Prof. Onkar Prasad

Designation: Professor

Institutional Address: University of Lucknow, Lucknow

Date of Birth: 10 th July 1966

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Academic Qualification:

- **1996**: Doctor of Philosophy (Ph.D.) in Physics, University of Lucknow, Lucknow, India.
- **1987**: Master of Science (M.Sc. Special) in Physics, *secured First position* in the Department of Physics, University of Lucknow, Lucknow, India.
- **1986**: Bachelor of Science (B.Sc. Hons) in Physics, *secured First position* in the Department of Physics, University of Lucknow, Lucknow, India.
- **1985**: Bachelor of Science (B.Sc.), University of Lucknow, Lucknow, India.

Awards and Scholarships:

- National Merit Scholarship.
- P.N. Sharma Memorial Prize for securing highest marks in B.Sc. Hons Physics examination 1986.
- Ward Memorial Vidyant Gold Medal for best student in M.Sc. (Special) and M.Sc. Part II Physics examination 1987.
- Qualified C.S.I.R. J.R.F. examination 1988.

Academic Appointments:

- **1990 - 1998**: Lecturer in Physics, University of Lucknow, Lucknow.
- **1998 - 2001**: Senior Lecturer in Physics, University of Lucknow, Lucknow.
- **2001 - 2007**: Reader in Physics, University of Lucknow, Lucknow.
- **2007 Onwards:** Professor of Physics, University of Lucknow, Lucknow.

Administrative Positions:

- **2001- 2002**: Assistant Provost Balrampur Hostel, University of Lucknow, Lucknow.
- **November 19, 2024 - till date**: Head, Department of Physics, University of Lucknow, Lucknow.

Committee/Society Services at University of Lucknow:

- Member, Executive Council, University of Lucknow, Lucknow (2024-2025).
- Member, Faculty Board of Science, University of Lucknow, Lucknow.
- Member, Board of Studies, Department of Physics, University of Lucknow, Lucknow.
- Member, Departmental Research Committee, Department of Physics, University of Lucknow, Lucknow.
- Member, various departmental committees, Department of Physics, University of Lucknow, Lucknow.
- Member, Faculty Board of Science, Department of Physics and Astro-Physics, University of Allahabad, Prayagraj.

Academic Contributions:

- Designed and developed the Choice Based Credit System (CBCS) syllabi for the M.Sc. Physics program for University of Lucknow, Lucknow, aligning course structure with current academic and industry standards effective from 2020 to 2025.

- Contributed to restructuring the Choice Based Credit System (CBCS) syllabi for the two years M.Sc. Physics program at the University of Lucknow, ensuring alignment with current academic and industry standards, effective from 2025 onwards.

- Played a key role in Designing and developing the Choice Based Credit System (CBCS) syllabi for the M.Sc. Physics one year program for University of Lucknow, Lucknow, aligning course structure with current academic and industry standards, effective from 2025 onwards.

- Designed and developed the Credit Based System syllabi for the B.Sc. four years program (Physics) for University of Lucknow, Lucknow, aligning course structure with National Education Policy (N.E.P. 2020) standards, effective from 2021 to 2024.

- Restructured the Credit Based System syllabi for the B.Sc. four years program (Physics), Lucknow, aligning course structure with National Education Policy (N.E.P. 2020) standards, effective from 2024 onwards.

- Planned and Coordinated Academic Time tables for undergraduate and postgraduate programs since 2019, ensuring optimal utilization of faculty expertise, classrooms, and course schedules.

Teaching Experience:

More than 35 years of experience in teaching Undergraduate and Postgraduate-level courses.

Undergraduate Level:

- Mechanics
- Electromagnetic Theory
- Optics
- Electronics

Postgraduate Level:

- Nuclear Physics

Supervision and Mentorship:

- Guided Undergraduate and Postgraduate students in their term papers and master thesis projects respectively.
- Supervised **7** Research scholars for their Ph.D. degrees.

Ph.D. Thesis

- **Ph.D. Thesis Title:** The Study of Phonons in Poly (β benzyl – L Aspartate), Poly (L Methionine) and Poly (α Amino – Iso-butyric Acid).

Nature of Research Work:

Actively engaged in exploring and identifying novel anti-cancer agents through a combination of molecular docking and molecular dynamics (MD) simulations. The studies focus on predicting how potential compounds interact within the active site of target biomolecules, evaluating key non-covalent interactions such as hydrogen bonding and van der Waals forces that contribute to binding stability. Long-timescale MD simulations are employed to confirm the structural stability of the biomolecule–ligand complexes, while binding energy calculations and residue-wise decomposition analyses provide deeper insights into the

strength and nature of these interactions. Additionally, all compounds are rigorously screened through pharmacokinetic and drug-likeness filters, ensuring that only the most promising candidates advance further in the development of anti-cancer agents. The research encompasses advanced quantum-chemical and spectroscopic investigations, combining density functional theory with experimental methods to study molecular structures, vibrational behavior, and non-linear optical responses.

Nanoclusters are also explored, investigating their unique physicochemical properties for potential applications in catalysis, materials science, and nanomedicine. Interest in Normal Mode Analysis enables probing of the vibrational behavior of molecules, thus enhancing the understanding of molecular motions and their relation to function and stability.

Technical Proficiency:

- Operating Systems: Windows (10, XP, Vista), Ubuntu, macOS.
- Computational Chemistry Software: Gaussian, Gauss View, Virtual Nano-Lab, Auto Dock Vina, Gromacs, Chem-craft.
- Data Analysis Tools: MS Office Suite (Word, Excel, PowerPoint), Origin Pro.
- Additional Skills: Software installation, system maintenance, computational cluster management

Memberships and Affiliations:

- Life Member of Materials Research Society of India (MRSI)
- Life Member of Indian Science Congress

Research Experience and Metrics:

- Total number of published research papers: **85**
- Highest impact of publication: **5.9**
- Total number of citations: **1733**
- ORCID: **ORCID.org/0000-0001-5961-5868**
- h-Index: **23,** i10-Index: **45**

Research Publications:

2025

1. Unveiling a novel thiazolo [2,3-c] [1,2,4] triazole scaffolds as a dual cyclooxygenase and cholinesterase inhibitors: Spectral analysis, DFT calculations, in vitro and in silico studies. Parveen Rajesab, Basavarajaiah Suliphuldevara Mathada, Vidya Niranjan, Leena Sinha, Anagha S. Setlur, Anushree Maurya, K. Chandrashekar, Onkar Prasad. Journal of Molecular Structure. https://doi.org/10.1016/j.molstruc.2025.143166

2. *In Silico and in Vitro Evaluation of (1H-indol-3-ylmethylene)-pyridin-3-yl-amine as a Potent Inhibitor for VEGFR2, EGFR and Progesterone Receptors, Zohra Siddiqui, Anushree Maurya, Mamta Pal, Raj Shukla, Shilendra K. Pathak, Ruchi Srivastava, Vikas K. Shukla, Onkar Prasad Leena Sinha, Physical Chemistry Research. 10.22036/pcr.2025.500025.2629.*

3. Insights into Novel Isoniazide Encompassing triazolo [4, 3-b] [1, 2, 4] triazoles as Anti-TB, antioxidant and antidiabetic agents: A spectral analysis, DFT calculations, ADME P Rajesab, BS Mathada, V Niranjan, A Maurya, AS Setlur, O Prasad, Journal of Molecular Structure 1334, 141876.

4. Synthesis, Structural, DFT studies, Biological Effectiveness, and Molecular Docking Aspects of Multitarget Novel N-(4-Phenylthiazol-2-yl) hydrazine carboxamide Hybrids as COX inhibitors, Anti-TB, and Anti-oxidant activity. B Hiremath, A Maurya, Nagesh GY, O Prasad, P Karunakar, L Sinha, M Ahmed, Basavarajaiah SM; Journal of Molecular Structure 1321, 140081.

5. In silico insights into dual COX inhibition by fluoro-substituted indole derivative using DFT, molecular docking, and MD simulation studies. M Pal, R Shukla, A Maurya, Z Siddiqui, R Srivastava, SK Pathak, VK Shukla, O Prasad, L Sinha. Journal of the Chinese Chemical Society. 2025 72(6), 653-676. https://doi.org/10.1002/jccs.70020 .

6. Drug delivery potential of γ-graphyne, 6, 6, 12-graphyne and γ-graphdiyne for 5-Fluorouracil: insights from DFT calculations. A Maurya, AN Mishra, J Srivastava, S Mishra, M Pal, R Shukla, Z Siddiqui, M Kurban, O Prasad, L Sinha. Composite Interfaces, 1-21.

2024

7. Computational Study of Coumarin Compounds as Potential Inhibitors of Casein Kinase 2: DFT, 2D-QSAR, ADMET and Molecular Docking Investigations. HY Chennai, S Belaidi, M Ouassaf, L Sinha, O Prasad, G Serdaroğlu, S Chtita. Polycyclic Aromatic Compounds, 1-20, 1.

8. A comprehensive analysis of the spectroscopic and drug-like properties of dimethyl 5-hydroxybenzene-1, 3-dicarboxylate: insights from DFT and MD simulations. M Pal, A Maurya, R Shukla, Z Siddiqui, SK Pathak, R Srivastava, L Sinha, O Prasad, Molecular Simulation 50 (15), 1246-1261.

9. Structural Characterization, Spectroscopic Profile, Molecular Docking, ADMET Properties, Molecular Dynamics Simulation Studies, and Molecular Mechanics Generalized Born Surface. L Sinha, O Prasad, LH Al-Wahaibi, AA El-Emam, M SM Abdelbaky, S Garcia-Granda, ACS omega 9 (24), 26651-26672.

10. Synthesis, Spectroscopic Analysis, Molecular Docking, Molecular Dynamics Simulation of 5-(Adamantan-1-yl)-4-(3-Chlorophenyl)-2,4-Dihydro-3H-1,2,4-Triazole-3. L Sinha, O Prasad, AS Abdelrazeq, HA Ghabbour, LH Al-Wahaibi, MSM Abdelbaky, Polycyclic Aromatic Compounds 44 (4), 2553-2575,1.

11. A Thermo-acoustical And DFT Exploration Of Physio-Chemical Properties For N, N-Dimethylacetamide (DMA) With Water L Kumari, A Hussain, H Agarwal, A Mishra, R Gautam, R Singh, Leena Sinha, Onkar Prasad, Manisha Gupta, Oriental Journal Of Chemistry 40 (2). DOI : Http://Dx.Doi.Org//10.13005/Ojc/400209.

2023

12. DFT Study of the Adsorption Behaviour of Adenine on the Nano-SiO2 Cluster. L Sinha, O Prasad, Meftah, N., Keressa, A., Belaidi, S. et al. Silicon https://doi.org/10.1007/s12633-023-02292-y.

2022

13. Spectroscopic, electronic structure, molecular docking, and molecular dynamics simulation study of 7-Trifluoromethyl-1H-indole-2-carboxylic acid as an aromatase inhibitor. Isha Singh, Ruchi Srivastava, Vikas K Shukla, Shilendra K Pathak, Tanay Burman, Aamal A Al-Mutairi, Ali A El-Emam, Onkar Prasad, Leena Sinha; Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy; Volume 280, 121530.

2021

14. Study of molecular association in binary mixtures of poly(vinyl pyrrolidone) (PVP) with ethanol, 1-propanol and 1-butanol through thermo-acoustical, FT-IR, UV–Vis spectroscopy and DFT studies. Laxmi Kumari, Leena Sinha, Onkar Prasad & Manisha Gupta; Eur. Phys. J. D 75, 296.

15. Surface modification and characterization of h-BN-doped PVP thin film and its application as humidity sensor with theoretical DFT calculations. Laxmi Kumari, Utkarsh Kumar, Leena Sinha, Onkar Prasad, B. C. Yadav & Manisha Gupta, Chemical Papers volume 75, pages 4055–4068.

16. Thermoacoustic and DFT Analysis of N, N-Dimethylacetamide (DMA) with 1-Propanol and Methanol at 293.15, 303.15, and 313.15 KH Agarwal, L Kumari, L Sinha, O Prasad, M Gupta - Brazilian Journal of Physics, 51(3) 515-526

2020

17. DFT study on the electronic properties, spectroscopic profile, and biological activity of 2-Amino-5-trifluoromethyl-1, 3, 4-thiadiazole with anticancer properties, Isha Singh, Lamya H Al-Wahaibi, Ruchi Srivastava, Onkar Prasad, Shilendra K Pathak, Saurabh Kumar, Shama Parveen, Monisha Banerjee, Ali A El-Emam, Leena Sinha, ACS omega, 5(46) 30073-30087.

18. Thermodynamic, spectroscopic and DFT studies of binary mixtures of poly (vinylpyrrolidone)(PVP) with ethanol, 1-propanol and 1-butanol. L Kumari, S Gupta, I Singh, O Prasad, L Sinha, M Gupta. Journal of Molecular Liquids 299, 112237

2019

19. Experimental and theoretical DFT (B3LYP, X3LYP, CAM-B3LYP and M06-2X) study on electronic structure, spectral features, hydrogen bonding and solvent effects of 4-methylthiadiazole-5-carboxylic acid. I Singh, AA El-Emam, SK Pathak, R Srivastava, VK Shukla, O Prasad, and Leena Sinha, Molecular Simulation 45 (13), 1029-1043

2017

20. First principle study of a potential bioactive molecule with tetrahydroisoquinoline, carbothiomide and adamantane scaffolds. MM Al-Shehri, ARA Al-Majed, HI Aljohar, AA El-Emam, SK Pathak, Alok K.Sachan, Onkar Prasad, Leena Sinha, Journal of Molecular Structure 1143, 204-216

21. A combined experimental and theoretical DFT (B3LYP, CAM-B3LYP and M06-2X) study on electronic structure, hydrogen bonding, solvent effects and spectral features of methyl 1H-indol-5-carboxylate. R Srivastava, FAM Al-Omary, AA El-Emam, SK Pathak, M Karabacak, Vijay Narayan, Satish Chand, Onkar Prasad, Leena Sinha, Journal of Molecular Structure, 1137, 725-741.

2016

22. Spectroscopic and electronic structure calculation of a potential antibacterial agent incorporating pyrido-dipyrimidine-dione moiety using first principles. S Fatma, A Bishnoi, V Singh, FAM Al-Omary, AA El-Emam, S Pathak, Ruchi Srivastava, Onkar Prasad, Leena Sinha, Journal of Molecular Structure 1110, 128-137 (2016).

23. Conformational search, spectral analysis and electronic properties of 5-(4-Pyridinyl)-1, 3, 4-thiadiazol-2-amine. VK Shukla, MA Al-Alshaikh, AA El-Emam, AK Sachan, R Srivastava, Onkar Prasad, Leena Sinha. Journal of Molecular Structure 1108, 112-125

24. Investigations on Molecular Structure, Electronic Properties, NLO Properties and Comparison of Drug-Likeness of Triazolothiadiazole Derivatives by Quantum Methods and QSAR Analysis, A Kerassa, S Belaidi, D Harkati, T Lanez, O Prasad, L Sinha, Reviews in Theoretical Science 4 (1), 85-96

25. Prediction of molecular properties and spectroscopic profile of Riluzole with different functionals (B3LYP, M06-2X, MPWLYP): A combined theoretical and experimental study,VK Shukla, AK Sachan, SK Pathak, R Srivastava, O Prasad, L Sinha. Journal of Molecular Structure 1106, 265-276

2015

26. Spectroscopic and electronic structure calculation of a potential chemotherapeutic agent 5-propyl-6-(p-tolylsulfanyl) pyrimidine-2, 4 (1H, 3H)-dione using first principles. MA Al-Alshaikh,

OA Al-Deeb, NZ Alzoman, AA El-Emam, R Srivastava, AlokK. Sachan, Onkar Prasad, LeenaSinha, Journal of Molecular Structure 1100, 225-236.

27. Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid, M Karabacak, L Sinha, O Prasad, S Bilgili, AK Sachan, AM Asiri, A Atac, Journal of Molecular Structure 1095, 100-111.

28. Structure activity relationship and quantitative structure-activity relationships modeling of antitrypanosomal activities of alkyldiamine cryptolepine derivatives. S Belaidi, T Salah, N Melkemi, L Sinha, O Prasad. Journal of Computational and Theoretical Nanoscience 12 (9), 2421-2427.

29. Study on molecular structure, spectroscopic behavior, NBO, and NLO analysis of 3-methylbezothiazole-2-thione. S Chand, FAM Al-Omary, AA El-Emam, VK Shukla, O Prasad, L Sinha. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 146, 129-141.

30. Exploring QSARs of some benzenesulfonamides incorporating cyanoacrylamide moieties as a carbonic anhydrase inhibitors (specifically against tumor-associated isoforms IX and XII). AM Alafeefy, HA Abdel-Aziz, F Carta, CT Supuran, SK Pathak, O Prasad, and Leena Sinha, Journal of enzyme inhibition and medicinal chemistry 30 (4), 519-523.

31. A Combined theoretical and experimental study of conformational and spectroscopic profile of 2-acetamido-5-aminopyridine. SK Pathak, R Srivastava, AK Sachan, O Prasad, L Sinha, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 143, 147-157.

32. Conformational and spectroscopic behaviors of 2, 4-xylyl isothiocyanate. M Cinar, M Karabacak, S Chand, VK Shukla, L Sinha, O Prasad, Journal of Molecular Structure 1087, 113-120.

33. FT-IR and FT-Raman spectroscopic signatures, vibrational assignments, NBO, NLO analysis and molecular docking study of 2-{[5-(adamantan-1-yl)-4-methyl-4H-1, 2, 4-triazol-3-yl]sulfanyl}-N,N-dimethylethanamine. L Sinha, O Prasad, MS Almutairi, AM Alanazi, ES Al-Abdullah, AA El-Emam, SK Pathak, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 140, 1-14.

34. Development of certain novel N-(2-(2-(2-oxoindolin-3-ylidene) hydrazinecarbonyl) phenyl)-benzamides and 3-(2-oxoindolin-3-ylideneamino)-2-substituted quinazolin-4 (3H)-ones as CFM-1 analogs: Design, synthesis, QSAR analysis and anticancer activity, AM Alafeefy, AE Ashour, O Prasad, L Sinha, S Pathak, FA Alasmari,European Journal of Medicinal Chemistry 92, 191-201.

35. Spectral features, electric properties, NBO analysis and reactivity descriptors of 2-(2-Benzothiazolylthio)-Ethanol: Combined experimental and DFT studies. R Srivastava, L Sinha, M Karabacak, O Prasad, SK Pathak, AM Asiri, M.Cinar, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 136, 1205-1215.

36. Experimental (FT-IR, FT-Raman, UV and NMR) and quantum chemical studies on molecular structure, spectroscopic analysis, NLO, NBO and reactivity descriptors of 3, 5-Difluoroaniline. S

K Pathak, R Srivastava, AK Sachan, O Prasad, L Sinha, AM Asiri, M Karabacak. Spectrosochimica Acta Part A: Molecular and Biomolecular Spectroscopy. 2015, 135 283-295.

37. Investigations on Molecular structure, electronic properties, NLO properties, HOMO-LUMO analysis and comparison of drug-likeness of Triazolothiadiazole derivatives by quantum methods and QSAR anaylsis. K Aicha, S Belaidi, H Dalal, T Lanez, L Sinha, O Prasad. Reviews in Theoretical Science. 2015, 3, 1-10.

2014

38. FT-IR, FT-Raman and UV spectroscopic investigation, electronic properties, electric moments, and NBO analysis of anethole using quantum chemical calculations. L Sinha, O Prasad, S Chand, AK Sachan, SK Pathak, VK Shukla, Spectro-chimica Acta Part A: Molecular and Biomolecular Spectroscopy 133, 165-177.

39. Spectroscopic (FT-IR, FT-Raman, and UV–visible) and quantum chemical studies on molecular geometry, Frontier molecular orbitals, NBO, NLO and thermodynamic properties of 1-acetylindole. VK Shukla, ES Al-Abdullah, AA El-Emam, AK Sachan, S K Pathak, A Kumar, O Prasad, A Bishnoi, L Sinha. - Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 133, 626-638.

40. Molecular structure, vibrational and electronic properties of 4-Phenyl-3H-1, 3-thiazol-2-ol using density functional theory and comparison of drug efficacy of keto and enol forms by QSAR analysis. AK Sachan, SK Pathak, S Chand, R Srivastava, O Prasad, S Belaidi, L Sinha. - Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 132, 568-581.

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42. Structural, spectroscopic (FT-IR, FT-Raman and UV) studies, HOMO–LUMO, NBO, NLO analysis and reactivity descriptors of 2, 3 Difluoroaniline and 2, 4-Difluoroaniline.SK Pathak, NG Haress, AA El-Emam, R Srivastava, O Prasad, L Sinha, Journal of Molecular Structure, 1074, 457-466.

43. Structural and spectroscopic characterization of a novel potential anti-inflammatory agent 3-(adamantan-1-yl)-4-ethyl-1H-1,2,4-triazole-5(4H)thione by first principle calculations. L Sinha, O Prasad, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 124 , (2014) 108–123.

44. FT-IR, FT-Raman, NMR, UV and Quantum Chemical Studies on Monomeric and Dimeric Conformations of 3,5-dimethyl-4-methoxybenzoic acid. L Sinha, O Prasad Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 123, 352–362, (2014).

45. Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone, L Sinha, O Prasad SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy 120, 126–136.

46. Structural, vibrational, and electronic properties of Succinimide, N-Hydroxy Succinimide and N-Methyl Succinimide by density functional theory: A comparative study. AK Sachan, S Chand, R Srivastava, VK Shukla, S K Pathak, A Kumar, O Prasad, L Sinha. J. Chem. Pharm. Res., 6(11), 211-227.

47. Quantum chemical study of molecular structure, non-linear optical and vibrational properties of pyridine and pentachloropyridine. S Chand, SK Pathak, AK Sachan, R Srivastava, VK Shukla V. Narayan, A Kumar, O Prasad, L Sinha. - J. Chem. Pharma. Res,6(3), 1434-1444,

2013

48. An experimental and theoretical investigation of Acenaphthene-5-boronic acid: Conformational study, NBO and NLO analysis, molecular structure and FT-IR, FT-Raman, NMR and UV spectra, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 115, 753–766.

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2012

50. Monomeric and dimeric structures, electronic properties and vibrational spectra of azelaic acid by HF and B3LYP methods. Journal of Molecular Structure 1022, 81–88.

51. Structural and spectroscopic characterization of a novel potential chemotherapeutic agent 3-(1-adamantyl)-1-{[4-(2-methoxyphenyl) piperazin-1-yl] methyl}-4-methyl-1H-1, 2, 4-triazole-5 (4H)-thione by first principle calculations. AA El-Emam, AMS Al-Tamimi, KA Al-Rashood, HN Misra, V Narayan, O Prasad, L Sinha- Journal of Molecular Structure, DOI:10.1016/j.molstruc.2012.04.074.

52. The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMO–LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid. O Prasad, L Sinha Spectro-chimica Acta Part A: Molecular and Biomolecular Spectroscopy, Volume 93, 33-46.

53. Theoretical Raman and FTIR vibrational analysis of 2-phenyl-1H-indene-1,3(2H)- dione by ab initio method. O Prasad, L Sinha Journal of At. Mol. Sci. Vol. 3, No. 2, 95-105.

54. Vibrational, Structural and Electronic properties of 6-methyl nicotinic acid by Density Functional Theory. O Prasad, L Sinha Journal of Chemical and Pharmaceutical Research, 4(6), 3287-3296.

55. Theoretical Studies on the Isomers of Quinazolinone by first Principles. O Prasad, L Sinha Research Journal of Recent Sciences, Vol. 1(3) , 11-18.

2011

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57. Electronic structure, electric moments and vibrational O analysis of 3-(2-methoxyphenoxy) propane-1, 2-diol by Π ab initio and density functional theory. L Sinha, A Kumar, V Narayan, RK Srivastava, O Prasad. J. At. Mol. Sci. Vol 2(3), 212-224.

58. Comparative study of frontier orbitals, molecular electrostatic potential surface of Oxygen Nano-clusters by first principles, O Prasad, L Sinha Chinese Journal of Physics, Vol. 49 (2) 664-671.

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60. Quantum Chemical study of Molecular structure, Non-Linear Optical and Vibrational Properties of ortho and meta - Fluorobenzaldehyde. O Prasad, L Sinha Journal of Chemical and Pharmaceutical Research, Vol. 3 Issue 5, 668-677.

2010

61. Electronic structure, non-linear properties and vibrationalanalysis of Acenaphthene and its carbonyl derivative Acenaphthenequinone by density functional theory. O Prasad, L Sinha Journal of Molecular Structure: Theochem, vol. 958, no. 1, 33-40.

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2009

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2007

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2006

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2005

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