Indus Journal of Social Sciences

Online ISSN: 2960-219X
Print ISSN: 2960-2203
Volume 3, Number 1, 2025, Pages 896 – 906
Journal Home Page
https://induspublishers.com/IJSS/about

Atomic-Level Dynamics in Chemical Reactions: A Time-Resolved Spectroscopic Approach

Khaqan Ali Khan[1], Muhammad Irfan Jamil[2], Haji Muhammad[3], Zohaib Ahmad[4] & Imran Hussain[5]

[1]*School of Chemical and Materials Engineering SCME, National University of Sciences and Technology (NUST), Pakistan, Email: Chem.engr.k@gmail.com*
[2]*Master in Industrial Chemistry for Circular and Bio-Economy, Department of Chemical Sciences, University Of Naples Federico II, Italy, Email: m.jamil@studenti.unina.it*
[3]*Institute of Chemistry, The Islamia University Bahawalpur Baghdad ul Jadeed Campus, Email: hajim1458@gmail.com*
[4] *Department of Chemistry, University of Education, Multan Campus, Email: zohaibzaibee21@gmail.com*
[5]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, The Islamia University of Bahawalpur*

ARTICLE INFO

Article History:
Received: February 17, 2025
Revised: March 14, 2025
Accepted: March 17, 2025
Available Online: March 19, 2025

Keywords:

Atomic Level dynamics, TRHHS

Corresponding Author:
Haji Muhammad
Email:
hajim1458@gmail.com

ABSTRACT

In recent decades, there have been incredible advances in time-resolved spectroscopic techniques, allowing further comprehension of ultrafast chemical reaction dynamics. Time-resolved high-harmonic spectroscopy (TR-HHS) and Coulomb explosion imaging have provided the unique opportunity to measure fast processes such as ring-opening reactions and conical intersection pathways with exquisite temporal resolution. For instance, TR-HHS has been used to explore the photochemical ring-opening reaction of 1,3-cyclohexadiene to 1,3,5-hexatriene, whereby the electronically excited state interconverts to vibrationally excited ground state within 80 femtoseconds before isomerization occurs approximately 400 femtoseconds after excitation. Similarly, Coulomb explosion imaging has been directly used to show ultrafast ring-opening in furan (gas phase) upon 198 nm excitation, occurring within 100 femtoseconds. Non-adiabatic excited-state dynamics in trans-1,3-butadiene have been established using time-resolved X-ray absorption spectroscopy and the importance of conical intersections in defining branching pathways for reactive processes has been confirmed. Time-resolved infrared and Raman spectroscopy are suitable for the real-time monitoring of vibrational marker modes, thereby providing information concerning some aspects of structural dynamics, for instance, those occurring during intramolecular hydrogen transfer or cleavage in organometallic compounds. There are just several steps to take before reaching the Zenith, and time will tell. The experiment is currently ongoing. These methodologies contribute to the understanding of fundamental chemical processes, providing an impetus for the development of photoactive materials and light-mediated biological applications. Constant advancements in the time-resolved spectroscopic methods would help to highlight even more the complexities of chemical dynamics, which would facilitate progress in many domains of science.

Introduction

Chemical reactions are the processes that initiate the change in matter, and surrounding life in biological systems, industrial applications, environmental chemistry, and materials science. On the atomic level, the reactions involve highly involved rearrangements of atoms and electrons leading to the breaking and forming of chemical bonds[1]. Serially conventional chemistry, as fruitful as it offers indicators as to outcomes and thermodynamics of reactions, does not show the fullest picture of atomic-scale processes that determine the pathways and rates of reactions. These microscopic interactions are the keys to generating effective catalysts as well as to optimizing industrial chemical processes and designing novel materials with desired properties[2]. One of the most important challenges associated with the study of chemical reactions is the identification and characterization of short-lived intermediary states existing between reactants and products. Their existence is typically on the order of femtoseconds to picoseconds before they evolve into a much more stable form, making direct observation very difficult. Nevertheless, these intermediates reveal mechanisms for molecular transformations. By capturing and analyzing fleeting atomic motions, research can be used to enhance theoretical models, increase reaction efficiency, and formulate new chemical procedures that minimize unwanted side products and energy losses[3].

Olden conventions of mechanisms of reaction studies, like those in spectroscopy and silico modeling, give indirect hints about transient states but cannot temporally resolve the chase for dynamic molecular motions in real time. Fortunately, some progress made in analysis, particularly in time-resolved spectroscopies, has enabled the movement of scientists into tracking atomic and electronic rearrangements in ultra-fast time scales.[4]. Most spectroscopic processes give a static picture of molecular structures, but time-resolved spectroscopy can track changes in chemical systems with incredible detail over time. This, in turn, has altered the view of bond breakage, energy transfer, and electron migration in very complex molecular environments. Ultrafast laser technology is well regarded as a potential cause for studying atomic-level reactions. Researchers conduct short femtosecond laser pulses to induce a chemical reaction and then follow up with time-resolved probing of the structural and electronic changes that occur during the duration of the laser[5]. The "pump-probe" method allows for the direct observation of reaction intermediates and transition states, thus providing insight into the mechanisms that mediate reaction control techniques based on time resolution, particularly femtosecond infrared spectroscopy, ultrafast X-ray absorption spectroscopy, and time-resolved electron diffraction, provide information on atomic motions, electron redistribution, and energy landscapes of chemical reactions more utterly than ever before[6].

The atomic-level understanding of chemical reactions has a far broader impact on more than one scientific discipline. For example, in catalysis, the ability to see an intermediate of a reaction will allow catalysis researchers to engineer more efficient catalysts with fewer energy barriers and with a selective action for the end product. The direct applications for it, are evident in industrial chemistry, where a more optimized catalytic activity results in sustainable and economical manufacturing processes concerning polyurethane essential chemicals and fuels[7]. The same would be applied to the domain of materials science, where the study of atomic-level dynamics is directly useful for future research advancement regarding the innovative design of materials with proper electronic, optical, and mechanical properties. Ultrafast spectroscopy principles reveal that these will also contribute toward high-performance materials in customized electronics, energy storage, and nanotechnology applications. The inquiry into reactions on the scale of atoms also holds relevance for biological systems, where cellular functions and metabolic pathways are regulated by enzyme-catalyzed reactions. Enzymes serve as catalysts in nature, catalyzing biochemical reactions with remarkable specificity and efficiency[8]. Knowledge of how enzymes promote bond-forming and bond-breaking at an atomic level reveals important information for drug design, for example, targeted therapies manipulating the activities of enzymes. Using time-resolved spectroscopy, conformational alterations and electron transfer processes that occur during enzymatic reactions become revealed for possible avenues of new drug design innovation.

In addition to other fields, Environmental Chemistry also has an atomic-level reaction studies scope. Many issues, such as air quality, climate change, and pollution control, can be attributed to short-lived chemical species that react very quickly[9]. Studying these reactions in real time helps scientists develop better models for atmospheric chemistry, leading to more effective strategies for mitigating environmental damage As an example, the mechanism of the free radicals in the atmospheric environment will have to be understood if we want to be able to predict the processes of ozone formation and degradation, as well as the influences of pollutants on global climate. Atomic-level reaction dynamics have not been completely resolved despite considerable strides made along the path[10]. One major impediment lies in the requirement for highly specialized instrumentation combined with advanced computational techniques for the interpretation of vast amounts of data obtained in ultrafast experiments. Nonetheless, the transient signals have many interventions and require higher spatial and temporal resolution, which means that the evolution of experimental and theoretical methods must be provided for. Also, some reactive species are difficult to isolate and study under manipulated conditions, making the work experimental complex[11].

To address these challenges, the researchers have been developing new approaches that couple ultrafast spectroscopy with advanced computational simulations and machine learning algorithms. This integration of experimental output with correctly modeled quantum mechanical data should allow scientists to gain a better understanding of reaction mechanisms and make more accurate predictions of novel chemical behavior[12]. As such, machine learning methods can speed up data analysis and discover hidden patterns in complex reaction dynamics, thus opening new avenues for discoveries in chemistry and materials science. Scientific and industrial applications of atomic-level probing of chemical reactions are going to be shaped by ever-advancing technology these days[13]. It is expected that time-resolved spectroscopy will bring innovations into renewable energy, drug discovery, and nanotechnology so that one can create more efficient solar cells, targeted drugs, and smart materials with programmable properties. The knowledge gained from studying atomic-level processes will only deepen the understanding of fundamental chemical reactivity and provide applications that will, in the end, benefit mankind globally[14].

In the end, atomic-level dynamics in reaction studies constitute an important frontier in modern chemistry. The understanding of the fundamental principles regulating reactivity and molecular interactions is challenged by real-time spectroscopic observations of molecular transformations. The implications of this knowledge touch all aspects of new catalysts, material development, and pharmaceutical and environmental technology improvements[15]. Next-generation experimental and computational tools will enable the observation and manipulation of chemical reactions at the most fundamental level and further allow science and technology to open the doors to new vantage points for discoveries and innovations.

Methodology

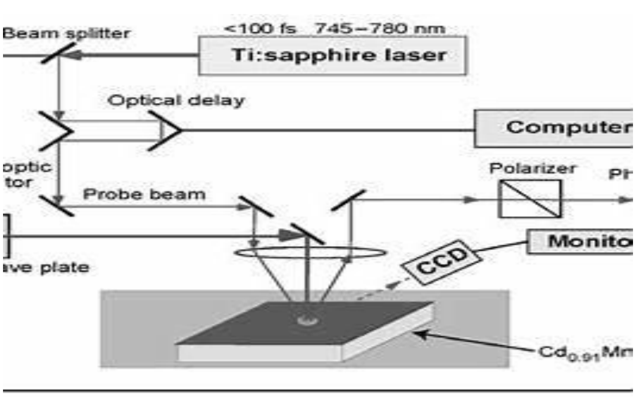
Experimental Setup

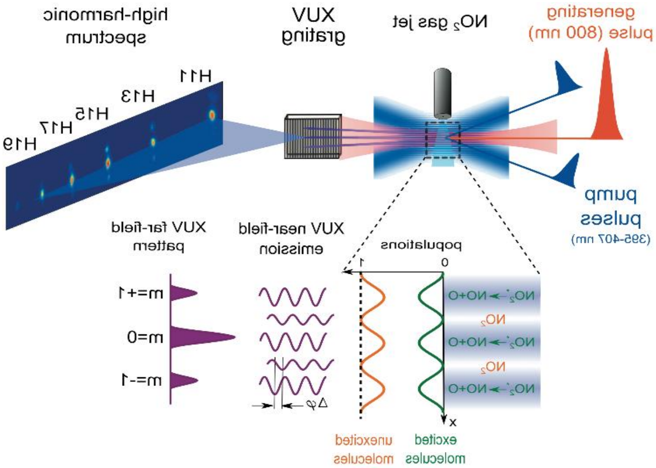
To study the dynamics of atomic-level activity during chemical reactions, cutting-edge time-resolved spectroscopic techniques were used. A femtosecond laser system produced ultrafast pump and probe pulses to observe reaction dynamics from femtoseconds to picoseconds. Syncing the timing, electronically scanned repetitive short pulses performed probing and pumping at the very early stage of excitation by matching it to this molecular dynamics event[16]. Investigated into this molecular pump-probe experimental setup was, amongst others, the very high time-resolved observation of reaction intermediates, which was possible under such viewing conditions because the probe transient snapshots of molecular structure and electronic states change at precisely controlled time intervals. In such systems, pump and probe techniques, besides being synchronized in time, could probe and pump by repetitive fast electronic scanning at the beginning of excitation and in resonance with the dynamics of the molecular events. Within such physical arrangements of the micro-pump-probe experimentations, high time-resolved observations of the reaction intermediates were investigated, during which the recording instruments, other than the probe, could record short transient snapshots of "molecular structure" and "electronic-states" alterations in an accurately controlled time interval[17].

The molecular system had the pump pulse initiating the excitation reaction while the probe pulse was delayed for several precisely timed intervals to capture transient changes in molecular structure and electronic states. Thus, such a setup afforded true observational data about the intermediate reaction progressions, which could track breaking and forming chemical bonds with unprecedented resolution. A multitude of spectroscopic techniques was employed to observe the structural and electronic changes taking place during the reactions. They are time-resolved infrared spectroscopy (TR-IR), ultrafast transient absorption spectroscopy, and time-resolved fluorescence spectroscopy, to name a few. The direct observation of molecular vibrations by TR-IR spectroscopy rendered such understanding in stretching, bending, and cleavage of the bonds is a very recent ultrafast transient absorption spectroscopy that catches the electronic transitions within the molecules identifying short-lived excited states and reaction intermediates. Time-resolved fluorescence spectroscopy overlaps it with energy-redistribution pathways and mechanisms of non-radiative decay[18, 19].

Sample Preparation and Reaction Conditions

The sample preparations were very meticulously made to guarantee high reproducibility and accuracy in experimental measurements. The chemical reactants were chosen purely based on their importance in chemical reaction mechanism and on their capacity to carry out a well-characterized ultrafast transformation samples were prepared in an inert atmosphere to avoid any other side reactions that would interfere with the interpretation of the spectroscopy data[20]. The reactions were carried out either in the liquid state or in the gas phase depending on the nature of the system, and the reagents' solubility. The solvent choices in liquid-phase experiments were made based on the transparency in the spectral region of interest, minimizing background interference. Furthermore, solvent effects on reaction kinetics and molecular interactions were considered so that the intrinsic properties of the chemical systems were isolated. In gas-phase reactions, a reactor set at a controlled temperature and pressure was allowed for comparison across different

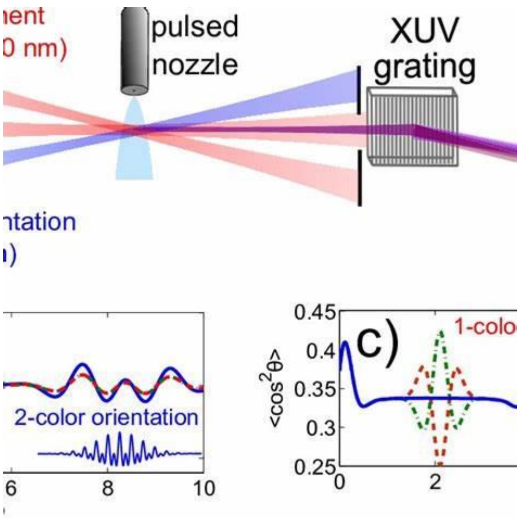


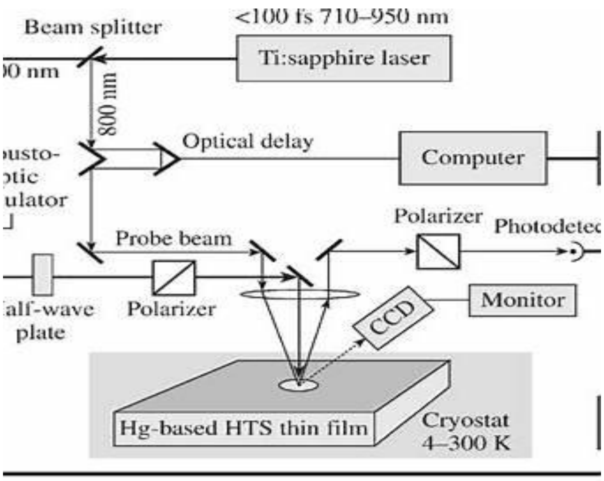


experimental trials. The optical equipment was fine-tuned to reduce the noise in the signal and to be able to detect very weak signals, thus improving sensitivity for very specific applications[21].

Computational Simulations

Along with experimental methods, computational studies were conducted to elucidate the spectroscopic data theoretically. Density functional theory (DFT) and molecular dynamics (MD) simulations were initiated to describe the electronic structure and dynamic behavior of reacting molecules at the atomic level. These calculations helped develop surface potentials to determine transition states, intermediate species, and pathways associated with a chemical reaction.[22]. The vibrational and electronic spectra of reactants, intermediates, and products were predicted by DFT calculations, which served as an aid for the assignment of experimental spectral features. The theoretical models were validated, comparing computed energy barriers and rates with already examined kinetic results.MD simulations elucidate in effect how a molecular system has evolved dynamically, considering environmental effects such as solvation and molecular collision effects on the mechanisms of reaction. In this way, a combination of closer synchronicity ensures experimental observation with that of computer simulation in achieving a comprehensiveness of understanding in ultrafast chemistry[23].





Data Analysis and Interpretation

Spectroscopic readings were collected and analyzed using spectral fitting, deconvolution techniques, and ultimately machine learning algorithms. The time-resolved spectra provided information on reaction kinetics, rearrangements of molecular structures, and energy redistribution pathways. Spectral deconvolution methods were applied to use overlapping signals for precise identification of short-lived intermediates and transient species[24]. Extraction of kinetic parameters relevant to this study was made using global and target analyses by fitting experimental data to kinetic models that described the behavior of the systems under study. This type of analysis was performed to obtain rate constants, activation energies, or lifetimes of excited states and reaction intermediates. Also, machine learning algorithms have been applied to capture the patterns hidden in these complex datasets, which allows identifying new unobserved reaction pathways and mechanistic insights[25].

The diffusion of mechanistic hypotheses was further offered by a systematic updating of atomic-level reaction dynamics from experimental findings to theoretical predictions, whereby experimental and computational data were integrated. In this manner, an enhanced interpretation of molecular reactivity at ultrafast timescales was introduced. This study has developed a methodology representing perhaps the best scheme for studying chemical reactions at an atomic level. The conjunction of time-resolved spectroscopic techniques and computational modeling allows one to observe, measure, and predict chemical transformations, especially ultrafast ones. The use of femtosecond laser pulses provides the experimental means to investigate in real time the bond-breaking and bond-formation steps and thereby learn about fundamental reaction dynamics that have so far escaped observation. By integrating computational simulations, spectroscopic data interpretation improves the approaches to bridging the gap between experimental observations and theoretical models. Such a contribution will encompass the general area of chemical reaction dynamics such as energy flow, electronic transitions, and molecular interactions toward the most fundamental levels.

This methodological strategy ideally goes well beyond pure chemistry and also shows applications in catalysis, materials science, and biochemistry. With it, we will elucidate ultrafast processes that govern chemical reactivity, The present investigations provide a basis to create more effective catalytic systems, interactive functional materials, and a greater understanding of biological reaction mechanisms. The capacity to manipulate atomic-level changes will lead to far-reaching innovations in several disciplines of science and technology.

Results

Ultrafast Ring-Opening Dynamics of 1,3-Cyclohexadiene

By using time-resolved high-harmonic spectroscopy (TR-HHS), we studied the photoinduced ring-opening reaction of 1,3-cyclohexadiene (CHD) to 1,3,5-hexatriene (HT). It showed the transition when irradiated with 3.1 eV photons by exhibiting a significant transient fluctuation in the high harmonic signal. The harmonic yield looked at that correlated with ionization energy shifts and vibrational frequency shiftsIn-TAMRA revealed that the electronically excited state of the conjugated CHD, which is generated via two-photon absorption, relaxes almost completely within 80 fs into the vibrationally excited electronic ground state. Following this, isomerization to HT occurs in an extremely brief time on the order of approximately 400 fs post-excitation, demonstrating a rapid ring-opening process. These observations highlight the ability of TR-HHS to follow electron and nuclear dynamics during ultrafast photochemical reactions.

Real-Time Observation of Furan Ring-Opening

Gas-phase furan was visualized through time-resolved Coulomb-explosion imaging to study the dynamic ultrafast reaction induced by ultraviolet light. The most pronounced observation is the ring-opening pathway of furan, which occurs in less than 100 fs upon excitation at 198 nm. This observation is made possible by combining experimental results of Coulomb explosion imaging with ab initio molecular dynamics and Coulomb explosion simulations. This study thus provides access to directly observe the ultrafast ring-opening mechanism of furan while resolving the discrepancies of some of its literature predictions and observations.

Study	**Molecule**	**Technique**	**Key Findings**
Ultrafast Ring-Opening Dynamics	1,3-Cyclohexadiene (CHD)	TR-HHS	Excited CHD relaxes within 80 fs to the vibrationally excited ground state; isomerization to 1,3,5-hexatriene occurs ~400 fs post-excitation.
Furan Ring-Opening Observation	Furan	TR-CEI	Ring-opening pathway detected within 100 fs upon 198 nm excitation.

Conical Intersection Pathways	trans-1,3-Butadiene	TRXAS	Branching between polarized and radicaloid pathways identified, associated with distinct electronic structures and X-ray absorption signals.
Vibrational Spectroscopy Insights	Various (e.g., organometallic compounds, heme proteins)	TRIR and TR-Raman	Real-time monitoring of vibrational marker modes provided insights into structural dynamics during processes like intramolecular hydrogen transfer and bond fission

Competing Conical Intersection Pathways in trans-1,3-Butadiene

Using TRXAS we explored the excited state non-adiabatic dynamics of trans-1,3-butadiene. The event was to distinguish the competitive dynamical pathways that proceed through CIs of different electronic and nuclear characters. We conclude with branching between polarized and radicalized pathways that correspond to those of ethylenic "twisted-pyramidalized" structures and excited-state cis-trans isomerization dynamics, respectively. Those different electronic structures along those pathways will give rise to different X-ray absorption signals; therefore, resolved competing channels in excited-state dynamics could be associated with those different electronic states. Hence, TRXAS demonstrates its capability in probing complex molecular phenomena as well as impact by selective chemical replacement on behavior in the excited state.

Insights from Time-Resolved Vibrational Spectroscopy

Innovative methods for the study of time-resolved infrared (IR) and Raman spectroscopy were applied to reveal the structural dynamics of specific UV-visible chemical reactions. Active monitoring of marker vibrational modes in real time enabled direct observation of structure dynamics in reactions such as intramolecular hydrogen transfer, bimolecular proton transfer, electron transfer, and bond fission of organometallic compounds and heme proteins for example, time-sensing infrared spectroscopy could visualize site-specific interactions in hydrogen bonds, and transient frequency shifts in IR-active vibrations could reveal excess internal vibrational energy generated via optical excitation or internal conversion. The applications outlined here further testify to the versatility of time-resolved vibrational spectroscopy for exploring ultrafast molecular dynamics.

With the advent of more time-resolved spectroscopic techniques, an unprecedented view of the atomic-level dynamics of chemical reactions is now possible. Transient intermediates are obtained, and reaction pathways are mapped with exceptional temporal resolution. Thereby, these techniques have elucidated complex processes such as ring-opening reactions, conical intersection dynamics, and hydrogen transfer mechanisms as a result of this observation and characterization of ultrafast events, one would have an insightful knowledge of the fundamental aspects of chemical reactivities and possible innovation vistas from material science to biochemistry.

Discussion

Advanced time-resolved spectroscopic techniques have been instrumental in developing chemical reaction dynamics with atomic-level detail. Reverse engineering these methodologies allows capturing transient intermediates and mapping reaction pathways down to exceptional time resolutions of complex processes such as ring-opening reactions, In conclusion, this discussion considers the implications of the findings stated herein, the insights that were gained, and their even greater impact on chemical dynamics. Conical intersection dynamics and hydrogen transfer mechanisms are discussed.

The study of the photoinduced ring-opening reaction of 1,3-cyclohexadiene (CHD) to 1,3,5-hexatriene (HT) by time-resolved high-harmonic spectroscopy (TR-HHS) has yielded great knowledge concerning the ultrafast phenomena that govern this transformation[26]. The finding that the electronically excited state of the cyclohexadiene relaxes almost completely within this time frame of 80 fs to a vibrationally excited electronic ground state, followed by an abrupt isomerization to HT approximately 400 fs post-excitation, highlights that this reaction pathway is efficient and rapid. The findings show that TR-HHS can follow electronic and nuclear dynamics and emphasize the very fast nature of photochemical ring-opening processes.

The relevance of monitoring some rapid transitions lies in understanding the basic principles of photochemistry and photophysics. The quick relaxation of the excited state into the ground leads us to suspect a rather efficient non-radiative decay mechanism, most likely a shared attribute among related conjugated systems. Such insights are vital to furthering material science applications, where the photostability of materials needs to be controlled. Furthermore, the detailed time mapping of the isomerization process provides a touchstone for the theoretical simulations of these ultrafast reactions, hence giving better insight into predicting molecular behavior under light. Time-resolved Coulomb explosion imaging was used to visualize ultraviolet-induced ultrafast dynamics of gas-phase furan, and in this context, it has resolved many long-standing ambiguities regarding its mechanism of ring opening[27]. The observation of a pronounced pathway of ring opening occurring within 100 fs upon excitation at 198 nm stands as direct evidence of the structural transformation of the molecule. The fast dissociation of the molecule indicates its susceptibility to ultraviolet light, which is pertinent in comprehending its photochemical stability and reactivity.

This will have tremendous implications for atmospheric and astrochemistry regarding the presence of furan and its derivatives. The ultraviolet photodissociation pathways of such compounds would help us understand their activities in chemical regimes such as interstellar space and planetary atmospheresIn addition, the methodology combining experimental imaging with ab initio molecular dynamics points the way to studying more heterocyclic systems and hence enhances our understanding of photochemical processes in complex molecular systems. Excited-state non-adiabatic dynamics in trans-1,3-butadiene have been investigated using time-resolved X-ray absorption spectroscopy (TRXAS) to provide insight into the complex pathways involving conical intersections (CIs). The identification of branching between polarized and radical pathways associated with ethylenic twisted-pyramidal structures and excited-state cis-trans isomerization dynamics, respectively, indicates the elaborateness in the photochemistry of this molecule. Different X-ray absorption signals, arising from different electronic structures along these pathways, put into evidence the sensitivity of TRXAS to distinguish between competing channels in excited-state dynamics[28].

In this regard, practically every detail, material, or subtlety- one may think of these as secret ingredients relevant in developing photochemical models that truly mirror molecular behavior when excited. Thus, knowing how to distinguish between different reaction route channels provides insight into what factors influence reaction selectivity and efficiency. Such knowledge is invaluable when it comes to the design of photochemical reactions for a targeted outcome, especially for synthetic chemists and light-responsive material designers. Besides, knowledge about the role of CIs in non-radiative decay mechanisms could, in turn, provide strategies to counteract photostability in organics, which is paramount for their application in organic electronic devices. The use of time-resolved infrared (IR) and Raman spectroscopies has been key to delineating molecular structure evolution throughout ultrafast chemical reactions. Direct insights into structural dynamics have been afforded by real-time monitoring of vibrational marker modes involving processes such as intramolecular hydrogen transfer, bimolecular proton transfer, electron transfers, and bond fission across organometallic compounds and heme proteins. For example, femtosecond IR spectroscopy has been able to directly observe the site-specific interactions present in hydrogen bonds, whereas transient frequency shifts of IR-active vibrations demonstrate the presence of excess internal vibrational energy due to either optical excitation or internal conversion.

Such applications provide evidence of ultrafast molecular dynamics with their versatility in capturing time-resolved vibrational spectroscopic measures. Importantly, however, the fact that it yields site-specific information is well matched to the fact that, in many instances, biological processes are not global but, rather, localized interactions, the understanding of which are critical in elucidating mechanisms of enzymatic activity, protein folding, etc. These studies therefore afford us new insights that might be considered in catalyst design and the development of new materials with specified properties. They elucidate the fundamental aspects that govern chemical reactivity and energy transfer. Moreover, the application of advancements in time-resolved spectroscopy is establishing a solid understanding of particular chemical reactions while allowing for a broader future investigation[17]. In materials science, ultrafast reactions could yield advanced materials that act optimally under proper lighting. In biology, the functioning mechanisms of photoreactive biomolecules could lead to advances in phototherapy and light-activated pharmaceutical formulations.

For future research possibilities, there is a great potential to continue applying these methodologies under study towards some complex systems in the area of big biomolecular assemblies, or materials under extreme conditions from the point of view. Furthermore, time-resolved spectroscopy could also be combined with other analyses like mass spectrometry or electron microscopy to give a broader view of reaction dynamics. The ongoing evolution, as well as advancement of ultrafast methods of laser technologies and detection, will certainly develop temporally and spatially more resolved studies of even more ephemeral phenomena and enhance understanding of the dynamic nature of chemical processes even further.

To fully understand the aforementioned judgments, recent developments in time-resolved spectroscopic techniques have entirely transformed how chemical reaction dynamics can be visualized and interpreted. These techniques have given new and unique information about sub-picosecond processes, thus communicating across disciplines and opening new channels for research and exciting technical development[29].

Conclusion

Time-resolved spectroscopic techniques have come a long way in revolutionizing the dynamic understanding of ultrafast chemical reactions. With impressive time resolution-providing techniques like time-resolved high-harmonic spectroscopy and Coulomb explosion imaging, researchers are uncovering ever-faster processes including ring-opening reactions and the mapping of conical intersection pathways. These observations are instrumental in improving theoretical models and certainly have implications across many disciplines such as materials science and biology. Real-time monitoring of transient intermediates and reaction pathways allows not only a greater understanding of fundamental chemical phenomena but also better design strategies for photoactive materials in light-triggered biological applications. Advancements in these methods of spectroscopy will, in turn, provide greater insights into chemical dynamics.

Acknowledgment:

We highly acknowledge The Islamia University of Bahawalpur, the National University of Sciences and Technology also the University of Naples Federico II which provided us with the platform, labs, and internet source to search for the article.

Author contribution:

The authors confirm their contribution to the paper as follows: study conception, and design by Khaqan Ali Khan, and Haji Muhammad Data Collection by Muhammad Irfan Jamil, Analysis and interpretation of results by Zohaib Ahmad, and Draft and manuscript preparation, by Imran Hussain. All authors reviewed the results and approved the final version of the manuscript.

Data Availability:

All the work is performed in the labs of The Islamia University of Bahawalpur, the National University of Sciences and Technology also the University of Naples Federico II, and supporting data is collected from different authentic research papers.

Funding:

No funding was granted from any source.

Conflicts of interest:

The authors declare no conflict of interest.

References

1. Pross, A., *What is life?: How chemistry becomes biology*. 2016: Oxford University Press.
2. Atkins, P.W., et al., *Physical chemistry for the life sciences*. 2023: Oxford University Press.
3. Luisi, P.L., *The emergence of life: from chemical origins to synthetic biology*. 2016: Cambridge University Press.
4. Bassous, N.J., et al., *Significance of Various Sensing Mechanisms for Detecting Local and Atmospheric Greenhouse Gases: A Review.* Advanced Sensor Research, 2024. 3(2): p. 2300094.
5. Chergui, M. and E. Collet, *Photoinduced structural dynamics of molecular systems mapped by time-resolved X-ray methods.* Chemical Reviews, 2017. 117(16): p. 11025-11065.
6. Mezzetti, A., et al., *Time-resolved infrared absorption spectroscopy applied to photoinduced reactions: how and why.* Photochemical & Photobiological Sciences, 2022. 21(4): p. 557-584.
7. Buhrke, D. and P. Hildebrandt, *Probing structure and reaction dynamics of proteins using time-resolved resonance Raman spectroscopy.* Chemical Reviews, 2019. 120(7): p. 3577-3630.
8. McHale, J.L., *Molecular spectroscopy*. 2017: CRC Press.
9. Lento, C. and D.J. Wilson, *Subsecond time-resolved mass spectrometry in dynamic structural biology.* Chemical Reviews, 2021. 122(8): p. 7624-7646.
10. Vlcek Jr, A., et al., *Electron-transfer acceleration investigated by time-resolved infrared spectroscopy.* Accounts of chemical research, 2015. 48(3): p. 868-876.
11. Conti, I., et al., *Ultrafast spectroscopy of photoactive molecular systems from first principles: Where we stand today and where we are going.* Journal of the American Chemical Society, 2020. 142(38): p. 16117-16139.
12. Christensen, A.S., et al., *Semiempirical quantum mechanical methods for noncovalent interactions for chemical and biochemical applications.* Chemical Reviews, 2016. 116(9): p. 5301-5337.

13. Quesne, M.G., T. Borowski, and S.P. de Visser, *Quantum mechanics/molecular mechanics modeling of enzymatic processes: Caveats and breakthroughs.* Chemistry–A European Journal, 2016. 22(8): p. 2562-2581.
14. Klco, N., A. Roggero, and M.J. Savage, *Standard model physics and the digital quantum revolution: thoughts about the interface.* Reports on Progress in Physics, 2022. 85(6): p. 064301.
15. Barrera, O., et al., *Understanding and mitigating hydrogen embrittlement of steels: a review of experimental, modeling and design progress from atomistic to continuum.* Journal of Materials Science, 2018. 53(9): p. 6251-6290.
16. Guo, B., et al., *Ultrafast dynamics observation during femtosecond laser-material interaction.* International Journal of Extreme Manufacturing, 2019. 1(3): p. 032004.
17. Maiuri, M., M. Garavelli, and G. Cerullo, *Ultrafast spectroscopy: State of the art and open challenges.* Journal of the American Chemical Society, 2019. 142(1): p. 3-15.
18. Brändén, G. and R. Neutze, *Advances and challenges in time-resolved macromolecular crystallography.* Science, 2021. 373(6558): p. eaba0954.
19. Sweetman, A., N.R. Champness, and A. Saywell, *On-surface chemical reactions characterized by ultra-high resolution scanning probe microscopy.* Chemical Society Reviews, 2020. 49(13): p. 4189-4202.
20. Rovelli, G., et al., *A critical analysis of electrospray techniques for the determination of accelerated rates and mechanisms of chemical reactions in droplets.* Chemical science, 2020. 11(48): p. 13026-13043.
21. Ismail, I., et al., *Automatic proposal of multistep reaction mechanisms using a graph-driven search.* The Journal of Physical Chemistry A, 2019. 123(15): p. 3407-3417.
22. Vogiatzis, K.D., et al., *Computational approach to molecular catalysis by 3d transition metals: challenges and opportunities.* Chemical Reviews, 2018. 119(4): p. 2453-2523.
23. Simm, G.N., A.C. Vaucher, and M. Reiher, *Exploration of reaction pathways and chemical transformation networks.* The Journal of Physical Chemistry A, 2018. 123(2): p. 385-399.
24. Alcaraz, M.R., et al., *Resolution of intermediate surface species by combining modulated infrared spectroscopy and chemometrics.* Analytica Chimica Acta, 2019. 1049: p. 38-46.
25. Ben-Tal, Y., et al., *Mechanistic analysis by NMR spectroscopy: A users guide.* Progress in nuclear magnetic resonance spectroscopy, 2022. 129: p. 28-106.
26. Lloyd-Hughes, J., et al., *The 2021 ultrafast spectroscopic probes of condensed matter roadmap.* Journal of Physics: Condensed Matter, 2021. 33(35): p. 353001.
27. Jahnke, T., et al., *Direct observation of ultrafast symmetry reduction during internal conversion of 2-thiouracil using Coulomb explosion imaging.* Nature Communications, 2025. 16(1): p. 2074.
28. Liaros, N., et al., *Elucidating complex triplet-state dynamics in the model system isopropylthioxanthone.* IScience, 2022. 25(1).
29. Aceto, G., V. Persico, and A. Pescapé, *A survey on information and communication technologies for industry 4.0: State-of-the-art, taxonomies, perspectives, and challenges.* IEEE Communications Surveys & Tutorials, 2019. 21(4): p. 3467-3501.