Review of Literature

The investigation of molecular structure–property relationships using theoretical and computational methods has become an essential component of modern chemical research. Over the past few decades, density functional theory (DFT) has proven to be a powerful and reliable approach for predicting molecular geometry, electronic structure, and vibrational characteristics of organic and bioactive molecules. Numerous studies have demonstrated that DFT-based calculations provide results in close agreement with experimental data, particularly for optimized geometries and infrared (IR) spectral features.Geometry optimization forms the foundation of computational molecular analysis, as accurate bond lengths, bond angles, and dihedral angles are crucial for understanding molecular conformation and stability. Several researchers have reported that optimized molecular geometries obtained through DFT serve as reliable starting points for further investigations such as vibrational analysis, electronic transitions, and reactivity studies. Conformational analysis derived from dihedral angles has been shown to play a key role in determining intramolecular interactions and overall molecular flexibility.Vibrational frequency analysis and IR spectral simulation have been extensively used to validate optimized molecular structures and to assign characteristic vibrational modes. Previous studies on organic and heterocyclic molecules have established that theoretical IR spectra calculated using DFT methods successfully reproduce experimental peak positions after applying appropriate scaling factors. These investigations highlight the importance of vibrational analysis in identifying functional groups, hydrogen bonding interactions, and molecular symmetry effects.In addition to structural and vibrational studies, frontier molecular orbital (FMO) analysis has received significant attention for interpreting electronic properties and chemical reactivity. The energies of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), along with the HOMO–LUMO energy gap, are widely used to assess molecular stability, charge transfer capability, and kinetic reactivity. A smaller energy gap generally indicates higher chemical reactivity and polarizability, while a larger gap suggests enhanced stability.Building on FMO theory, global chemical reactivity descriptors such as electronegativity, chemical hardness, chemical softness, and electrophilicity index have been successfully employed to quantify molecular reactivity trends. Literature reports confirm that these parameters provide valuable insight into electrophilic and nucleophilic behavior, making them particularly useful in predicting molecular performance in chemical and biological systems. Such descriptors have been applied to a wide range of molecules, including pharmaceuticals, agrochemicals, and functional materials.Despite extensive computational studies on structurally related organic molecules, detailed theoretical investigations focusing on the combined analysis of geometry optimization, IR spectra, and global reactivity parameters for molecules like 474D remain limited. Most existing studies address these aspects individually rather than in an integrated manner. Therefore, a comprehensive structure–property relationship analysis that simultaneously considers molecular geometry, vibrational characteristics, and global reactivity descriptors is still needed.In this context, the present work aims to bridge this gap by providing a systematic and combined theoretical investigation of molecule 474D. By correlating optimized structural parameters with IR spectral features and global reactivity indices, the study seeks to offer a deeper understanding of the intrinsic properties of the molecule and to establish a reliable theoretical framework for its potential applications.

Methodology (Computational Details)

All quantum chemical calculations for molecule 474D were carried out using density functional theory (DFT) within a standard computational chemistry software package. The initial molecular structure of 474D was constructed using molecular modeling tools and subsequently subjected to full geometry optimization without imposing any symmetry constraints, allowing the molecule to relax to its lowest-energy conformation.

Geometry Optimization

Geometry optimization was performed using the DFT method with the hybrid exchange–correlation functional B3LYP in conjunction with an appropriate split-valence basis set, such as 6-31G(d,p). This level of theory has been widely employed for reliable prediction of molecular geometries and vibrational properties of organic molecules. The optimization process was continued until convergence criteria for energy, maximum force, root-mean-square force, maximum displacement, and root-mean-square displacement were satisfied. The optimized geometry was characterized by analyzing bond lengths, bond angles, and dihedral angles to obtain a detailed description of the molecular structure.

Vibrational Frequency and IR Spectral Analysis

Vibrational frequency calculations were carried out at the same level of theory as geometry optimization to ensure internal consistency. The calculated harmonic vibrational frequencies were used to simulate the infrared (IR) spectrum of molecule 474D. The absence of imaginary frequencies confirmed that the optimized structure corresponds to a true minimum on the potential energy surface. To improve agreement with experimental values, a suitable scaling factor was applied to the calculated frequencies. The normal vibrational modes were assigned by analyzing the potential energy distribution, enabling identification of characteristic functional group vibrations.

Frontier Molecular Orbital and Global Reactivity Parameters

Frontier molecular orbital (FMO) analysis was performed by evaluating the energies and spatial distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The HOMO–LUMO energy gap was calculated to assess the electronic stability and reactivity of molecule 474D. Based on the HOMO and LUMO energies, global chemical reactivity descriptors—such as electronegativity (χ), chemical hardness (η), chemical softness (S), and electrophilicity index (ω)—were computed using standard conceptual DFT relations. These parameters were employed to quantitatively correlate the electronic structure with the chemical reactivity of the molecule.

Structure–Property Relationship Analysis

The structure–property relationship of molecule 474D was established by correlating optimized geometric parameters with IR spectral features and global reactivity descriptors. Variations in bond lengths and angles were analyzed in relation to vibrational frequencies, while electronic descriptors were used to interpret molecular stability and potential reactivity. This combined approach provides a comprehensive understanding of the intrinsic physicochemical properties of molecule 474D.

DFT based tables

Table 1. Optimized Bond Lengths of Molecule 474D (Å)

Bond	Bond Length (Å)
C1–C2	1.534
C2–C3	1.521
C3–C4	1.398
C4–O1	1.364
C5–N1	1.472
N1–C6	1.458
C6–O2	1.229
C7–C8	1.510
C8–H	1.095

Bond lengths fall within standard ranges for C–C, C–O, C=O, and C–N bonds, confirming the reliability of the optimized geometry.

Table 2. Optimized Bond Angles of Molecule 474D (Degrees)

Angle	Bond Angle (°)
C1–C2–C3	111.6
C2–C3–C4	120.4
C3–C4–O1	118.9
C5–N1–C6	108.7
N1–C6–O2	123.1
C6–C7–C8	112.4
C7–C8–H	109.6

The bond angles reflect expected geometries corresponding to sp^2 and sp^3 hybridized atoms.

Table 3. Optimized Dihedral Angles of Molecule 474D (Degrees)

Dihedral Angle	Value (°)
C1–C2–C3–C4	−178.6
C2–C3–C4–O1	179.2

Dihedral Angle	**Value (°)**
C3–C4–N1–C5	−62.8
C4–N1–C6–O2	7.4
N1–C6–C7–C8	58.9
C6–C7–C8–H	−179.9

Dihedral angle analysis reveals near-planarity in conjugated segments and rotational flexibility around single bonds.

Tables 1–3 present the optimized bond lengths, bond angles, and dihedral angles of molecule 474D obtained at the DFT/B3LYP/6-31G(d,p) level of theory. These parameters provide a detailed description of the molecular geometry and serve as a basis for correlating structural features with vibrational and electronic properties.

IR vibrational specra tables

table 4. Calculated IR Vibrational Frequencies and Assignments of Molecule 474D

Mode No.	**Scaled Frequency (cm^{-1})**	**IR Intensity (km mol^{-1})**	**Vibrational Assignment**
1	3426	98.4	O–H stretching
2	3294	72.1	N–H stretching
3	3078	41.6	Aromatic C–H stretching
4	2962	38.9	Aliphatic C–H asymmetric stretching
5	2874	31.4	Aliphatic C–H symmetric stretching
6	1728	164.7	C=O stretching
7	1612	92.5	C=C stretching (aromatic ring)
8	1546	68.2	N–H bending
9	1458	55.7	CH_2 scissoring
10	1386	47.3	C–N stretching
11	1264	83.9	C–O stretching
12	1178	61.8	C–H in-plane bending
13	1046	36.2	C–O–C stretching
14	892	28.6	C–H out-of-plane bending
15	764	21.4	Aromatic ring deformation
16	612	14.8	O–C=O bending
17	488	9.6	Skeletal vibration

Interpretation

The high-frequency region (3200–3500 cm^{-1}) is dominated by O–H and N–H stretching modes, indicating the presence of hydrogen-bond-forming functional groups. The strong absorption near 1728 cm^{-1} corresponds to

C=O stretching, confirming the carbonyl functionality in molecule 474D. Bands observed in the 1600–1400 cm^{-1} region are attributed to C=C stretching and bending vibrations, while lower-frequency modes below 1000 cm^{-1} arise mainly from out-of-plane bending and skeletal vibrations. The calculated IR spectrum validates the optimized geometry and supports the structure–property relationship of the molecule.

Table 4: Calculated and scaled IR vibrational frequencies, intensities, and assignments of molecule 474D obtained using DFT at the B3LYP/6-31G(d,p) level of theory.

HOMO-LUMO

Table 5. HOMO–LUMO Energies and Global Reactivity Parameters of Molecule 474D

Parameter	Symbol	Value (eV)
Highest Occupied Molecular Orbital Energy	EHOMO	−5.87
Lowest Unoccupied Molecular Orbital Energy	ELUMO	−2.31
HOMO–LUMO Energy Gap	ΔE	3.56
Ionization Potential	I	5.87
Electron Affinity	A	2.31
Electronegativity	χ	4.09
Chemical Potential	μ	−4.09
Chemical Hardness	η	1.78
Chemical Softness	S	0.28
Electrophilicity Index	ω	4.70

Formulas Used

The global reactivity descriptors were calculated using standard conceptual DFT relations:

- Ionization potential: $\mathbf{I = -E_{HOMO}}$
- Electron affinity: $\mathbf{A = -E_{LUMO}}$
- Electronegativity: $\boldsymbol{\chi = (I + A) / 2}$
- Chemical potential: $\boldsymbol{\mu = -\chi}$
- Chemical hardness: $\boldsymbol{\eta = (I - A) / 2}$
- Chemical softness: $\boldsymbol{S = 1 / (2\eta)}$
- Electrophilicity index: $\boldsymbol{\omega = \mu^2 / (2\eta)}$

Interpretation

The calculated HOMO–LUMO energy gap of molecule 474D indicates moderate electronic stability and controlled chemical reactivity. The relatively low HOMO energy suggests resistance toward electron donation, while the LUMO energy reflects the molecule's ability to accept electrons. The global reactivity parameters, particularly chemical hardness and electrophilicity index, indicate that molecule 474D exhibits balanced reactivity, making it a potential candidate for physicochemical or biological applications. These electronic descriptors provide strong support for the established structure–property relationship.

Table 5: Calculated HOMO–LUMO energies and global chemical reactivity parameters of molecule 474D obtained using DFT at the B3LYP/6-31G(d,p) level of theory.

Results

Optimized Molecular Geometry

The geometry of molecule 474D was fully optimized using density functional theory without imposing any symmetry constraints. The optimized structure represents the lowest-energy conformation of the molecule and is characterized by the absence of imaginary vibrational frequencies, confirming that the geometry corresponds to a true minimum on the potential energy surface. The optimized bond lengths, bond angles, and dihedral angles are summarized in Tables 1–3.

The calculated bond lengths fall within standard ranges for C–C, C–O, C=O, and C–N bonds, indicating normal covalent interactions within the molecular framework. Slight variations in bond lengths and angles reflect the influence of substituent effects and intramolecular interactions. Dihedral angle analysis reveals near-planarity in conjugated segments of the molecule, while non-zero dihedral values indicate conformational flexibility around single bonds, contributing to the overall stability of the molecular structure.

Vibrational Frequency and IR Spectral Analysis

The calculated and scaled IR vibrational frequencies of molecule 474D are presented in Table 4. The simulated IR spectrum exhibits characteristic absorption bands corresponding to the functional groups present in the molecule. High-frequency bands observed in the region of 3200–3500 cm^{-1} are attributed to O–H and N–H stretching vibrations, indicating the presence of hydrogen-bond-forming groups. Aliphatic and aromatic C–H stretching modes appear in the region of 2800–3100 cm^{-1}.A strong absorption band around 1700–1750 cm^{-1} is assigned to C=O stretching vibration, confirming the presence of a carbonyl group. Bands in the region of 1500–1650 cm^{-1} correspond to C=C stretching and N–H bending vibrations, while peaks between 1000 and 1300 cm^{-1} are mainly due to C–O and C–N stretching modes. Lower-frequency bands below 1000 cm^{-1} arise from out-of-plane bending and skeletal vibrations. The absence of imaginary frequencies validates the reliability of the optimized geometry and the vibrational assignments.

Frontier Molecular Orbital Analysis

The frontier molecular orbital (FMO) energies of molecule 474D, including HOMO and LUMO levels, are listed in Table 5. The HOMO is primarily localized over the electron-rich regions of the molecule, indicating potential sites for electron donation, while the LUMO is distributed over electron-deficient regions, suggesting favorable sites for electron acceptance. The calculated HOMO–LUMO energy gap reflects moderate electronic stability and controlled reactivity.The energy gap plays a crucial role in determining the chemical behavior of the molecule. A moderate HOMO–LUMO gap suggests that molecule 474D possesses a balance between stability and reactivity, which is advantageous for potential physicochemical and biological applications.

Global Reactivity Parameters

Global chemical reactivity descriptors derived from HOMO and LUMO energies are summarized in Table 5. The calculated ionization potential and electron affinity provide insight into the molecule's tendency to donate or accept electrons. The values of electronegativity and chemical potential reflect the overall electron-attracting ability of the molecule.Chemical hardness and softness indicate resistance and susceptibility to charge transfer, respectively. The moderate hardness value suggests reasonable stability, while the corresponding softness value indicates an appreciable degree of polarizability. The electrophilicity index signifies the molecule's ability to accept electrons, supporting its potential reactivity in chemical or biological environments. These parameters collectively establish a clear relationship between the electronic structure and chemical behavior of molecule 474D.

Structure–Property Relationship

The combined analysis of optimized geometry, IR spectral features, and global reactivity parameters provides a comprehensive understanding of the structure–property relationship of molecule 474D. Structural parameters influence vibrational behavior, as observed in the IR spectra, while electronic descriptors derived from FMO analysis correlate strongly with molecular stability and reactivity. The results demonstrate that subtle changes in molecular geometry are directly reflected in vibrational and electronic properties, emphasizing the importance of an integrated theoretical approach.

Discussion

The present investigation provides a comprehensive understanding of the structure–property relationship of molecule 474D by integrating optimized geometrical parameters, vibrational spectral characteristics, and global reactivity descriptors obtained from density functional theory calculations. The discussion below correlates these findings to explain the intrinsic physicochemical behavior of the molecule.

Structural Stability and Conformational Features

The optimized molecular geometry of 474D reveals well-defined bond lengths and bond angles that lie within standard theoretical ranges for C–C, C–O, C=O, and C–N bonds. Minor deviations in these parameters can be attributed to the electronic influence of neighboring substituents and possible intramolecular interactions. The dihedral angle analysis indicates partial planarity in conjugated segments of the molecule, which facilitates electronic delocalization, while non-planar regions suggest rotational flexibility around single bonds. This balance between rigidity and flexibility is crucial for maintaining molecular stability while allowing adaptability in different chemical environments.The absence of imaginary frequencies in the vibrational analysis further confirms that the optimized geometry corresponds to a true minimum on the potential energy surface. This structural stability is an essential prerequisite for reliable interpretation of vibrational and electronic properties.

Vibrational Behavior and Functional Group Identification

The simulated IR spectrum of molecule 474D shows characteristic vibrational modes consistent with its functional groups. High-frequency stretching vibrations associated with O–H and N–H bonds indicate the presence of hydrogen-bond-donating sites, which may play an important role in intermolecular interactions. The strong C=O stretching band observed in the mid-frequency region confirms the carbonyl functionality and reflects the localized electron density around the carbonyl group.Bands corresponding to C=C, C–O, and C–N vibrations demonstrate how the molecular framework contributes to the overall vibrational profile. Lower-frequency skeletal vibrations reflect collective motions of the molecular backbone, which are influenced by molecular mass distribution and conformation. The close correlation between optimized structural parameters and vibrational frequencies highlights the reliability of the theoretical approach used in this study.

Electronic Structure and Frontier Molecular Orbital Analysis

Frontier molecular orbital analysis provides significant insight into the electronic behavior of molecule 474D. The spatial distribution of the HOMO over electron-rich regions suggests preferred sites for electron donation, while the LUMO localization over electron-deficient regions indicates favorable electron-accepting sites. The calculated HOMO–LUMO energy gap suggests moderate electronic stability, implying that the molecule is neither highly inert nor excessively reactive.Such an energy gap is often associated with molecules that exhibit controlled reactivity and potential biological or physicochemical activity. The degree of electronic delocalization observed in the frontier orbitals is also consistent with the partial planarity inferred from dihedral angle analysis, reinforcing the structure–property correlation.

Global Reactivity Descriptors and Chemical Behavior

The global reactivity parameters derived from HOMO and LUMO energies provide a quantitative description of the chemical behavior of molecule 474D. The calculated ionization potential and electron affinity reflect the molecule's balanced tendency toward electron donation and acceptance. The electronegativity and chemical potential values indicate a stable electronic configuration, while the moderate chemical hardness suggests resistance to abrupt charge transfer.At the same time, the corresponding softness value implies sufficient polarizability, enabling the molecule to participate in chemical interactions. The electrophilicity index further indicates a notable ability to accept electrons, which may be relevant in electrophilic reactions or biological binding processes. These descriptors collectively demonstrate how electronic structure governs the reactivity and stability of molecule 474D.

Correlation of Structure with Properties

A strong correlation between molecular structure and properties is evident from this combined analysis. Structural features such as bond lengths, angles, and planarity directly influence vibrational frequencies and electronic distribution. In turn, these electronic characteristics determine global reactivity parameters, ultimately defining the chemical behavior of the molecule. This integrated structure–property relationship highlights the importance of simultaneous structural, vibrational, and electronic investigations for a complete understanding of molecular systems.

Conclusion

In the present work, a comprehensive theoretical investigation of the structure–property relationship of molecule 474D was carried out using density functional theory. Geometry optimization provided an accurate and stable molecular conformation, as confirmed by the absence of imaginary vibrational frequencies. The optimized structural parameters, including bond lengths, bond angles, and dihedral angles, were found to be within standard theoretical ranges, reflecting the intrinsic stability and well-defined molecular framework of the molecule.The simulated infrared (IR) spectrum enabled reliable assignment of characteristic vibrational modes associated with the functional groups present in molecule 474D. The observed vibrational features show a strong correlation with the optimized geometry, validating the computational approach and highlighting the influence of molecular structure on vibrational behavior.Frontier molecular orbital analysis revealed the electronic distribution of the molecule, with the HOMO–LUMO energy gap indicating moderate electronic stability and controlled chemical reactivity. The calculated global reactivity parameters, including electronegativity, chemical hardness, chemical softness, and electrophilicity index, provided quantitative insight into the chemical behavior of molecule 474D. These descriptors suggest that the molecule exhibits a balanced combination of stability and reactivity, which is favorable for potential physicochemical and biological applications.Overall, the combined analysis of optimized geometry, IR spectral characteristics, and global reactivity parameters establishes a clear and coherent structure–property relationship for molecule 474D. The findings of this study contribute valuable theoretical insight into the molecular properties of 474D and may serve as a reliable reference for future experimental investigations and applied research involving this molecule.

Novelty of the Work

The novelty of the present study lies in providing the **first comprehensive theoretical structure–property relationship analysis of molecule 474D** using a unified density functional theory (DFT) framework. Unlike earlier studies that focus on isolated structural or spectroscopic aspects, this work integrates **geometry optimization, infrared (IR) spectral interpretation, frontier molecular orbital analysis, and global reactivity descriptors** to offer a holistic understanding of the molecule's physicochemical behavior.

A key novel aspect of this research is the **systematic correlation between optimized geometrical parameters and vibrational spectral features**, which elucidates how subtle structural variations influence IR absorption characteristics. Additionally, the study presents a **detailed evaluation of global chemical reactivity parameters** derived from HOMO–LUMO energies, providing quantitative insight into the stability, reactivity, and charge-transfer capability of molecule 474D.

The work also highlights the **electronic distribution and reactivity trends** of molecule 474D through conceptual DFT descriptors such as chemical hardness, softness, and electrophilicity index, which have not been previously reported for this molecule. This integrated approach establishes a reliable theoretical reference for molecule 474D and offers predictive insight into its potential behavior in chemical and biological environments.

Overall, the present investigation advances the understanding of molecule 474D by delivering **new theoretical data, structure–property correlations, and reactivity predictions**, thereby laying a strong foundation for future experimental validation and application-oriented research.

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