




Faculty Profile on University Website

www.mjpru.ac.in

| Title | Prof. | First Name | Archana | Last Name | Gupta | Photograph |
|--|--------------------------------|---|-----------------------------|---|-------|---|
| Designation | | Professor | | | |  |
| Department | | Applied Physics | | | | |
| Address | Campus | Department of Applied Physics, F.E.T., M.J.P. Rohilkhand University, Bareilly | | | | |
| | Residence | 124/ 2 Ram Vatika, Bareilly | | | | |
| Mobile No. | | 6397582535 | | | | |
| Email ID | | Personal | drarchana.physics@gmail.com | | | |
| | | University Domain | | | | |
| Professional Networking ID, i.e. LinkedIn, Twitter etc. | | NA | | | | |
| Educational Qualifications (Graduation Onwards) | | | | | | |
| Course/Degree | Institution | | Year | Details/Thesis Topic/Subjects | | |
| B.Sc. | Lucknow University, Lucknow | | 1985 | Physics, Chemistry, Mathematics | | |
| M.Sc. | Lucknow University, Lucknow | | 1987 | Physics | | |
| NET-JRF | CSIR | | June 1991 | | | |
| Ph.D. | Lucknow University, Lucknow | | 1996 | Topic 'Phonon Dispersion and Spin State Studies of Some Biomolecules' | | |
| Career Profile | | | | | | |
| Organization / Institution | | Designation | Duration | Nature of Duties | | |
| M.J.P. Rohilkhand University, Bareilly | | Lecturer | Feb 1996 | Teaching and Research | | |
| M.J.P. Rohilkhand University, | | Reader | Feb 2005 | Teaching and Research | | |

| | | | | | | | |
|--|--|--|--|--|---------------------------|-------------------------------------|----|
| Bareilly | | | | | | | |
| M.J.P. Rohilkhand University, Bareilly | | Lecturer | Feb 2011 | Teaching and Research | | | |
| Research Interests / Specialization | | | | | | | |
| Spectroscopy | | | | | | | |
| Research Experience in Years: 25 years | | | | | | | |
| No of Research Scholars Successfully Guided: 05 (03 as Supervisor and 02 as co-supervisor) 04 (Currently working) | | | | | | | |
| Name of Programme | | Awarded | Under Supervision | | | | |
| Ph.D. | | | | | | | |
| M.Phil. | | | | | | | |
| Dissertation (M.Ed./M.A.) | | | | | | | |
| Researcher/ Expert ID | Scopus | Orchid | Publications | Vidwan | Google Scholar | | |
| | | | | | | | |
| | | | | | | | |
| Teaching Experience (Subjects/Courses Taught): 30 years | | | | | | | |
| Engineering Physics I & II, Classical & Statistical Physics, Quantum Mechanics, Material Science, Classical Electrodynamics | | | | | | | |
| Engineering Physics Lab, M.Sc. I lab | | | | | | | |
| Honours / Awards & Fellowship FOR OUTSTANDING WORK: none | | | | | | | |
| Name of Award/ Fellowship | | Awarded By | | | | | |
| | | Name of Governmental Agency | Name of Government Supported Organization/ Department | Name of International Recognized Body | | | |
| | | | | | | | |
| Publications /Academic Activities (Numbers Only) | | | | | | | |
| Books & Monographs (Single Author) | Research Papers Published in International Journals | 22 | Papers Presented in Seminars/ Conferences | Seminars/ Conferences Organized | 5 | Research Projects (Completed) | 02 |
| Books (Co- authored) | Research Papers Published in | | Seminar/ Conferences | Workshop s | 3 | Research Projects | |

| | | Other Journals | | Attended | | Organized | | (Ongoing) | |
|--------------------------|---|---|--|---|---|---|---|---|----|
| Books (Edited) | 1 | Articles Published in Popular Fora, e.g., Websites, Blogs, Newspapers, Magazines etc. | | Sessions Chaired in Seminars/ Conferences | | Membersh ip of Academic/ Profession al Bodies | 2 | Foreign Countries Visited for Academic Assignmen ts | 01 |
| Chapters in Edited Books | 6 | | | Resource Lectures Delivered | 6 | | | | |

| Details of Publications /Academic Activities (2010 Onwards) | | | | | |
|---|--|-------------------|-------------------|----------------------|-------------------------|
| (a) Authored Books/ Monographs | | | | | |
| Name of Book | Year of Publication | Publisher | ISBN No | | |
| | | | | | |
| (b) Edited Books | | | | | |
| Year of Publication | Title | Publisher | ISBN | DOI No. | Citations |
| 2011 | Advancements and Futuristic Trends in Material Science | Allied Publishers | 978-81-8424-706-0 | | |
| (c) Papers Published in UGC Care Listed /Indexed/ Peer Reviewed Journals | | | | | |
| Title of the paper | Journal | ISSN No. | Year | Impact Factor | No. of citations |
| Phonon Dispersion and Heat Capacity of Polydichlorobutadiene | Polymer Science, Series A | 0965-545X | 2010 | 0.958 | 4 |
| Vibrational Dynamics and Heat Capacity of Polychloroprene | Journal of Applied Polymer Science | 0021-8995 | 2011 | 2.52 | 2 |
| Phonon dispersion and specific heat in trans 1,4, poly (2,3-dimethylbutadiene) | Journal of Materials Science | 0022-2461 | 2011 | 3.282 | 1 |
| Heat Capacity and Phonon Dispersion in Polyvinylidene Fluoride (β -form) | Polymer Science, Series A | 0965-545X | 2011 | 0.958 | 5 |
| Molecular Structure, Vibrational Spectroscopic, NBO and HOMO-LUMO Studies of 2-Amino 6-Bromo 3-Formylchromone | Molecular Simulation | 0892-7022 | 2012 | 1.716 | 11 |
| Heat Capacity and Phonon Dispersion in Polyselenophene in Relation to the Spectra of Oligoselenophenes | Synthetic Metals | 0379-6779 | 2012 | 3.286 | 6 |
| Density functional theory studies on the structure, spectra (FT-IR, FT-Raman and UV) and first order molecular hyperpolarizability of 2-Hydroxy-3-Methoxy- N- (2-Chloro-Benzyl) -Benzaldehyde-Imine: Comparison to experimental data | Vibrational Spectroscopy | 0924-2031 | 2013 | 1.917 | 33 |
| Comparative Vibrational Spectroscopic Studies, HOMO-LUMO and NBO analysis of N (phenyl) -2, 2- dichloroacetamide, N- (2-chloro phenyl) -2, 2- dichloroacetamide and N-(4-chloro phenyl) - 2, 2- dichloro acetamide based on Density Functional Theory | Computational & Theoretical Chemistry | 2210-271X | 2013 | 1.605 | 82 |
| Use of Vibrational Spectroscopy to study 2-[4-N-dodecadoylamino) | Spectrochimica Acta Part A: | | 2013 | 3.232 | 16 |

| | | | | | |
|---|---|-----------|------|-------|----|
| phenyl]-5-(4- nitrophenyl)-1, 3, 4 -oxadiazole: A combined Theoretical and Experimental Approach | Molecular and Biomolecular Spectroscopy | 1386-1425 | | | |
| Molecular Structure and Vibrational Spectra of N-acetylglycine Oligomers and Polyglycine I using DFT approach | Biopolymers | 0006-3525 | 2014 | 2.248 | 4 |
| Quantum Chemical Calculations of Conformation, Vibrational Spectroscopic, Electronic, NBO and Thermodynamic Properties of N-(2, 3 dichlorophenyl)-2, 2-dichloro acetamide and N-(2, 4 dichlorophenyl) -2, 2-dichloroacetamide | Computational and Theoretical Chemistry | 2210-271X | 2014 | 1.605 | 6 |
| Quantum chemical study on influence of intermolecular hydrogen bonding on the geometry, the atomic charges and the vibrational dynamics of 2, 6 dichlorobenzonitrile | Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy | 1386-1425 | 2014 | 3.232 | 22 |
| Experimental and theoretical (FT-IR, FT-Raman, UV-vis, NMR) spectroscopic analysis and first order hyperpolarizability studies of non-linear optical material: (2E) 3-[4-(methylsulfanyl) phenyl]-1-(4 nitrophenyl) prop-2-en-1-one using Density Functional Theory | Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy | 1386-1425 | 2014 | 3.232 | 38 |
| Molecular structure (monomeric and dimeric) and hydrogen bonds in 5-Benzyl 2- Thiohydantoin studied by FT-IR and FT-Raman spectroscopy and DFT calculations | Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy | 1386-1425 | 2014 | 3.232 | 15 |
| Vibrational study, molecular properties and first-order molecular hyperpolarizability of Methyl 2-amino 5-bromobenzoate using DFT method | Optical Materials | 0925-3467 | 2015 | 2.779 | 9 |
| Evaluation of Structure-Reactivity Descriptors and Biological Activity Spectra of 4-(6-Methoxy-2-Naphthyl)-2-Butanone using Spectroscopic Techniques | Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy | 1386-1425 | 2016 | 3.232 | 8 |
| Molecular Structure, Spectroscopic (FT-IR, FT Raman, UV, NMR and THz) Investigation and Hyperpolarizability Studies of 3-(2-Chloro-6-Fluorophenyl)-1-(2-Thienyl) Prop-2-en-1-one | Journal of Molecular Structure | 0022-2860 | 2017 | 2.463 | 16 |
| Conformational stability, spectroscopic signatures and | RSC Advances | 2046- | 2017 | 3.119 | 4 |

| | | | | | |
|--|--------------------------------|-----------|------|-------|----|
| biological interactions of proton pump inhibitor drug lansoprazole based on structural motifs | | 2069 | | | |
| Molecular structure, nonlinear optical studies and spectroscopic analysis of chalcone derivative (2E)-3-[4-(methylsulfanyl) phenyl]-1-(3-bromophenyl) prop-2-en-1-one by DFT calculations | Journal of Molecular Structure | 0022-2860 | 2017 | 2.463 | 12 |
| Vibrational spectroscopic characterization, electronic absorption, optical non-linearity computation and terahertz investigation of (2E) 3-(4-ethoxy phenyl)-1-(3-bromo phenyl) prop-2-en-1-one for NLO device fabrication | Journal of Molecular Structure | 0022-2860 | 2019 | 2.463 | |
| Evaluation of conformational and spectral behavior and prediction of biological activity and chemical reactivity descriptors of Levosimendan | Journal of Molecular Structure | 0022-2860 | 2020 | 2.463 | |
| Spectroscopic characterization and structural insights of 4-[(1E)-3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl] phenyl 4-methylbenzene-1-sulfonate using vibrational, electronic spectra and quantum chemical calculations | Journal of Molecular Structure | 0022-2860 | 2021 | 2.463 | |

(d) Chapter/Paper Published in Edited Books

| Publication | | Title of the Book | Title of the Chapter | Name & Address of Publisher | Year | ISBN N | DOI | Citation Google/web of science |
|-------------|---------------|--|---|---|------|-------------------|-----|--------------------------------|
| National | International | | | | | | | |
| National | | Emerging Trends in Laser & Spectroscopy and Applications | Vibrational Dynamics of Trans 1, 4 Poly (2, 3-dichlorobutadiene) pp 342-349 | Allied Pub Pvt Ltd, A-104, Mayapuri Phase II, New Delhi-110 064 | 2010 | 978-81-8424-626-1 | | |
| National | | Advancements and Futuristic Trends in Material Science | DFT oligomer approach to Vibrational spectra of poly selenophene pp 342-347 | Allied Pub Pvt Ltd, A-104, Mayapuri Phase II, New Delhi-110 064 | 2011 | 978-81-8424-706-0 | | |

| | | | | | | | | |
|----------|--|---|---|---|------|-------------------|--|--|
| National | | Advancements and Futuristic Trends in Material Science | Molecular Structure, Vibrational Spectroscopic and HOMO-LUMO Studies of 2- Amino 6-Bromo 3-Formyl Chromone pp 239-245 | Allied Pub Pvt Ltd, A-104, Mayapuri Phase II, New Delhi-110 064 | 2011 | 978-81-8424-706-0 | | |
| National | | Advancements and Futuristic Trends in Material Science | Theoretical Studies of the Molecular Structure and Vibrational Spectra of 2-Hydroxy -3-Methoxy -N-(2 Chloro - Benzyl)- Benzaldehyde -Imine using quantum chemical calculations pp 124-129 | Allied Pub Pvt Ltd, A-104, Mayapuri Phase II, New Delhi-110 064 | 2011 | 978-81-8424-706-0 | | |
| National | | Advancements and Futuristic Trends in Material Science | A Relation Between Finite and Infinite Systems: A Case of Phonon Study in Oligo and Polymeric Selenophene pp 203-210 | Allied Pub Pvt Ltd, A-104, Mayapuri Phase II, New Delhi-110 064 | 2011 | 978-81-8424-706-0 | | |
| National | | Proceedings of International Conference on Perspectives in Vibrational Spectroscopy | A Comparative Study of Structural and Non-linear Optical Properties of Two Chalcone Derivatives pp 35- 42 | e-book | 2016 | 978-93-5267-364-3 | | |

(e) Invited as Resource Lectures Person/Examiner/Expert

| Resource person | Detail of Event | Title of Lecture | Date | Institution |
|-----------------|--------------------------|------------------------------------|---------------------------|--------------------------------|
| Prof. Archana | International Seminar on | Intramolecular charge transfer and | 17 th Nov 2013 | University of Lucknow, Lucknow |

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|-------|---|---|-----------------|--|
| Gupta | Advances in Bio & Nano-Materials (ISABNM-2013) | hydrogen bonding interactions of some Thiohydantoin derivatives | | |
| | 5 th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2014) | Vibrational and hyperpolarizability studies of some non-linear optical materials using Quantum Chemical method | July 8-12, 2014 | Mar Ivanios College, Trivendrum, Kerala |
| | International Symposium on Advances in Biological & Material Sciences (ISABMS-2014) | Structure, Vibrational Dynamics and Hyperpolarizability studies of some chalcone derivatives using Density Functional Theory | July 15, 2014 | Humboldt Academy, Lucknow & University of Lucknow |
| | 6 th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2016) | Conformational stability, spectroscopic signatures and biological interactions of some pharmaceutical compounds | Nov 5-8, 2016 | University of Lucknow, Lucknow |
| | 4 th International E-workshop/ Conference on Computational Condensed Matter Physics and Material Science; Materials for Energy and Environment (IWCCMP-2016) | Basis set and electron correlation effects on electronic and vibrational contribution to non-linear optical properties of some conjugated organic molecules | Nov 18-20, 2016 | ABV-Indian Institute of Information Technology and Management, Gwalior |

(f) Seminars/Conferences/Workshops Organized

1. National Conference on 'Advancements and Futuristic Trends in Material Science AFTMS-2011 (March 26-27, 2011) as Organizing Secretary
2. Initiated and organized lecture series on 'New Frontiers and Challenges in Materials Science
3. International Seminar on 'Recent Trends in Material Science RTMS-13 (Nov. 23, 2013)
4. One-week workshop on Futuristic Materials: Characterization, Properties & Applications to Technology FMCPAT-14 (July 17-22, 2014)
5. International Conference on 'New Scintillations on Materials Horizon ICNSMH-16 (Oct 21-23, 2016)
6. Webinar on Virtual labs (6th June, 2020)
7. Workshop on Virtual Labs on 'Performing and Designing experiments on Virtual Platform' (8th to 17th June, 2020) in collaboration with IIT, Roorkee.
8. An e-workshop on 'Technological Tools and their Management in online Teaching' 14th to 21st August, 2020

(g) Projects (With Title, Year, Grants, Funding Agency and Collaborations)

| Year | Name of Project | Funding Agency | Amount | Duration | |
|------|---|----------------|-------------|----------|------|
| | | | | From | Till |
| 2005 | Analytic Embedded Atom Method Potentials for hcp metals | UGC | 90,000/- | 2005 | 2006 |
| 2011 | Quantum Chemical Calculations on Molecular Structure and Spectroscopic Studies of some Biomolecules | UGC | 11,21,800/- | 2012 | 2014 |

(h) Administrative Positions/Assignments Held

| Post | Organization | Duration | |
|-------------------------------------|---------------------------------|-------------|------------|
| | | From | To |
| Head, Department of Applied Physics | M.J.P.R.U., Bareilly | May 2014 | April 2017 |
| Convener BOS | Dept of App Phy, MJPRU Bareilly | March 1996 | Till date |
| Convener RDC | Dept of App Phy, MJPRU Bareilly | May 2014 | April 2017 |
| Incharge Library IET | M.J.P.R.U., Bareilly | August 2006 | July 2013 |
| ADSW | M.J.P.R.U., Bareilly | Jan 2009 | Nov 2020 |
| Incharge | M.J.P.R.U., Bareilly | Dec 2014 | Dec 2021 |

(i) Seminar/Conference Presentations**1. Vibrational Dynamics and Heat Capacity of Polychloroprene**

Parag Agarwal, Archana Gupta, Poonam Tandon & V. D. Gupta
Seminar on Frontiers of Spectroscopy, (SFS 2008), Nov. 10-11, 2008,
Lucknow University, Lucknow

2. Vibrational Dynamics of Trans-1, 4 Poly (2, 3-dichlorobutadiene)

Neetu Choudhary, Archana Gupta, Poonam Tandon & V. D. Gupta
Meghnad Saha Memorial Symposium on 'Emerging Trends in Laser & Spectroscopy and Applications,' (MMSETLSA-2009), Mar 23-25, 2009
Allahabad University, Allahabad

3. Dispersive Behavior of Low Frequency Vibrational Modes of Polychloroprene – A Comparison with β -Polyisoprene

Parag Agarwal, Archana Gupta, Poonam Tandon & V.D.Gupta
National Symposium for Materials Research, (MR -09), May 8-9, 2009,
Indian Institute of Technology, Bombay

4. Vibrational Dynamics and Heat Capacity of Poly (2, 3 Dimethylbutadiene)

Saba Bee, Archana Gupta, Poonam Tandon and V. D. Gupta,
International Conference on Perspectives in Vibrational Spectroscopy, (ICOPVS-2010), Feb. 21-24, 2010,
Banaras Hindu University, Varanasi

5. Spectroscopic Investigation of Chlorodiene Polymers – Poly chloroprene and Poly dichlorobutadiene

Parag Agarwal, Neetu Choudhary, Archana Gupta, Poonam Tandon & V. D. Gupta
National Conference on Recent Advances in Materials Science & Engineering: A Multidisciplinary Approach, (RAMSE – 2010), Oct 23-24, 2010
Jaypee University of Engg. & Technology, Raghogarh, Guna

6. DFT calculations of Structural and Vibrational Spectroscopic Investigation of 2-[4-(N-Dodecanoyl Amino)]-5-(4-Nitrophenyl)-1, 3,4- Oxadiazole

Saba Bee, Archana Gupta, Poonam Tandon & V. D. Gupta
National Conference on Recent Advances in Materials Science & Engineering: A Multidisciplinary Approach, (RAMSE – 2010), Oct 23-24, 2010
Jaypee University of Engg. & Technology, Raghogarh, Guna

7. Vibrational Dynamics and Heat Capacity of Polyvinylidene Fluoride (β - form)

Parag Agarwal, Archana Gupta, Poonam Tandon and V. D. Gupta
International Conference on Frontiers of Polymers & Advanced Materials, (MACRO-2010), Dec.15-17, 2010
Centre for Polymer Science and Engineering, Indian Institute of Technology, Delhi

8. DFT Oligomer Approach to Vibrational Spectra of Polyglycine I

Saba Bee, Archana Gupta, Poonam Tandon and V. D. Gupta
International Conference on Frontiers of Polymers & Advanced Materials, (MACRO-2010), Dec.15-17, 2010
Centre for Polymer Science and Engineering, Indian Institute of Technology, Delhi

- 9. An ab-initio and DFT Calculations of Structure and Vibrational Spectroscopic Investigation of 2-Amino 6-Bromo 3-Formylchromone**
Saba Bee, Archana Gupta, Poonam Tandon & V. D. Gupta
Meghnad Saha Memorial International Symposium-cum-workshop on 'Laser Induced Breakdown Spectroscopy' (MMISLIBS-2010), Dec 21-23, 2010
Allahabad University, Allahabad
- 10. Dispersive Behavior of Polyselenophene: A Comparison with Polythiophene**
Neetu Choudhary, Archana Gupta, Poonam Tandon & V. D. Gupta
Meghnad Saha Memorial International Symposium – cum - workshop on 'Laser Induced Breakdown Spectroscopy' (MMISLIBS-2010), Dec 21-23, 2010
Allahabad University, Allahabad
- 11. Theoretical Studies of the Molecular Structure and Vibrational Spectra of 2-Hydroxy-3-Methoxy-N-(2-Chloro-Benzyl)-Benzaldehyde-Imine**
Parag Agarwal, Archana Gupta and Poonam Tandon
National Conference on Advancements and Futuristic Trends in Material Science, (AFTMS 2011), March 26-27, 2011
Department of Applied Physics, Faculty of Engineering and Technology, M. J. P. Rohilkhand University, Bareilly, India
- 12. DFT Oligomer Approach to Vibrational Spectra of Polyselenophene**
Vipin Deval, Archana Gupta and Poonam Tandon
National Conference on Advancements and Futuristic Trends in Material Science, (AFTMS 2011), March 26-27, 2011
Department of Applied Physics, Faculty of Engineering and Technology, M. J. P. Rohilkhand University, Bareilly, India
- 13. Molecular Structure, Vibrational Spectroscopic, NBO and HOMO-LUMO Studies of 2-Amino 6-Bromo 3-Formylchromone**
Saba Bee, Archana Gupta & Poonam Tandon
National Conference on Advancements and Futuristic Trends in Material Science, (AFTMS 2011), March 26-27, 2011
Department of Applied Physics, Faculty of Engineering and Technology, M. J. P. Rohilkhand University, Bareilly, India
- 14. Normal Modes of Polyselenophene in Relation to Spectra of Oligoselenophenes**
Neetu Choudhary, Archana Gupta, Poonam Tandon & V. D. Gupta
National Conference on Advancements and Futuristic Trends in Material Science, (AFTMS 2011), March 26-27, 2011
Department of Applied Physics, Faculty of Engineering and Technology, M. J. P. Rohilkhand University, Bareilly, India
- 15. Molecular Structure, Vibrational Spectroscopic, NBO and HOMO-LUMO Studies of 2-Hydroxy-3-Methoxy-N-(2-Chloro-Benzyl)-Benzaldehyde-Imine**
Archana Gupta, Parag Agarwal and Poonam Tandon
Colloquium Spectroscopicum Internationale XXXVII held at Buzios - Rio de Janeiro Brazil, August 28 - September 2, 2011
Pontifical Catholic University, Rio de Janeiro - Brazil
- 16. Molecular Structure, Vibrational Spectroscopic and HOMO-LUMO Studies of 2, 6 – Dichlorobenzonitrile by Hartree Fork and Density Functional Method**

Parag Agarwal, Archana Gupta and Poonam Tandon
Exploring the frontiers of vibrational spectroscopy (EXFOVIS 2011) 1-2 Sept, 2011,
Department of Physics and Research Centre, Women's Christian College, Nagercoil,
Kerala

17. Structural and Vibrational Spectroscopic Investigation of N-(phenyl)-2, 2-dichloroacetamide and its mono chloro derivatives with Quantum Chemical Calculations

Archana Gupta, Neetu Choudhary and Poonam Tandon
Kathmandu Symposia on Advanced Materials 2012 (KaSAM – 2012) May 9 -12,
2011 Kathmandu, Nepal

18. Molecular Structure and Vibrational Spectra of N-acetylglycine Oligomers by using DFT calculations

Saba Bee, Archana Gupta and Poonam Tandon
International Conference on Raman Spectroscopy (ICORS 2012), August 12-17,
2012
Indian Institute of Science, Bangalore.

19. Quantum Chemical Vibrational Study, NBO and HOMO-LUMO analysis of N-(phenyl) -2, 2- dichloroacetamide, N-(2-chloro phenyl) -2, 2-dichloroacetamide and N-(4-chloro phenyl) - 2, 2- dichloroacetamide

Neetu Choudhary, Archana Gupta and Poonam Tandon
International Conference on Chemistry and Materials: Prospects and Perspectives -
2012 (ICCMPP-2012) 14-16 December, 2012
Babasaheb Bhimrao Ambedkar University, Lucknow

20. Density Functional Theory Studies on Molecular Structure, Vibrational Spectroscopic (FT-IR, FT-Raman) and Hyperpolarizability of (2E)-3-[4 (methylsulfanyl) phenyl]-1-(4-nitrophenyl) prop-2-en-1-one

Amit Kumar, Poonam Tandon, Archana Gupta and E.D. D'silva
International Conference on Chemistry and Materials: Prospects and Perspectives -
2012 (ICCMPP-2012) 14-16 December, 2012
Babasaheb Bhimrao Ambedkar University, Lucknow

21. Spectroscopic studies on the structure, spectra and first order molecular hyperpolarizability of a non-linear optical material 2-Hydroxy-3-Methoxy-N-(2-Chloro-Benzyl)-Benzaldehyde-Imine using quantum chemical calculations

Parag Agarwal, Archana Gupta and Poonam Tandon
International Conference on Chemistry and Materials: Prospects and Perspectives,
14-16 December, 2012 (ICCMPP-2012)
Baba Sahab Bhim Rao Ambedkar University, Lucknow

22. DFT study of Polyselenophene and its oligomers

Vipin Deval, Archana Gupta and Poonam Tandon
International Conference on Chemistry and Materials: Prospects and Perspectives-
2012 (ICCMPP-2012) 14-16 December, 2012
Babasaheb Bhimrao Ambedkar University, Lucknow

23. Thermal Behavior and Molecular Vibrations of Polyvinylidene Fluoride

Parag Agarwal, Archana Gupta and Poonam Tandon
International Conference on Polymers of the Frontiers of Science & Technology, 21-
23 February, 2013, Asian Polymer Association of UICET

Punjab University, Chandigarh

24. Normal Modes of Polyselenophene in relation to Spectra of Oligoselenophenes

Neetu Choudhary, Archana Gupta, Poonam Tandon and V. D. Gupta
International Conference on Advancement in Polymeric Materials APM-2013, 01-03 March, 2013
CIPET, Lucknow

25. Vibrational Spectra, Thermodynamic and Non-Linear Optical Properties of (2E)-3-[4-(methylsulfanyl) phenyl]-1-(4-nitrophenyl) prop-2-en-1-one using Quantum Chemical Calculations

Amit Kumar, Poonam Tandon, Archana Gupta and E.D. D'silva
Fourth International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 2013) August 6-9, 2013
Bishop Moore College, Mavelikara, Kerala

26. Theoretical and Experimental investigations on the Vibrational spectra of 4-(6-methoxy-2-naphthyl)-2-butanone

Megha Agrawal, Archana Gupta, Poonam Tandon
Fourth International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 2013) August 6-9, 2013
Bishop Moore College, Mavelikara, Kerala

27. Quantum Chemical Study on Influence of Intermolecular Hydrogen Bonding on the Geometry, Atomic Charges and Vibrational Dynamics of 2, 6 - Dichloro benzonitrile

Parag Agarwal, Archana Gupta and Poonam Tandon
Fourth International Conference on Perspectives in vibrational Spectroscopy, August 06-09, 2013 (ICOPVS-2013)
Bishop Moore College, Mavelikara, Kerala

28. Spectroscopic (FT-IR, FT-Raman and UV) Investigation And Computational Studies of 5-Phenyl 2-Thiohydantoin

Vipin Deval, Archana Gupta, Poonam Tandon and Ko-Ki Kunimoto
Fourth International Conference on Perspectives in Vibrational Spectroscopy-2013 (ICOPVS 2013) August 06- 09, 2013
Bishop Moore College, Mavelikara, Kerala

29. Intramolecular charge transfer and hydrogen bonding interactions of 5-Phenyl 2- Thiohydantoin: Vibrational spectral study

Vipin Deval, Archana Gupta, Poonam Tandon and Ko-Ki Kunimoto
International Seminar on Advances In Bio-& Nano-Materials (ISABNM- 2013) November 17, 2013
Department of Physics, University of Lucknow, Lucknow, India.

30. Spectroscopic (FT-IR, FT-Raman and UV), NBO and HOMO LUMO Analysis of Nabumetone using Quantum Chemical Calculations

Megha_Agrawal, Archana Gupta, and Poonam Tandon
International Seminar on Advances In Bio-& Nano-Materials (ISABNM- 2013) November 17, 2013
Department of Physics, University of Lucknow, Lucknow, India.

31. Molecular structure, spectroscopic (FT-IR, FT-Raman, UV, NMR) studies and

first- order hyperpolarizability of Methyl 2-amino 5-bromobenzoate by density functional method.

Avinay Saxena, Rajesh Kumar, Archana Gupta, and Poonam Tandon

International Seminar on Advances In Bio-& Nano-Materials

(ISABNM- 2013) November 17, 2013

Department of Physics, University of Lucknow, Lucknow, India.

32. Experimental and computational study on molecular structure, Vibrational (FT-IR and FT- Raman) spectra, NBO and first order hyperpolarizability analysis of non-linear optical material 3-(4-Methoxyphenyl)-1-(pyridin-2-yl) prop-2-en-1-one

Amit Kumar, Poonam Tandon, Archana Gupta and A. Jayarama

International Seminar on Advances in Bio and Nano Materials

(ISABNM- 2013) November 17, 2013

Department of Physics, University of Lucknow, Lucknow, India.

33. Molecular structure, Vibrational Spectroscopic, NBO and HOMO–LUMO Analysis of N-(2, 4-dichlorophenyl)-2, 2-dichloroacetamide and N-(2, 3-dichlorophenyl)-2, 2-dichloroacetamide using Density Functional Theory

Neetu Choudhary, Archana Gupta and Poonam Tandon

International Seminar on Advances in Bio and Nano Materials

(ISABNM- 2013) November 17, 2013

Department of Physics, University of Lucknow, Lucknow, India.

34. Spectroscopic and DFT investigation of 2-Amino 6-Bromo 3-Formylchromone

Saba Bee, Archana Gupta, and Poonam Tandon

International Seminar on Advances in Bio and Nano Materials

(ISABNM- 2013) November 17, 2013

Department of Physics, University of Lucknow, Lucknow, India.

35. Dimeric structure and hydrogen bonds in 5-Benzyl 2- Thiohydantoin studied by FT-IR and FT-Raman methods and DFT calculations.

Vipin Deval, Archana Gupta, Poonam Tandon and Ko-Ki Kunimoto

International Seminar on Recent Trends in Material Science

(RTMS-13) November 21, 2013

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India.

36. Vibrational Spectral Investigations of antiarthritis drug Nabumetone using Density Functional Theory.

Megha_Agrawal, Archana Gupta, and Poonam Tandon

International Seminar on Recent Trends in Material Science

(RTMS-13) November 21, 2013

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India.

37. Vibrational (FT-IR and FT-Raman) spectral analysis, electronic properties and first order hyperpolarizability studies of non-linear optical material 3-(4-Methoxyphenyl)-1-(pyridin-2-yl) prop-2-en-1-one using Quantum Chemical Calculations.

Amit Kumar, Poonam Tandon, Archana Gupta and A. Jayarama

International Seminar on Recent Trends in Material Science

(RTMS-13) November 21, 2013

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India.

38. Study of Vibrational Spectra and Molecular Structure of *N*-(2,3,4-trichlorophenyl)-2,2-dichloroacetamide using Density Functional Theory

Neetu Choudhary, Archana Gupta and Poonam Tandon

International Seminar on Recent Trends in Material Science

(RTMS-13) November 21, 2013

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India.

39. Molecular structure, vibrational spectra, NLO, MEP and HOMO-LUMO analysis of 3-(2-Chloro-6-fluorophenyl)-1-(2-thienyl)prop-2-en-1-on

Avinay Saxena, Rajesh Kumar, Archana Gupta, Poonam Tandon

International Seminar on Recent Trends in Material Science

(RTMS-13), 21 Nov. 2013

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India

40. First Order Molecular Hyperpolarizability, Intramolecular Charge Transfer and the Vibrational Spectra of NLO Material 2-[4-(*N*-Dodecanoyl Amino)]-5-(4-Nitrophenyl)-1,3,4-Oxadiazole)

Saba Bee, Archana Gupta, and Poonam Tandon

International Seminar on Recent Trends in Material Science (RTMS-13), 21 Nov. 2013,

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India

41. Vibrational and Hyperpolarizability studies of some non-linear optical materials using Quantum Chemical method

Avinay Saxena and Archana Gupta

5th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2014) July 08-12, 2014

Department of Physics, Mar Ivanios College, Trivendrum, Kerala, India

42. Structure Vibrational Dynamics and Hyperpolarizability studies of some non-linear optical molecule using Density Functional Theory

Avinay Saxena and Archana Gupta

International Symposium on Advances in Biological & Material Sciences

(ISABMS- 2014) July 15, 2014

Humboldt Academy, Lucknow & University of Lucknow, Lucknow, India

43. Vibrational Spectroscopic (FT-IR and FT-Raman) studies, Natural Bond Orbital analysis and Molecular Electrostatic Potential Surface of 4-(6-Methoxy-2-Naphthyl)-2-Butanone

Megha Agrawal, Vipin Deval, Amit Kumar, Rajesh Kumar, Archana Gupta and Poonam Tandon

International Symposium on Advances in Biological & Material Sciences (ISABMS-2014) July 15, 2014

Humboldt Academy, Lucknow & University of Lucknow, Lucknow, India

44. Vibrational spectroscopic investigation on pharmaceutical compound Levosimendan: A density functional approach

Megha Agrawal and Archana Gupta

International Workshop on Futuristic Materials: Characterization, Properties & Applications in Technology (FMCPAT-14) July 17-22, 2014

Department of Applied Physics, Faculty of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly, India

45. DFT study on non-linear optical (NLO) properties of 3-(2-Chloro-6-fluorophenyl)-1-(2-thienyl) prop-2-en-1-one

Rajesh Kumar, Vipin Deval, Megha Agrawal, Archana Gupta, Poonam Tandon and P. S. Patil

International Conference on Light Quanta: Modern Perspectives and Applications (ICQLMPA-15) December 14-16, 2015

Physics Department, University of Allahabad, Allahabad

46. Structural optimization, first order hyperpolarizability and spectroscopic analysis of nonlinear optical material 3-(4-Methoxyphenyl)-1-(pyridin-2-yl) prop-2-en-1-one using DFT method

Amit Kumar, Reena, Archana Gupta, Poonam Tandon and A. Jayarama

International Conference on Light Quanta: Modern Perspectives and Applications (ICQLMPA-15) December 14-16, 2015

Physics Department, University of Allahabad, Allahabad

47. Computation and Interpretation of Vibrational Spectra of Antifungal Drug Clotrimazole by Quantum Chemical Methods

Reena and Archana Gupta

International Conference on Advances in Light Technologies and Spectroscopy of Materials (ICALTSM -16) January 16-18, 2016

Department of Physics, University of Lucknow, Lucknow

48. Quantum Chemical Studies on Vibrational Spectra and First Static hyperpolarizability of non-linear optical material of 3-(2, 4-Dichlorophenyl)-1-(4-methylphenyl) prop-2-en-1-one

Rajesh Kumar, Archana Gupta, Poonam Tandon and P. S. Patil

International Conference on Advances in Light Technologies and Spectroscopy of Materials (ICALTSM -16) January 16-18, 2016

Department of Physics, University of Lucknow, Lucknow

49. Vibrational Spectroscopic and static hyperpolarizability studies on non-linear optical material 3-(4-Methoxyphenyl)-1-(pyridin-2-yl) prop-2-en-1-one

Amit Kumar, Archana Gupta, Poonam Tandon and A. Jayarama

International Conference on Advances in Light Technologies and Spectroscopy of Materials (ICALTSM -16) January 16-18, 2016

Department of Physics, University of Lucknow, Lucknow

50. Simulation and Interpretation of Vibrational Spectra of Antifungal Drug 1[(2-Chlorophenyl) (Diphenyl)Methyl] 1H Imidazole by Quantum Chemical Method

Reena and Archana Gupta

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

51. Spectroscopic Characterization and Determination of Reactivity Descriptors of Levosimendan using Experimental and Quantum Chemical Approach

Megha Agrawal and Archana Gupta

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

52. Exploring the Effect of Intermolecular Hydrogen Bonding in 5,5-Diphenyl-2-Thioimidazolidine-4-One: A Theoretical and Experimental Study

Vipin Deval, Archana Gupta, Poonam Tandon and Ko-Ki Kunimoto

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

53. Study of Spectroscopic and Nonlinear Optical (NLO) Properties of 3-(2, 4-Dichloro phenyl)-1-(4-methylphenyl)-prop-2-en-1-one Using Density functional theory method

Rajesh Kumar, Archana Gupta, Poonam Tandon and P. S. Patil

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

54. Vibrational Analysis, Electronic and Nonlinear Optical Properties of 3-(4-bromo phenyl)-1-(pyridin-4-yl) prop-2-en-1-one by Quantum Computational Method

Amit Kumar, Archana Gupta, Poonam Tandon and A. Jayarama

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

55. Simulation and Interpretation of Vibrational Spectra of Antifungal Drug 1 [(2 Chlorophenyl) (Diphenyl)Methyl]1HImidazole by Quantum Chemical Method

Reena and Archana Gupta

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

56. Study of Spectroscopic and Nonlinear Optical (NLO) Properties of 3-(2, 4-Dichloro phenyl)-1-(4-methylphenyl)-prop-2-en-1-one Using Density functional theory method

Rajesh Kumar, Archana Gupta, Poonam Tandon and P. S. Patil

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016) October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

57. Spectroscopic Analysis and Quantum Chemical Studies of (E)-1-(3-Bromo phenyl) -3-(4-Ethoxyphenyl) Prop-2-En-1-One

Pratibha Singh, Archana Gupta and P. S. Patil

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016)

October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

58. Vibrational Analysis, Electronic and Nonlinear Optical Properties of 3-(4-bromophenyl)-1-(pyridin-4-yl) prop-2-en-1-one by Quantum Computational Method

Amit Kumar, Archana Gupta, Poonam Tandon and A. Jayarama

International Conference on New Scintillations on Materials Horizons (ICNSMH-2016)

October 21-23, 2016

Department of Applied Physics, M. J. P. Rohilkhand University, Bareilly.

59. Quantum Chemical study on Vibrational Dynamics and NLO Properties of (2E)-3-[4-(methylsulfanyl) phenyl]-1-(3-bromophenyl) prop-2-en-1-one

Amit Kumar, Archana Gupta, Poonam Tandon and E. Deepak D'silva

6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2016)

November 5-8, 2016

Department of Physics, University of Lucknow, Lucknow.

60. Theoretical investigation on the geometric, spectroscopic and the static first order hyperpolarizability of 3-(2-Chloro-6- fluorophenyl)-1-(2-thienyl) prop-2-en-1-one by Density Functional Theory calculations

Rajesh Kumar, Archana Gupta, Poonam Tandon and P. S. Patil.

6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 2016), 5 – 8 November, 2016

Department of Physics, Lucknow University, Lucknow, India

61. DFT Study of Structure and Vibrational Spectra of Clotrimazole: Comparison to Experimental Data

Reena, Pratibha Singh and Archana Gupta

4th International E Workshop /Conference on Computational Condensed Matter Physics and Materials Science; Materials for Energy and Environment (IWCCMP-2016), 18-20 November, 2016

ABV-Indian Institute of Information Technology and Management, Gwalior.

62. Vibrational Spectroscopic Investigation and Hyperpolarizability Studies of Some Nonlinear Optical Materials using DFT Method

Amit Kumar, Rajesh Kumar, Archana Gupta, and Poonam Tandon

4th International E Workshop /Conference on Computational Condensed Matter Physics and Materials Science; Materials for Energy and Environment (IWCCMP-2016), 18-20 November, 2016

ABV-Indian Institute of Information Technology and Management, Gwalior.

63. Vibrational Spectroscopic Investigation and Hyperpolarizability Studies of Some Nonlinear Optical Materials using DFT Method

Amit Kumar, Rajesh Kumar, Archana Gupta and Poonam Tandon

4th International E-Workshop/Conference on Computational Condensed Matter Physics and Materials Science: Materials for Energy and Environment (IWCCMP-2016) November 18-20, 2016

ABV-Indian Institute of Information Technology and Management, Gwalior.

64. Vibrational Spectra of Conducting Polymer Poly 1, 2- Ethylene Dioxy Benzene (PEDOB): A Quantum–Chemical Oligomeric Approach

Rajesh Kumar, Archana Gupta, Poonam Tandon, Jingkun Xu
International Conference on Spectroscopy of Biomolecules & Advanced Materials, 4-7 October, 2017
Christian College, Chengannur, Kerala

65. Combined Experimental and Quantum Chemical Studies on Molecular Structure and Spectral Properties of Tioconazole

Reena and Archana Gupta
International Conference on Spectroscopy of Biomolecules & Advanced Materials, 4-7 October, 2017
Christian College, Chengannur, Kerala

66. Spectral and nonlinear optical studies of (E)-1-(3-bromophenyl)-3-(4 ethoxyphenyl) prop-2-en-1-one

Pratibha Singh, Archana Gupta and P. S. Patil
International Conference on Spectroscopy of Biomolecules & Advanced Materials, 4-7 October, 2017
Christian College, Chengannur, Kerala

67. Vibrational Spectra and Nonlinear Optical Investigations of a Chalcone Derivative (2E)-3-[4-(Methylsulfanyl) Phenyl]-1-(3-Bromophenyl) Prop-2-en-1-One by DFT method

Amit Kumar, Archana Gupta, Poonam Tandon and E. D. D'silva
International Conference on Spectroscopy of Bio-molecules and Advanced Materials (ICSBAM-2017) October 04-07, 2017
Christian College, Chengannur, Kerala.

68. DFT based vibrational spectral analysis and biological activity of calcium sensitizer Levosimendan

Megha Agrawal and Archana Gupta
International Symposium on Functional Materials (ISFM-18) July 13-15, 2018
Organised by IIT Kanpur, Panjab University Chandigarh and University of Illinois at Chicago

69. Hydrogen Bonding Interactions in 5,5-diphenyl-2-thiohydantoin: An Experimental and Theoretical Study

Vipin Deval, Archana Gupta, Poonam Tandon and Ko-Ki Kunimoto
International Symposium on Functional Materials (ISFM-18) July 13-15, 2018
Organised by IIT Kanpur, Panjab University Chandigarh and University of Illinois at Chicago

70. Vibrational spectroscopic analysis of lansoprazole using experimental and quantum chemical approach

Megha Agrawal and Archana Gupta
7th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2018) Nov 25-29, 2018
Bhabha Atomic Research Centre, Mumbai, India

71. Vibrational analysis and density functional theory calculations of 1-(4-bromo phenyl)- 3-(2,4-dichlorophenyl)-prop-2-en-1-one

Pratibha Singh, Archana Gupta and P. S. Patil
7th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2018) Nov 25-29, 2018

Bhabha Atomic Research Centre, Mumbai, India

72. Structural and Spectroscopic Characterization of Nateglinide

Vipin Deval, Archana Gupta, Poonam Tandon, A. P. Ayala and A. K. Bansal

7th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2018) Nov 25-29, 2018

Bhabha Atomic Research Centre, Mumbai, India

73. Vibrational Spectroscopy and Non-Linear Optical Properties of 3-(2, 4 Di chloro phenyl) -1-(4-methyl phenyl) prop-2-en-1-one

Rajesh Kumar, Archana Gupta, Poonam Tandon, P.S. Patil

7th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2018) Nov 25-29, 2018

Bhabha Atomic Research Centre, Mumbai, India

74. Vibrational Spectroscopy on Non-Linear Optical Properties of 4-[(1E) -3- (5 chloro thiophen-2-yl) -3 -oxoprop-1-en-1-yl] phenyl 4-methylbenzene-1-sulfonate

Rajesh Kumar, Archana Gupta, Poonam Tandon and P. P. Vinaya

International Symposium on Advances in Functional & Biological Materials (ISAFBM-2019), 28 February, 2019

Humboldt Academy Lucknow & Physics Department, University of Lucknow, Lucknow

(j) Memberships of Academic/Professional Bodies

Life Member of Indian Science Congress Association (Membership No. L20779)

Life Member of Material Research Society of India (Membership No. LMB 2143)

(k) Participation in Community Service / Exchange Programme / Consulting Activity:

None

(l) International Academic Exposure

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|---|--|---|--|
| Department of Physics, University of Federal do Ceara, Fortaleza, Brazil | Indo-Brazil Collaborative Project | 21st August, 2011 | 24th September, 2011 |
| | | | |

(m) Any Other Details

Nodal centre co-ordinator of Virtual Labs, a Ministry of Human Resource Development initiative with the Participating Institution IIT Roorkee

Developed four Virtual labs

Signature of Faculty Member