
CURRICULUM VITAE

Atanu Bhattacharya

Institute Affiliation:

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Academic Career Summary

Education

2010 PhD (Best Thesis Award), Department of Chemistry, Colorado State University, USA, Advisor: Prof. Elliot R. Bernstein.

PhD Thesis: (a) Excited Electronic State Decomposition of Energetic Molecules, Probed using Nanosecond Energy Resolved Time of Flight Mass Spectrometry and Femtosecond Pump-Probe Transient Ionization Spectroscopy; (b) Conformation Specific Reactivity of Radical Cation Intermediates of Bioactive Molecules, Probed using IR-VUV Spectroscopy and CASSCF/CASMP2/CASPT2 Calculations.

2005 MSc, Department of Chemistry, Indian Institute of Technology, Bombay, Specialization: Physical Chemistry, 1st Class (7.5/10)

2003 BSc, R. K. Mission Vidyamandira, Belur (Calcutta University), Chemistry (Hons) with Physics and Mathematics, 1st Class (63%)

Academic Appointments

2023-2024 Visiting Scientist, Joint Quantum Institute, University of Maryland, College Park, Maryland, USA

2013-2023 Assistant Professor, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India

2012-2013 Program Specific Researcher, Kyoto University and RIKEN, Japan

2010-2012 Research Associate (Post-Doctoral Work), Brookhaven National Laboratory, USA

Current Professional Appointments

2021-Present Advisor, Chemical Applications in Quantum Computer, IBM Quantum Computing Initiative, Bangalore, India

2018-Present Editorial Board Member, Electronic Structure, an Institute of Physics (IOP-UK) Journal

Honours and Awards

2016-2018 Young Associate, Indian Academy of Science, as a Promising Young Scientist at Early Age (less than 35 Years) with Exceptional Scientific Ability, India

2014-2015 Liverpool-India Fellowship, as an Outstanding Young Researcher from India to Strengthen the Research and Teaching in Liverpool University, UK

2013 Young Scientist Research Award, for Outstanding Research Proposal, Department of Atomic Energy, India.

2009 Teresa Fonseca Memorial Prize, as an Outstanding Researcher in Physical Chemistry, Department of Chemistry, Colorado State University, USA

Current Research Area

Experimental Chemical Dynamics

(a) **Surface Chemical Dynamics** of Heterogeneous Catalysis using Surface Science Approach (which couples surface science study with femtosecond laser spectroscopy)

(b) Surface Science Study of CO_2 Capture and Conversion to Fuel (which involves Synchrotron-based X-ray absorption spectroscopy study to decipher structure of catalyst and surface science study of reaction)

(c) **High Harmonic Generation Spectroscopy** to Explore Strong Field-Molecule Interaction and Attosecond Dynamics (this involves a femtosecond/attosecond X-ray beamline constructed in our lab)

Computational Quantum Dynamics

(a) **Electronically Nonadiabatic Dynamics** of Energetic Molecules through Conical Intersection (using ab initio multiple spawning dynamics)

(b) Theoretical High Harmonic Generation Spectroscopy (calculating the dipole acceleration response of molecules due to strong field ionization by solving time-dependent Schrödinger equation using molecular electrostatic potential)

(c) **Theoretical Attosecond Dynamics of Chemical Bonding** (using time-dependent natural bond orbital analysis)

(d) Theoretical Surface Chemical Dynamics (using two-temperature model coupled with frictional energy transfer)

Services to National Academy/Organization

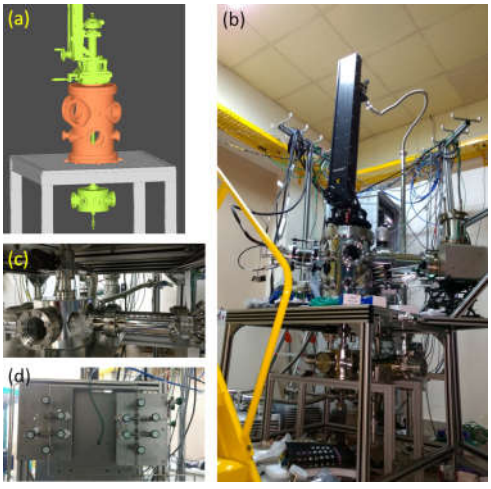
2021-Present Teaching (30 Hours) Physical Chemistry to Pre-university Teachers at Challakere Talent Development Center, Indian Institute of Science, Bangalore

2015-Present Mentoring Summer Interns of Indian Academy of Sciences, Bangalore

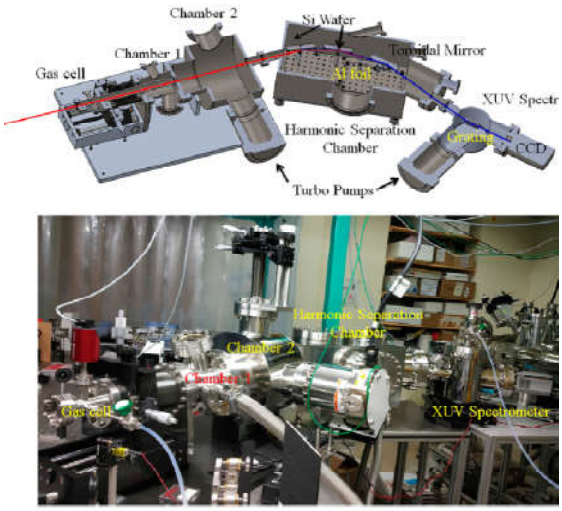
I. Executive Summary of Research Contributions

After obtaining rigorous doctoral and post-doctoral training on molecular beam experiments, molecular spectroscopy, vacuum technology, femtosecond laser spectroscopy, surface science study, catalysis, X-ray spectroscopy, photoelectron spectroscopy and quantum chemical calculations, I have established a novel experimental chemical dynamics program independently at Indian Institute of Science (IISc). This program has two major directions: **Surface Chemical Dynamics** (**Facility # 1**) and **High Harmonic Generation Spectroscopy (Facility # 2)**. Both areas are completely different from my doctoral work. To establish these two fields, I have built two experimental facilities, for the first time, at IISc. To the best of my knowledge, these two unique experimental facilities are not present at any other institute in India. Furthermore, I have developed certain unique theoretical/computational schemes which are novel to augment and to validate the experimental efforts. Using these facilities, I have trained several young researchers (5 PhD students graduated and more than 20 summer interns mentored). My research program at IISc was funded by 6 research projects.

The outcomes of the experimental research in surface chemical dynamics have significant relevance for **Net Zero Carbon Emission technologies**. The computational work in my group is of general significance for the emerging **quantum computing**.



Surface Chemical Dynamics
Facility # 1 at IISc



High Harmonic Generation Spectroscopy
Facility # 2 at IISc

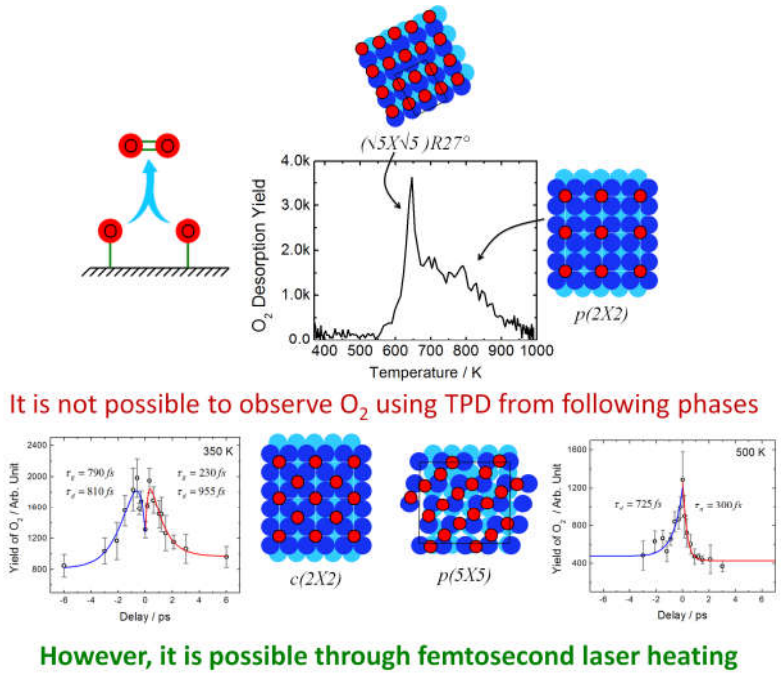
II. Key Details of Research Work

II.1 Surface Chemical Dynamics:

Thermally activated catalysis at the gas-solid heterogeneous interface plays an important role in chemical production, pollution elimination, and many technologically important catalytic conversion processes. For example, a catalytic converter is used in automobile exhaust to convert toxic CO to CO_2. This CO to CO_2 conversion process occurs at the active catalyst surface of palladium in catalytic converter. For a long time, physical chemists, with the help of surface science approach, have played important role in exploring mechanistic details of a catalytic process because improvement or alteration of a catalytic process is possible only through better understanding the mechanisms and dynamics of the process. Surface science approach involves a model catalytic surface (often an idealized single crystal surface) under ultra-high vacuum (UHV) conditions (10^{-10} Torr level of vacuum) because under such low pressure (note that atmospheric pressure is 760 Torr), a model catalytic surface can be kept atomically clean for several hours to perform detailed experiment without contaminating the catalyst surface.

Traditionally, surface science study of a catalytic process involves a technique called temperature programmed desorption (TPD) spectroscopy. The major problem associated with the TPD technique is that it cannot capture the reaction intermediates because reaction intermediates are short-lived and transiently prepared during a chemical reaction. As a result, many important aspects (both in terms of mechanisms and dynamics) of a catalytic process remain unseen if TPD technique is used. The only route to overcome the shortcoming of a TPD technique is to couple surface science technique with femtosecond laser spectroscopy (this coupled approach is named by us as **surface chemical dynamics**). In other words, instead of registive heating, femtosecond pulse-induced heating should be used as sophisticated heating technique to drive the catalytic reaction. In India, to the best of my knowledge, nobody other than our group has coupled surface science technique and femtosecond laser spectroscopy before to explore the catalytic reaction mechanisms and dynamics.

It is well-known, for a long time, that TPD measurements can monitor recombinative $O_{adsorbed} + O_{adsorbed} = O_{2,gas}$ desorption only from the $(\sqrt{5}X\sqrt{5})R27^{O}$-O and p(2x2)-O phases on the single crystal Pd(100) surface. Both the c(2X2)-O and p(5X5)-O phases remain silent in this overall thermally activated recombinative desorption process. With the help of femtosecond laser excitation, for the first time, we have demonstrated that both c(2X2)-O and p(5X5)-O phases can be made active for the recombinative $O_{adsorbed} + O_{adsorbed} = O_{2,gas}$ desorption. (Chem. Phys. Lett. 784, 139117 (2021) or DOI: **https://doi.org/10.1016/j.cplett.2021.139117**). Thus, femtosecond laser excitation opens door to the investigation of the surface chemical reactions which otherwise cannot be observed with the help of conventional thermal heating process.



Superior performance of surface chemical dynamics study

Although above demonstration has been given for the simplest model catalytic reaction, namely $O_{adsorbed} + O_{adsorbed} = O_{2,gas}$, the same technique can be used to explore complex high value industrial catalytic reaction mechanisms and dynamics. One of our recent works (J. Phys. Chem. C, 122, 26528 (2018) or DOI: https://doi.org/10.1021/acs.jpcc.8b09162) shows that Fe–Pd multicomponent core–shell nanoparticles capture CO_2 at the room temperature; however, corresponding single component analogue nanoparticles fabricated following the same procedure do not capture CO_2 at the room temperature. To the best of our knowledge, this is the first report on converting easily available iron oxide system to an active material for CO_2–capture at room temperature. This work has significant relevance to **Net Zero Emission technologies** and **room temperature CO_2 capture technologies**. I envision that using surface chemical dynamics study**,** several novel aspects of mechanism and dynamics of CO_2-capture and its conversion to fuel on modified iron oxide surfaces can be explored in near future. Furthermore, surface chemical dynamics study of CO_2 conversion to ethanol on Rh surfaces (broadly selective conversion of syngas to ethanol) would be invaluable because lack of detailed mechanistic knowledge of this process hinders its wide-spread industrial implementation. This process is at the heart of proposed **carbon-based economy**. Currently nobody other than our group in even international scientific community has taken up surface chemical dynamics study of the proposed catalytic conversion process. **The unique facility built by our group is expected to generate many hitherto-unexplored aspects of fuel-related catalytic conversion processes in future**.

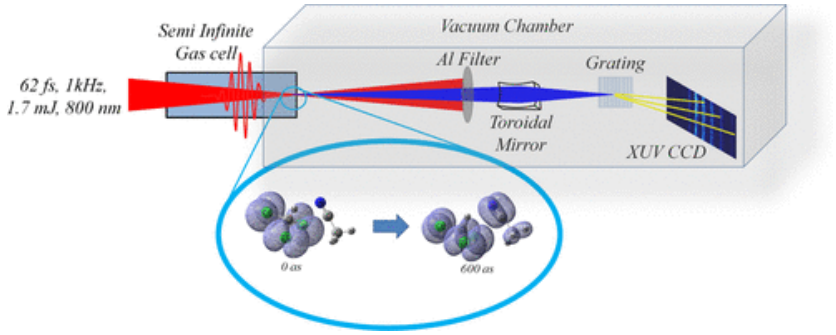
II.2 High Harmonic Generation Spectroscopy:

The chemical bonding in molecules and molecular clusters is determined by the nature of the electron density distribution between the atoms. Over the past century, our thinking of the nature of the chemical bonding revolved around the "static" (*time-independent*) aspects of the chemical bonding. Modern chemistry even continues the legacy using either the valence bond (VB) or the molecular orbital (MO) theory as a starting point for the theoretical prediction of the molecular structure and reactivity. Both theories deal with "static" (*time-independent*) descriptions of orbitals.

Schematic representation of the historical development of the field of "**chemical bonding**", featuring important milestones over the past 100 years. The purpose of this figure is to highlight hitherto-unexplored part of the subject "chemical bonding": the **attosecond electronic scale dynamics of chemical bonding** which serves as a prelude to chemical reactivity (leading to chemical reaction).

The discussion of the "dynamic" nature of a chemical bond over the past century has mostly kept *time-dependent* atomic and molecular orbitals out of focus. The ultimate triumph of understanding the "dynamic" nature of the chemical bond will only be achieved by directly monitoring the *time-dependent* atomic or molecular orbitals (or in other words, *time-dependent* change of the electron density) during formation or rupture of a chemical bond. With this consensus,

I have made an attempt to start phase-wise development of an attosecond spectroscopy facility to explore the attochemistry of chemical bonding, for the first time, in India and in international scientific community. In the first phase of this highly ambitious effort, I have built facility for high harmonic generation spectroscopy (Int. Rev. Phys. Chem., 40, 405 (2021) or DOI: **https://doi.org/10.1080/0144235X.2021.1976499).** Furthermore, we have found that higher order harmonic yield can be enhanced due to attosecond charge transfer in noncovalently bonded clusters (J. Phys. Chem. A, 123, 5144 (2019) or DOI: **https://doi.org/10.1021/acs.jpca.9b03295**). **This is a unique observation which has not been reported before in chemical bonding literature**.



High harmonic generation spectroscopy and its connection to attosecond dynamics.

Our work is a significant move towards fundamental science. One of the important next directions is to capture orbital hybridization dynamics. Hybridization is a very popular concept in chemical bonding literature. Thus far, secondary kinetic isotope effect is considered to be an indirect evidence of dynamical change of orbital hybridization during chemical reaction. **However, thus far, nobody has observed hybridization dynamics in real time**. This requires intervention of attosecond spectroscopy. One of our future directions is to explore attosecond change of hybridization in H_2 bond and Li_2 bond following vertical ionization. The motivation behind this work comes from the fact that 1 electron Li-Li is stronger than 2 electron Li-Li bond while 2 electron H-H bond is stronger than 1 electron H-H bond. To the best of our knowledge, nobody other than our group in India and in international science community is working on attochemistry of chemical bonding. Our unique presence in international scientific community is evidenced by the request for a review article from the Editor of **prestigious journal, International Reviews in Physical Chemistry.** Furthermore, one of our theoretical works on attosecond dynamics appeared at the **front cover of Journal of Physical Chemistry A**. This highlights the visibility of our attosecond program in the international science community, even through the program is at the first phase. Second phase of the program is to enable the beamline for attosecond pump-probe study.

III. Thematically Classified Research Publications

III.1 Summary

(1) Author of 37 peer-reviewed research publications in the area of molecular spectroscopy, femtosecond spectroscopy, chemical dynamics, catalysis, surface science, quantum dynamics through conical intersection, attosecond dynamics.

(2) Citation profile, as per Google Scholar 726 citations with h-index of 13 (**https://scholar.google.co.in/citations?user=L86LTeAAAAAJ&hl=en**)

III.2 Most Important 5 Experimental Papers in Last 5 Years

Research Publication	Statement of Significance
S. Banerjee, J. Ghosh, A. Chakraborty, A. Bera and A. Bhattacharya*, "*Catalytic $O_{adsorbed}+O_{adsorbed}=O_{2,gas}$ Desorption from c(2x2)-O and p(5x5)-O Phases on Single Crystal Pd(100) Surface: Observing the Unseen using Femtosecond Laser Spectroscopy*" Chem. Phys. Lett., 784, 139117 (2021) **https://doi.org/10.1016/j.cplett.2021.139117**	This work, for the first time, shows that temperature programmed desorption spectroscopy which is conventionally used to study catalysis mechanisms and kinetics fails to explore the catalytic reaction for certain adsorbate phase; while coupling of surface science approach and femtosecond laser spectroscopy can overcome the limitation. This is an important demonstration because this shows surface chemical dynamics as defined in my CV already is a unique route to understand details of catalysis.
S. Banerjee, A. Bera, A. Chakraborty, J. Ghosh, S. M. Varghese and A. Bhattacharya*, "*Ultrafast Dynamics of Recombinative Desorption of Molecular Oxygen from the Single Crystal Pd(110) Surface*" Chem. Phys., 551, 111332 (2021) **https://doi.org/10.1016/j.chemphys.2021.111332**	Instrumentation for coupling surface science study and femtosecond laser spectroscopy is a challenging task because one cannot purchase a stand-alone commercially available equipment to perform surface chemical dynamics study. This work documents details of the instrumentation which we have used to perform surface chemical dynamics study for the first time in India.
S. Chandra, I. Ansari, G. Dixit, F. Lepine and A. Bhattacharya*, "*Experimental Evidence of Sensitivity of the High Harmonic Generation to the Hydrogen Bonding*" J. Phys. Chem. A, 123, 5144 (2019) **https://doi.org/10.1021/acs.jpca.9b03295**	High harmonic generation (HHG) spectroscopy is an excellent route to explore attosecond dynamics because it can probe the electronic structure in atoms and molecules with attosecond or a few femtosecond resolution. Thus far, many efforts have been directed towards understanding the factors which can enhance the HHG yield. A common mechanism of enhancing the HHG yield involves the simultaneous use of an XUV field with the driving IR laser field for harmonic generation. Our work, for the first time, shows that

	higher order harmonic yield can also be enhanced due to attosecond charge transfer in noncovalently bonded clusters. This is a key concept which can be used further to explore attosecond dynamics of hybridization dynamics. The general appeal of this work was so high that the Editor of International Reviews in Physical Chemistry contacted us to write a review article on this general theme of attosecond chemical bonding.
S. Banerjee, A. Bera and A. Bhattacharya*, "*Femtosecond Laser-Induced Recombinative $O+O=O_2$ Reaction on Single Crystal Pd(100) Surface Requires Thermal Assistance*" J. Phys. Chem. C, 122, 26039-26046 (2018) https://doi.org/10.1021/acs.jpcc.8b08653	In the past, many efforts were directed by many scientists to observe a simple surface reaction, $O+O=O_2$, using femtosecond laser heating. All of them were in vain. We have, for the first time, shown that other scientists were in vain because this reaction can be carried out using femtosecond laser heating only at elevated surface temperature. Thereby, we have proved that thermal activation is needed to drive this reaction using femtosecond pulse heating with absorbed fluence of 2.86 mJ/cm^2 which was used by earlier scientists.
A. Bera, S. Banerjee, A. Bhattacharya,* Nidhi Tiwari, Shambhu Nath Jha, Dibyendu Bhattacharyya, "*Morphology, Stability, Structure and CO_2-Surface Chemistry of Micelle Nanolithographically Prepared Two-Dimensional Arrays of Core-Shell Fe-Pd Multicomponent Nanoparticles*" J. Phys. Chem. C, 122, 26528-26542 (2018) https://doi.org/10.1021/acs.jpcc.8b09162	Room temperature CO_2 capture is an important goal of current catalysis community. Iron oxide nanoparticles are not active for room capture of CO_2, but our work, for the first time, shows that if iron oxide is doped with palladium, the material becomes active for room temperature capture of CO_2. Thereby our work shows that iron oxide-based materials which are inexpensive, easy to synthesize, and abundant can be made active material for room temperature capture of CO_2.

III.3 Complete List of Publications

III.3.1 Experimental Surface Chemical Dynamics

1. S. Banerjee, J. Ghosh, A. Chakraborty, A. Bera and A. Bhattacharya*, "*Catalytic $O_{adsorbed}+O_{adsorbed}=O_{2,gas}$ Desorption from c(2x2)-O and p(5x5)-O Phases on Single Crystal Pd(100) Surface: Observing the Unseen using Femtosecond Laser Spectroscopy*" Chem. Phys. Lett., 784, 139117 (2021).
2. S. Banerjee, A. Bera, A. Chakraborty, J. Ghosh, S. M. Varghese and A. Bhattacharya*, "*Ultrafast Dynamics of Recombinative Desorption of Molecular Oxygen from the Single Crystal Pd(110) Surface*" Chem. Phys., 551, 111332 (2021).
3. S. Banerjee, A. Bera and A. Bhattacharya*, "*Femtosecond Laser-Induced Recombinative $O+O=O_2$ Reaction on Single Crystal Pd(100) Surface Requires Thermal Assistance*" J. Phys. Chem. C, 122, 26039-26046 (2018)

4. A. Bera, S. Banerjee, A. Bhattacharya,* Nidhi Tiwari, Shambhu Nath Jha, Dibyendu Bhattacharyya, "*Morphology, Stability, Structure and CO_2-Surface Chemistry of Micelle Nanolithographically Prepared Two-Dimensional Arrays of Core-Shell Fe-Pd Multicomponent Nanoparticles*" J. Phys. Chem. C, 122, 26528-26542 (2018).
5. A. Bera, A. Bhattacharya*, N. Tiwari, S. N. Jha and D. Bhattacharyya, "*Morphology, Stability, and X-ray Absorption Spectroscopic Study of Iron Oxide (Hematite) Nanoparticles Prepared by Micelle Nanolithography*" Surf. Sci., 669, 145 (2018).

III.3.2 Experimental High Harmonic Generation Spectroscopy

6. J. Ghosh, S. Chandra and A. Bhattacharya*, "High Harmonic Generation Spectrum of Energetic Molecule Nitromethane", Chem. Phys. Lett., 806, 139999 (2022).
7. S. Bag, S. Chandra, S. Chakraborty and A. Bhattacharya*, "*On The Analysis of High Harmonic Generation Spectra of Atoms and Molecules Using Molecular Electrostatic Potential*" J. Phys. Chem. A, 125, 3689-3695 (2021).
8. S. Chandra, I. Ansari, G. Dixit, F. Lepine and A. Bhattacharya*, "*Experimental Evidence of Sensitivity of the High Harmonic Generation to the Hydrogen Bonding*" J. Phys. Chem. A, 123, 5144 (2019).

III.3.3 Computational Quantum Dynamics

9. J. Ghosh, H. Gajapathy, A. Jayachandran, E. R. Bernstein and A. Bhattacharya*, "*On the Electronically Nonadiabatic Decomposition Dynamics of Furazan and Triazole Energetic Molecules*" J. Chem. Phys., 150, 164304 (2019).
10. J. Ghosh, S. Bhaumik and A. Bhattacharya*, "*Comparison of Internal Conversion Dynamics of Azo and Azoxy Energetic Moieties through the $(S_1/S_0)_{CI}$ Conical Intersection: An Ab Initio Multiple Spawning Study*" Chem. Phys., 513, 221-229 (2018).
11. J. Ghosh, A. Bera and A. Bhattacharya, "*AIMS Simulation Study of Ultrafast Electronically Nonadiabatic Chemistry of Methyl Azide and UV-VIS Spectroscopic Study of Azido-Based Energetic Plasticizer Bis(1,3-diazidoprop-2-yl)malonate*" Chem. Phys., 494, 78 (2017).
12. S. Bag, S. Chandra and A. Bhattacharya, "*Molecular Attochemistry in Non-polar Liquid Environment: Ultrafast Charge Migration Dynamics through Gold-Thiolate and Gold-Selenolate Linkages*", Phys. Chem. Chem. Phys., 19, 26679 (2017).
13. J. Ghosh, H. Gajapathy, A. Konar , G. Narasimhaiah and A. Bhattacharya, "*Sub-500 fs Electronically Nonadiabatic Chemical Dynamics of Energetic Molecules from the S_1 Excited State: Ab Initio Multiple Spawning Study*", J. Chem. Phys., 147, 204302 (2017)**.**
14. A. Bera, J. Ghosh and A. Bhattacharya "*Ab Initio Multiple Spawning Dynamics Study of Dimethylnitramine and Dimethylnitramine-Fe Complex to Model Their Ultrafast Nonadiabatic Chemistry*" J. Chem. Phys., 147, 044308 (2017).
15. S. Chandra and A. Bhattacharya*, "*Attochemistry of Ionized Halogen, Chalcogen, Pnicogen, and Tetrel Non-Covalent Bonded Clusters*" J. Phys. Chem. A, Feature Article, 120, 10057-10071 (2016), Appeared in Cover Art.
16. S. Banerjee, S. A. Shetty, M. N. Gowrav, C. Oommen, and A. Bhattacharya, "*Decomposition of Monopropellant HAN on Pd(100) and Ir(100) Surfaces: A DFT Study*", Surf. Sci. 653, 1-10 (2016).
17. S. Chandra, M. M. Iqbal and A. Bhattacharya, "*On the Attosecond Charge Migration in Cl⋯N, Cl⋯O, Br⋯N, and Br⋯O Halogen Bonded Clusters: Effect of Donors, Acceptor, Vibration, Rotation, and Electron Correlation*", J. Chem. Sci. 128, 1175-1189 (2016).
18. S. Chandra, B. Rana, G. Periyasamy and A. Bhattacharya "*On the Ultrafast Charge Migration Dynamics in Isolated Ionized Halogen, Chalcogen, Pnicogen, and Tetrel Bonded Clusters*" Chem. Phys. 472, 61-71 (2016).

19. J. Ghosh and A. Bhattacharya "*Prediction of Electronically Nonadiabatic Decomposition Mechanisms of Isolated Gas Phase Nitrogen-Rich Energetic Salt: Guanidium-Triazolate*" Chem. Phys., 464, 26-39 (2016).
20. S. Chandra, G. Periyasamy and A. Bhattacharya "*On the Ultrafast Charge Migration and Subsequent Charge Directed Reactivity in Cl···N Halogen Bonded Clusters Following Vertical Ionization*" J. Chem. Phys., 142, 244309 (2015).
21. A. Bera and A. Bhattacharya, "*Excited Electronic State Processes of a Model Metalized Energetic Material: Dimethylnitramine-Aluminum (DMNA-Al) Complex*" J. Chem. Sci., 127, 71-82 (2015).
22. A. Bera, S. Maroo, and A. Bhattacharya, "*Electronically Nonadiabatic Decomposition Mechanisms of Clusters of Zinc and Dimethylnitramine*" Chem. Phys., 446, 47-56 (2015)
23. A. Bhattacharya and E. R. Bernstein "*Excited Electronic State Decomposition of Gas Phase RDX: An ONIOM-CASSCF Study*" J. Phys. Chem. A. 115, 4135 (2011)

III.3.4 Experimental Molecular Spectroscopy and Laser Spectroscopy

24. A. Bhattacharya, Y. Q. Guo, and E. R. Bernstein, "*A Comparison of the Decomposition of Electronically Excited Nitro-Containing Molecules with Energetic Moieties C-NO_2, N-NO_2, and O-NO_2.*" J. Chem. Phys. 136, 024321 (2012)
25. A. Bhattacharya and E. R. Bernstein, "*Influence of turn (or fold) and Local Charge in the Fragmentation of Peptide Analogue Molecule, CH_3CO-Gly-NH_2 Following Single Photon Ionization at 10.5 eV*" J. Phys Chem. A. 115, 10679 (2011).
26. Y. Q. Guo, A. Bhattacharya, and E. R. Bernstein "*Decomposition of Excited Electronic State s-Tetrazine and its Energetic Derivatives*" J. Chem. Phys. 134, 024318 (2011).
27. A. Bhattacharya, J.-W. Shin, K. Clawson, and E. R. Bernstein, "*Conformation Specific and Charge Directed Reactivity of Radical Cation Intermediates of α-substituted (hydroxyl, amino, keto) Bioactive Carboxylic Acids*" Phys. Chem. Chem. Phys. 12, 9700 (2010).
28. A. Bhattacharya, Y. Q. Guo, E. R. Bernstein, "*Unimolecular Decomposition of Tetrazine-N-oxide Based High Nitrogen Content Energetic Materials from Excited Electronic States*" J. Chem. Phys. 131, 194304 (2009).
29. A. Bhattacharya, Y. Q. Guo, E. R. Bernstein "*Experimental and Theoretical Exploration of the Initial Steps in the Decomposition of a Model Nitramine Energetic Material: Dimethylnitramine*" J. Phys. Chem. A, 113, 811 (2009).
30. Y. Q. Guo, A. Bhattacharya, E. R. Bernstein "*Photodissociation Dynamics of Nitromethane at 226 and 271 nm at Both Nanosecond and Femtosecond Time Scales*" J. Phys. Chem. A, 113, 85 (2009).
31. Y. Q. Guo, A. Bhattacharya, E. R. Bernstein, "*Excited Electronic State Decomposition of Furazan Based Energetic Materials: 3,3′-Diamino-4,4′-Azoxyfurazan and its Model Systems, Diaminofurazan and Furazan*", J. Chem. Phys. 128, 034303 (2008).
32. Y. Q. Guo, M. Greenfield, A. Bhattacharya, E. R. Bernstein, "*On the Excited Electronic State Dissociation of Nitramine Energetic Materials and Model Systems*", J. Chem. Phys. 127, 154301 (2007).

III.3.5 Experimental Femtosecond Laser Spectroscopy

33. T. Katayama, Y. Inubushi, Y. Obara, T. Sato, T. Togashi, K. Tono, T. Hatsui, T. Kameshima, A. Bhattacharya, Y. Ogi, N. Kurahashi, K. Misawa, T. Suzuki, M. Yabashi, "*Femtosecond X-ray Absorption Spectroscopy with Hard X-ray Free Electron Laser*" Appl. Phys. Lett. 103, 131105 (2013).
34. Y. Q. Guo, A. Bhattacharya, and E. R. Bernstein, "*Ultrafast S_1 to S_0 Internal Conversion Dynamics for Dimethylnitramine through a Conical Intersection*" J. Phys. Chem. A, 115,

9349 (2011)

III.3.6 Review Articles

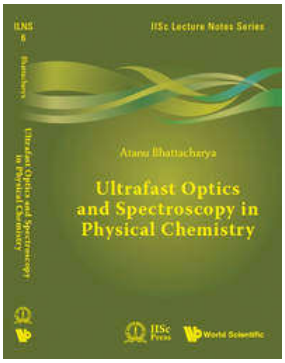
35. S. Bag, S. Chandra, J. Ghosh, A. Bera, E. R. Bernstein and A. Bhattacharya*, "*The Attochemistry of Chemical Bonding*" Intl. Rev. Phys. Chem., 40, 405-455 (2021).
36. A. Bhattacharya, Y. Q. Guo, and E. R. Bernstein "*Nonadiabatic Chemistry of Energetic Molecules*" Acc. Chem. Res. *invited article*, 43, 1476 (2010).

III.3.7 Book and Book Chapter

37. Atanu Bhattacharya, "*Ultrafast Optics and Spectroscopy in Physical Chemistry*", 2018, IISc-Press in association with World Scientific.
38. Elliot R. Bernstein and Atanu Bhattacharya, "*Exploring Intra- and Inter-molecular Interactions Between Non-Covalently Bonded Species Through Investigations of Clusters: Past, Present and Future*" in the Book "Intra- and Inter-molecular Interactions Between Noncovalently Bonded Species" 2020, Page 189-234.

IV Authored Textbooks

IV.1 Atanu Bhattacharya, Ultrafast Optics and Spectroscopy in Physical Chemistry, 2018, World Scientific, ISBN: 978-981-3223-67-7



This is a text book for new physical chemistry students who have background of chemistry or physical chemistry and who are interested in learning what ultrafast spectroscopy is, why optics related to the subject requires special attention, how to use the basic ideas of the subject in laboratory based ultrafast spectroscopy experiments, and how to interpret the experimental observations, etc. Sold more than 200 copies globally. Incorporated as a text book at IIT Madras and IIT Roorkee.

IV.2 Atanu Bhattacharya and Elliot R. Bernstein, Time-Dependent Quantum Chemistry, Under Review with World Scientific, 2022

This is a text book to introduce basic concepts behind time-dependent quantum chemistry revolving around the topics including time-dependent Schrodinger equation, stationary and superpositions states, Ehrenfest theorem and Bohmian mechanics, wavepacket dynamics, matrix representation of time-dependent Schrodinger equation, time evolution operator and its numerical implementation, adiabatic theory, light-atom interaction, quantum dissipative theory, wavepacket correlation function, etc. Hands-on exercises with Python programming are included so that students can practically solve simple selected quantum dynamical problems.

V Sponsored Research Project

V.1 Completed Projects (as PI)

Title	Funding Agency	Total Grant	Duration	Sanction Date	Other Investigator
5. On the Development of Liquid Phase Photoelectron Spectroscopy	DST-SERB	419.9 lakh INR	5 Years	24.03.2015	Not Any
4. Towards Ultrafast Investigation of Laser Initiated Decomposition Mechanism, Kinetics, and Dynamics of Metalized Energetic Materials	ISRO-STC	19.55 Lakh INR	3 Years	01.04.2014	Not Any
3. Size Controlled Synthesis of Supported Bimetallic Nanoparticles via Micelle Nanolithography	DAE-BRNS	17.00 lakh INR	3 Years	31.03.2014	Prof. Dibyendu Bhattacharya, BARC, Mumbai
2. Ultrafast Photocatalytic Reaction Mechanisms and Dynamics at the Semiconductor-Supported Metal Nanoparticle Surfaces in ultra high vacuum	DST-Nano Mission	264.196 Lakh INR	3 Years	10.12.2014	Not Any
1. Start-up grant towards procurement of UHV based surface analysis system equipped with quadrupole mass spectrometer, plasma cleaning facility and electron energy analyzer.	Indian Institute of Science	185.00 lakh INR	3 Years	19.07.2013	Not Any

V.2 Ongoing Projects (as PI)

Title	Funding Agency	Total Grant	Duration	Sanction Date	Other Investigator
6. Room Temperature Capture Followed by Photocatalytic Reduction of CO_2 on Iron Oxide-Based Nanomaterial Surfaces	MHRD-STAR	44.5 Lakh INR	3 Years	16.09.2020	Not Any

VI Scientific Talent Mentoring

VI.1 PhD Students Advised as Sole Supervisor at IISc

Name of the Student	Thesis Title	Awards/Honors/Distinction Secured by the Student	Current Status
Anupam Bera (30.07.2013-07.06.2019)	Thermal and Femtosecond Laser-Induced CO_2-Surface Chemistry on Supported Iron Oxide-Based Nanoparticle Surfaces Under UHV	1. **JRF** from CSIR (2013) 2. **SRF** from CSIR (2015) 3.**Raman-Charpak Fellowship** by Indo-French Centre for the Promotion of Advanced Research (IFCPAR), 2015	**Postdoctoral Appointment**: with Professor Eckart Hasselbrink, Surface Dynamics Group, University of Duisburg, Essen, Germany
Sourav Banerjee (01.08.2014-14.01.2020)	Femtochemistry of Heterogeneous Catalysis: Recombinative $O+O=O_2$ Reaction on Single Crystal Palladium Surfaces	**Best Poster Award**, Conference on Optics, Photonics and Synchrotron Radiation for Technological Application, Raja Ramanna Centre for Advanced Technology, Indore, India, 2018	**Appointed as Assistant Professor**, in the Department of Chemistry, Visva-Bharati University, W.B.
Jayanta Ghosh (01.08.2014-02.05.2020)	Ultrafast Processes in Energetic Molecules	---	**Postdoctoral Appointment**: with Professor Thomas Baumert, Ultrafast Laser Control Experimental Physics Group, University of Kassel, Kassel, Germany
Sankhabrata Chandra (01.08.2015-19.10.2020)	Attosecond Charge Migration in Noncovalently Bonded Clusters	**SERB International Travel Support Award** by DST for attending Ultrafast X-ray summer school conference, USA, 2018	**Postdoctoral Appointment**: with Professor Ralf I. Kaiser, Astrochemical Reaction Dynamics Group, University of Hawaii, Honolulu, USA
Sampad Bag (01.01.2017-31.01.2022)	Towards Electronic Scale Dynamics of Chemical Bonding in Isolated Molecules and Solvated Species	---	**Postdoctoral Appointment**: with Professor Martina Havenith, Terahertz Spectroscopy (THz) Group, Ruhr-University, Bochum, Germany

VI.2 Undergraduate Students Mentored at IISc

Name of the Student	UG Project Title	Current Status
Harshad Gajapathy (2016-2018)	High Harmonic Generation	Doctoral Appointment: Department of Chemistry, Ohio State University, USA

VI.3 Research Interns Mentored at IISc

From 2013-2022: Total 32 Interns

Ajay Jayachandran, Anish Mukhopadhyay, Arghyadeb Roy, Anirban Konar, Arnab Nandi, Ayush Gupta, Bhanu Tanej, Bhaskar Rana, Dabbiru Sai Suraj, Daniel, Dhiman Roy, Imran Khan, Jayesree Bhagabati, Krishanu Ghosal, Mahamed Musthafa Iqbal, Nabojit Kar, Rahul Kumar, Saunak Kumar Das, Sharath Shetty, Shrinivas Jayaram, Sophy Mariam Varghese, Soumajyoti Chakraborty, Subhajit Bhattachajee, Sudhakar Chennu, Suman Bhaumik, Sunil Samanta, Yoshada Singh, Tuhin Samanta, Thabassum Ahammad, Suvranil Ghosh, Sushant Reddy, Suraj Sai.

VII Teaching and Outreach Activities

VII.1 Teaching Undergraduate and Postgraduate Courses at IISc

Title of the Course	Level	Number of Students Registered
Chemical Kinetics (Fall 2014, Fall 2015)	UG	10
General Chemistry Laboratory (Fall 2020, Fall 2021, Fall 2022)	UG	50
Group Theory and Molecular Spectroscopy (Fall 2016, Fall 2017, Fall 2018, Fall 2019)	PG	15

VII.2 Self-Created Postgraduate Courses at IISc

Title of the Course	Level	Number of Students Registered
Ultrafast Optics and Spectroscopy (Spring 2016, Spring 2017, Spring 2018, Spring 2020)	PG	15
Time-Dependent Quantum Chemistry (Spring 2022)	PG	10

VII.3 NPTEL Courses

Two new courses created and taught independently at NPTEL

1. Ultrafast Optics and Spectroscopy in Physical Chemistry (30 Hours Lectures)
   YouTube link: **https://www.youtube.com/playlist?list=PLgMDNELGJ1Cb4_F7DZ9jJF5OjKLOZjRIk**

2. Time-Dependent Quantum Chemistry (30 Hours Lectures)
   YouTube link: **https://www.youtube.com/playlist?list=PLgMDNELGJ1Cbtd5MIUWUHvasydy7evigA**

VII.4 Teaching at Talent Development Center, IISc Challakere Campus (Teacher's Training Program)

Title of the Course	Level	Number of Students Registered
Thermodynamics and State of Matter (2021, 2022)	Pre-university Teachers	30

VIII Invited Lectures

Lecture Title	Event/Location	Date
Ultrafast Chemical Dynamics: Recombinative Desorption of O_2	Department of Chemistry, University of Sikkim	14.05.2022
Ultrafast Chemical	The Virtual Theme Meeting on Ultrafast	

Dynamics: Recombinative Desorption of O_2	Science (UFS) organized by UM-DAE Centre for Excellence in Basic Sciences, Mumbai	12.11.2021
Attosecond Charge Migration: Dynamics of Chemical Bonding	The Theme Meeting on Ultrafast Science (UFS) organized by IIT Bombay	08.11.2019
Synthesis, Characterization and Surface Chemical Dynamics of 2D Arrays of Supported Nanoparticles: Femtochemistry of Nanocatalysis	National Conference on Optics Photonics and Synchrotron Radiation (OPSR) at RRCAT, Indore	29.04.2018