

FACULTY PROFILE

Name: Dr. Anuradha Shukla
Designation: Assistant Professor
E_Mail: anuradhs1@srmist.edu.in
Orchid Id: 0000-0002-8537-4743
Scopus Author Id: 58591001300



- **Work Experience:** 9 Years
- **Professional Qualification:**

Degree	Institute/University	Specialization	Year of Passing
Ph.D.	Lucknow University, Lucknow	Spectroscopy and Quantum Chemical Calculations	2018
M.Sc.	Lucknow University, Lucknow	Electronics	2012
B.Sc.	C. M. S. Degree College, Lucknow	PCM	2010

- **Research Interest:**

- Spectroscopy
- Quantum Chemical Calculations
- Material Science

- **Journal Publications:**

1. Eram Khan, **Anuradha Shukla**, Muhammad Asim S Al-Hanafi, Poonam Tandon, Venu R Vangala: **Structural insights, spectral and H-bond analyses, of nitrofurantoin-phenazine cocrystal and comparison of its chemical reactivity with other nitrofurantoin cocrystals**, Journal of Molecular Structure, 2022, 1272, 131387.
2. Priya Verma, Anubha Srivastava, **Anuradha Shukla**, Poonam Tandon, and Manishkumar R. Shimpi: **Vibrational spectra, hydrogen bonding interactions and chemical reactivity analysis of nicotinamide-citric acid cocrystal by an experimental and theoretical approach**, New Journal of Chemistry, 2019, 43, 15956-15967.
3. Karnica Srivastava, **Anuradha Shukla**, Karthick Thangavel, Sitaram Velaga, Poonam Tandon, Kirti Sinha, Manishkumar Shimpi: **Molecular structure, spectroscopic signatures and reactivity analyses of paracetamol hydrochloride monohydrate salt using density functional theory calculations**, CrystEngComm, 21, 2019, 857-865.
4. Eram Khan, **Anuradha Shukla**, Karnica Srivastava, Debraj Gangopadhyay, Khaled H. Assi, Poonam Tandon, Venu R. Vangala: **Structural and reactivity analyses of nitrofurantoin 4-dimethylaminopyridine salt using spectroscopic and density functional theory calculations**, Crystals, 9, 2019, 413.
5. Eram Khan, **Anuradha Shukla**, Aditya N. Jhariya, Poonam Tandon, Venu R. Vangala: **Nitrofurantoin-**

melamine monohydrate (cocrystal hydrate): Probing the role of H-bonding on the structure and properties using quantum chemical calculations and vibrational spectroscopy, Spectrochimica Acta Part A, 2019, 221, 117170-117180.

6. **Anuradha Shukla**, Eram Khan, MHD. Bashir Alsirawan, Rajorshi Mandal, Poonam Tandon, Venu R. Vangala: **Spectroscopic (FT-IR, FT-Raman, 13C SS-NMR) and quantum chemical investigations to explore the structural insights of nitrofurantoin-4-hydroxybenzoic acid cocrystal**, New Journal of Chemistry, 2019, 49, 7136-7149.
7. Eram Khan, **Anuradha Shukla**, Poonam Tandon, Venu R. Vangala, Nitin Jadav, R. Telford, A. P. Ayala: **Study of molecular structure, chemical reactivity and H-bonding interactions in the cocrystal of nitrofurantoin with urea**, New Journal of Chemistry, 41, 2017, 11069-11078.
8. **Anuradha Shukla**, Eram Khan, Karnica Srivastava, Kirti Sinha, Poonam Tandon and Venu R. Vangala: **Study of molecular interactions and chemical reactivity of the nitrofurantoin–3-aminobenzoic acid cocrystal using quantum chemical and spectroscopic (IR, Raman, 13C SS-NMR) approaches**, CrystEngComm, 19, 2017, 3921-3930.
9. **Anuradha Shukla**, Eram Khan, Poonam Tandon and Kirti Sinha: **Study of vibrational spectra and hydrogen bonding network in dimeric and tetrameric model of Ampicillin using DFT and AIM approach**, Journal of Molecular structure, 1131, 2017, 225-235.
10. Neetu Singh, Prabhat Kumar, **Anuradha Shukla**, Satyendra Singh, Poonam Tandon: **Synthesis and Characterization of Nanostructured Magnesium Oxide: Insight from Solid-State Density Functional Theory Calculations**, J InorgOrganometPolym, 26, 2016, 1413-1420.
11. **Anuradha Shukla**, Eram Khan, Anubha Srivastava, Poonam Tandon, Kirti Sinha: **A computational study on molecular structure, multiple interactions, chemical reactivity and molecular docking studies on 6[D (-) α -amino-phenyl-acetamido] penicillanic acid (ampicillin)**, Molecular Simulation, 42, 2016, 863-873.
12. Eram Khan, **Anuradha Shukla**, Anubha Srivastava, Shweta, Poonam Tandon: **Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: a combined DFT and AIM approach**, New Journal of Chemistry, 39, 2015, 9800-9812.

➤ Books and Books Chapters:

1. Eram Khan, Karnica Srivastava, **Anuradha Shukla**, Jaya Pandey, Preeti Prajapati, Poonam Tandon: **Study of pharmaceutical cocrystal using experimental and computational techniques: An overview**, Proceedings of ICOPVS, Nov. 5-8, 2016, ISSN/ ISBN No.: 978-93-5267-364-3, pp. 8-14. (Peer-Reviewed)

➤ Awards and Achievements

1. Research Assistant, Department of Physics, Lucknow University, Under Promotion of University Research and Scientific Excellence (PURSE) Scheme by Department of Science & Technology, Govt. of India, Feb 2014 to Sept 2016
2. Ranked I in Electronics specialization and amongst Top 3 students in M.Sc. Physics program at University of Lucknow, 2012
3. Certificate of Merit for scoring highest marks in Physics, Mathematics in B. Sc. Examination 2010 at C.M.S.

Degree College, 2010

4. Certificate of Excellence for outstanding and consistent performance during the “Summer School on Laboratory Training and Management”, Department of Physics, University of Lucknow, 2015

➤ **Workshops/Seminars/FDPs/Professional Training**

1. **Refresher Course:** Refresher Course on National Education Policy (NEP), 2020, HRDC, Integral University, Lucknow, India, 24th Feb -3rd March 2021.
2. **Eight Days National e-workshop:** Technological Tools and their Management in online Teaching, Mahatma Jyotiba Phule Rohilkhand University, Bareilly, India, 14th -21st Aug 2020.
3. **Two Days Online Workshop:** Online Workshop on Computer-Aided Drug Design using BIOVIA Discovery Studio, Deen Dayal Upadhyaya Gorakhpur University, Department of Physics, 13th Aug-14th Aug 2020.
4. **One Week Workshop:** Moodle: Learning Management System (Department of Computer Application in association with Spoken Tutorial Project), IIT Bombay-Pandit Madan Mohan Malviya National Mission on Teachers and Teaching (PMMMNTT) under the aegis of Human Resource Development Center (HRDC) Integral University, Lucknow, 16th – 20th May 2020.
5. **Three Week Faculty Development Programme (FDP):** Teaching Skills and Communication Development Programme, Maxel Learning Pvt. Ltd, Lucknow, 3rd July – 20th July 2019.
6. **One Month Summer School:** Summer School on Laboratory Training and Management, University of Lucknow, Department of Physics, Lucknow 15th May – 15th June 2015
7. **Two Days Workshop:** Workshop on Frontiers of Spectroscopy, Banaras Hindu University, Department of Physics, Varanasi, 8th - 9th January 2015
8. **Two Days Workshop:** Molecular Modeling & Dynamics Simulation Analysis, University of Lucknow, Department of Biochemistry, Lucknow, 1st – 2nd August 2014

➤ **Work experience: 9 Years**

❖ **Teaching at Under Graduate Level: (4 Years)**

- Assistant Professor, Physics, SRM Institute of Science and Technology, Delhi- NCR Campus, Modinagar, Ghaziabad. **(Feb 2024 to till date)**
- Teaching Assistant, Physics, Lucknow University, Lucknow. **(July 2013 to June 2016)**
- Lecture, Physics, Isabella Thoburn College, Lucknow. **(July 2012 to March 2013)**

❖ **Teaching at Post Graduate Level: (5 Years)**

- Assistant Professor, Physics, Integral University & Lucknow. **(July 2018 to Jan 2024)**