

# Dr. Sumit Kumar

*Assistant Professor*

*Department of Chemistry, Magadh University, Bodh Gaya*

*Former Guest Scientist*

*Max-Planck Institute for Biophysical Chemistry (MPIBPC), Germany*



## Research Area:

- Computational study of Non-covalent interactions in the building blocks of biomolecules
- Surface study using Auger electron spectroscopy, temperature programmed desorption (TPD) spectroscopy and Transient pump-probe vibrational spectroscopy.
- Study of Non-covalent interactions in the building blocks of biomolecules and materials using R2PI (Resonantly Enhanced Two Photon Ionization), UV-UV and IR-UV double resonance spectroscopic techniques.

## Project Sanctioned:

**Nov 2019:** Research Grant under the Start-up Research Grant (SRG) Scheme from **Science and Engineering Research Board (SERB), Department of Science and Technology, Government of India.**  
(SERB Sanction order no.: SRG/2019/002284)

## Professional and Teaching Experience:

**Nov 2017 - Till date:** **Assistant Professor in Chemistry**  
Magadh University, Bodh Gaya

**Nov 2014-Nov 2017:** **Guest Scientist**  
Department of Dynamics at Surface  
**Max-Planck Institute of Biophysical Chemistry (MPIBPC), Goettingen, Germany.**

## Education:

**Aug 2009- Nov 2014:** **Ph.D. in Chemistry**  
Indian Institute of Science Education and Research (IISER), Pune, India.  
**Research Topic:** Probing non-covalent interactions in biomolecules and materials: A gas phase laser spectroscopy study of N-heterocyclic aromatic complexes. [Weblink](#)

**2007-2009:** **M. Sc. in Chemistry (Specialization: Physical Chemistry)**  
Centre of Advanced Study in Chemistry (CAS)  
Banaras Hindu University (BHU), Varanasi, India.

**2008-2009:** **Postgraduate Diploma in Spectroscopy**  
Centre of Advanced Study in Physics (CAS)  
Banaras Hindu University (BHU), Varanasi, India.

**2004-2007:** **B. Sc. (Honors) in Chemistry with Mathematics/Physics**  
Centre of Advanced Study in Chemistry (CAS)

### Membership:

- Lifetime Membership from **Indian Science Congress, Kolkata.**  
(Membership No.: L35712)
- Lifetime Membership from **Association of Chemistry Teachers (ACT), Mumbai.**  
(Membership No.: LM2102)
- Lifetime Membership from **Researchers Society of Chemical Sciences, Bhopal, India.**  
(Membership No.: RSCS/201/2018)
- Lifetime Membership from **All India Council For Technical Skill Development.**  
(Membership No.: AICTSD/PROFESSOR/25574)

### Awards/Achievements/National Fellowships/International Fellowships:

**July 2017:** **10th Rank** in the Selection list of Assistant Professor, organized by Bihar Public Service Commission (BPSC), Patna

**Nov 2014- Nov 2017:** **International Post-Doctoral Fellowship**  
Max-Planck Institute of Biophysical Chemistry, Germany

**Jan 2012 – Nov 2014:** **CSIR-UGC Senior Research Fellowship (SRF)** in Chemistry

**Jan 2010 – Jan 2012:** **CSIR-UGC Junior Research Fellowship (JRF)** in Chemistry

**2010:** Qualified **Graduate Aptitude Test Engineering (GATE)**, organized by IIT, Gauhati.

**2009:** CSIR-UGC NET-LS & JRF in Chemistry

**2007:** Qualified BHU-PET Entrance Exam organized at National Level

**2004:** Qualified BHU-UET Entrance Exam organized at National Level

**2003:** Qualified All India Engineering Entrance Examination, organized by CBSE, New Delhi

**1999:** Highest Marks in 10th Board at School Level, Organized by Bihar School Examination Board (BSEB), Patna

### List of Selected Publications in International Peer-Reviewed Journals:

1. **Sumit Kumar** and Alope Das, N-heterocyclic aggregation (**Invited Article**).
2. **Sumit Kumar**, Hongyan Jiang, Michael Schwarzer, Alexander Kandratsenka, Dirk Schwarzer and A. M. Wodtke, Vibrational relaxation lifetime of a physisorbed molecule at a metal surface. **Physics Review Letter** **2019**, 123, 156101. [Link](#) [**Impact Factor: 10**, Citation: 7]
3. Observation of the adsorption and desorption of vibrationally excited molecules on a metal surface, **Nature Chemistry** **2018**, 10, 592–598. [Link](#) [**Impact Factor: 26**, Citation: 39]

4. **Sumit Kumar**, Santosh K. Singh, Jamuna K. Vaishnav, J. Grant Hill and Alope Das, Interplay among electrostatic, dispersion and steric interactions: Spectroscopy and quantum chemical calculations of  $\pi$ -hydrogen bonded complexes, **ChemPhysChem** **2017**, 18, 828-838. [Link](#) [Impact Factor: 3, Citation: 1]
5. **Sumit Kumar**, Santosh K. Singh, Camilla Calabrese, Assimo Maris, Sonia Melandri and Alope Das, Structure of saligenin: Microwave, UV and IR spectroscopy studies in a supersonic jet combined with quantum chemistry calculations, **Phys. Chem. Chem. Phys.** **2014**, 16, 17163. [Link](#) [Impact Factor: 4.13, Citation: 10]
6. S. K. Singh, **Sumit Kumar** and Alope Das, Competition between  $n \rightarrow \pi^*$  and conventional hydrogen bonding (N-H...N) interactions: an ab initio study of the complexes of 7-azaindole and fluoro substituted pyridines, **Phys. Chem. Chem. Phys.** **2014**, 16, 8819. (*Appeared as a front inside cover page*) [Link](#) [Impact Factor: 4.13, Citation: 35]
7. **Sumit Kumar** and Alope Das, Observation of exclusively  $\pi$ -stacked heterodimer of indole and hexafluorobenzene in the gas phase, **J. Chem. Phys.** **2013**, 139, 104311. [Link](#) [Impact Factor: 3, Citation: 21]
8. **Sumit Kumar**, Ankita Mukherjee and Alope Das, Structure of indole...imidazole Heterodimer in a supersonic jet: A gas phase study on the interaction between the aromatic side chains of tryptophan and histidine residues in proteins, **J. Phys. Chem. A** **2012**, 116, 11573. [Link](#) [Impact Factor: 3, Citation: 17]
9. **Sumit Kumar** and Alope Das, Effect of acceptor heteroatoms on  $\pi$ -hydrogen bonding interactions: A study of indole...thiophene heterodimer in a supersonic jet, **J. Chem. Phys.** **2012**, 137, 094309. [Link](#) [Impact Factor: 3, Citation: 16]
10. **Sumit Kumar** and Alope Das, Mimicking trimeric interactions in the aromatic side chains of the proteins: A gas phase study of indole...(pyrrole)<sub>2</sub> heterotrimer, **J. Chem. Phys.** **2012**, 136, 174302. (*Selected for "Virtual Journal of Biological Physics Research 2012, 23, Section: Protein Conformational Dynamics/Folding"*) [Link](#) [Impact Factor: 3, Citation: 15]
11. **Sumit Kumar**, Vedant Pande, and Alope Das,  $\pi$ -hydrogen bonding wins over conventional hydrogen bonding interaction: A jet-cooled study of indole...furan heterodimer, **J. Phys. Chem. A** **2012**, 116, 1368. (*Selected for "top-cited and/or TOP-accessed articles from India" from American chemical society as an article published " J. Phys. Chem. A 121, 26, 4843"*) [Link](#) [Impact Factor: 3, Citation: 47]
12. **Sumit Kumar**, Indu Kaul, Partha Biswas and Alope Das, Structure of 7-azaindole...2-fluoropyridine dimer in a supersonic jet: Competition between N-H...N and N-H...F interactions, **J. Phys. Chem. A** **2011**, 115, 10299. [Link](#) [Impact Factor: 3, Citation: 17]
13. **Sumit Kumar**, Partha Biswas, Indu Kaul and Alope Das, Competition between hydrogen bonding and dispersion interactions in indole-pyridine dimer and (indole)<sub>2</sub>...pyridine trimer studied in a supersonic jet, **J. Phys. Chem. A** **2011**, 115, 7461. [Link](#) [Impact Factor: 3, Citation: 32]
14. **Sumit Kumar** and Alope Das, Non-covalent Interactions in Biomolecules and Materials: Gas Phase Laser Spectroscopy and Quantum Chemistry Calculations, **ISrapS Bulletin** **2013**, 25, 1&2, 48.

### Citations Report:

- **Total citations:** 294
- H-Index: 10
- I10-Index: 10
- Google Citation Page: <https://scholar.google.co.in/citations?user=bsUE6tAAAAAJ&hl=en>

### Reviewer's Committee:

- In the Reviewer's Committee of Journal of Emerging Technologies and Innovative Research.

### Induction/Orientation/Refresher Courses attended:

1. Completed UGC sponsored Refresher Course on 'Recent Advances in Chemical Sciences' organized by Refresher course by UGC HRDC, DHSU University Sagar from August 17 - August 29, **2020**
2. Completed 4-Week Induction/Orientation Programme for "Faculty in Universities/Colleges/Institutes of Higher Education" organized by Teaching Learning Centre, Ramanujan College, University of Delhi, Delhi under the aegis of Ministry of Human Resource Development and Pandit Madan Mohan Malviya National Mission on Teachers And Teaching from June 26 - July 24, **2020**.
3. Completed Faculty Induction Programme organized by School of Education, Faculty of Education, BHU under PMMMNMTT scheme from 3rd Sep to 29th Sep, **2018**.

### Organized Conference/Symposium/Meeting/Workshop/College Event:

4. Organized Online "National Science Day Quiz" on Feb 28, **2021** at PG Department of Chemistry, Magadh University, Bodh Gaya.
5. Organized an "Interdisciplinary Consortium for Research and Educational Cooperation" between Institute of Advanced Materials, Sweden and Magadh University, Bodh Gaya, India on Feb 21, **2021**.
6. Organized Online "Chemistry Quiz" between May 26, 2020 to June 03, **2020** at PG Department of Chemistry, Magadh University, Bodh Gaya.
7. Organized Online "COVID-19 AWARENESS QUIZ" between May 15, **2020** to May 25, 2020 at PG Department of Chemistry, Magadh University, Bodh Gaya.
8. **Mentored PG Project "LiFi Wireless Technology"** and presented at two-day State level Science Innovators' Exhibition, Workshop and Lecture series during 27th and 28th February **2020** at Rajendra Mandap Raj Bhawan, organized by Munger University, Munger.
9. Organized 1st Alumni Meet on August 25, **2019** at Anugrah Memorial College, Gaya.
10. Organized One-day Seminar on "Higher Education: Past, Present and Future (A Historical Perspective)" on August 27, **2019** at Anugrah Memorial College, Gaya.
11. Organized International e-Conference on Advanced and Innovative Materials for Sustainable Future (ICAISF-2020) between June 22- 23, **2020** at R. R. S. College, Mokama, Patliputra University, Patna.

## Poster/Oral Presentation in Conference/Symposium/Meeting/Workshop

### Poster/Oral Presentation in Conference/Symposium/Meeting/Workshop (Outside India):

12. Oral presentation in 2nd German-Chinese Young Scientist Symposium on Structures and Dynamics at Surfaces on " Time resolved studies of vibrational relaxation dynamics of small physisorbed molecules on noble metal surfaces" at Max-Planck Institute of Biophysical Chemistry, Goettingen, Germany during May 28- June 1, **2017**.
13. Summer school on interfaces and energy organized by EPFL center for molecular nanoscience and technology and Max-Planck Institute of Biophysical Chemistry, Goettingen during September 04-09, **2016**.
14. Poster presentation in Conference Retreat on the Dynamics at Surfaces Meeting on " Vibrational lifetime of small diatomic molecules physisorbed on noble metals: A new experimental setup" at Schloss Ringberg (Ringberg Castle), Germany during May 18-21, **2016**.
15. Oral presentation in Conference Retreat on the Dynamics at Surfaces Meeting on "Direct measurement of vibrational lifetime of CO on Au(111)" at Schloss Ringberg (Ringberg Castle), Germany during May 20-23, **2015**.
16. International Bunsen Discussion Meeting at Max-Planck Institute of Biophysical Chemistry, Goettingen, Germany during Nov 01-04, **2015**.

### Poster/Oral Presentation in Conference/Symposium/Meeting/Workshop (Inside India):

17. Attended International Webinar on Sustainable Chemistry Organized by Association of Chemistry Teachers(ACT), Homi Bhabha Centre for Science Education (TIFR) Mumbai on 18th March **2021**.
18. Attended International Webinar on Instrumental Methods of Analysis Organized Association of Chemistry Teachers (ACT), Department of Chemistry, Kamla Nehru Mahavidyalaya, Nagpur and International Research Centre and Department of Chemistry, Kalasalingam Academy of Research and Education, Krishnankoil on 17th and 18th October **2020**.
19. International Webinar entitled "Relevance of Dr. B.R. Ambedkar's Economic Thoughts in Special Reference of Indian Economy" held on July 26, **2020** organized by B. R. Social and Educational Welfare Society, Sitapur, U. P.
20. Attended 5 days certificate course on "Risk Management of Biological and Cascading Hazards: In the Context of Pandemics" organized by Resilience Innovation Knowledge Academy from 12th to 16th October **2020**.
21. Oral Presentation at National Conference on Education for Sustainable Development held at Central University of South Bihar from 22nd to 23rd March **2020** on "Current Challenges in Sustainable Development in India".

22. **Invited Talk** in “National Workshop on Research Ethics and Anti-Plagiarism” organized by Dept. of Chem., VKS University, Ara & Computer Centre VKSU, Ara -802301, Bihar, India on Feb 07-08, **2020**.
23. Attended DWIH Workshop on “Grant Writing & Management” held at Banaras Hindu University, Varanasi from 7th to 9th November **2019**, which is organized by India house of University of Cologne and Max Planck Society, Germany.
24. Attended One-day Regional Workshop on “Awareness, Adoption and Promotion of the MOOCs on Swayam platform” at the Ranchi University, Morabadi Campus, Aryabhatt Auditorium on September 3, **2019**.
25. Oral Presentation in National Conference on “Recent Advances in Chemical Science” organized by applied science department, Madan Mohan Malaviya University of Technology, Gorakhpur on "n→π\* interaction in biomolecules: A quantum chemical calculation study" during March 29-30, **2019**.
26. Oral presentation on the topic “N-heterocyclic aggregation: Insight and perspective” at the National Seminar on the topic entitled “Future India: Science & Technology” (NSFIST 2019), under Indian Science Congress Association, Patna Chapter, during April 3-4, **2019**, held at Munger University, R.D. & D.J. College Campus, Munger-811201, Bihar.
27. Attended Two-day National Seminar on “Blueprint of Higher Education in Bihar” in Rajbhavan, Patna organized by Patna University, Patna on February 4-5, **2019**.
28. Oral Presentation in International Seminar on Green Chemistry: Synthesis, Processing & Devices” organized by Dept. of Chemistry, VKS University, Ara, Bihar on April 6-7, **2018**.
29. Oral presentation in One-day Workshop Radhakrishnan Shabhar, DDE Building, M.U., Bodhgaya, Bihar on “Capacity Building of Teachers Researchers/ Students through Research Projects” organized by Magadh University on March 31, **2018**.
30. Poster presentation in 11th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters (SDMC) at the Hans Coco Palms, Puri, Orissa on "Effect of methyl substitution in the complexes of indole with methylated benzenes: Interplay among electrostatic, dispersion interactions and steric repulsion" organized during 20-23 February **2014**.
31. Poster presented in Humboldt Kolleg meeting on Surface Science & Engineered Surfaces at Lavasa Valley, Pune on "Observation of exclusively π-stacked heterodimer of indole and hexafluorobenzene in the gas phase" during Feb. 14-16, **2014**.
32. Poster Presentation in Trombay Symposium on Radiation & Photochemistry (TSRP - 2014) at Bhabha Atomic Research Centre (BARC), Mumbai on "Observation of exclusively π-stacked heterodimer of indole and hexafluorobenzene in the gas phase." during January 06-09, **2014**.
33. Poster Presentation in 10th meeting of Spectroscopy and Dynamics of Molecules and Clusters (SDMC) on “Tailor Made Synthesis of T-shaped or π-Stacked Dimer in the Gas Phase: Concept for Efficient Drug Design and Material Synthesis” organized in Chunda Palace, Udaipur, Rajasthan during February 21-24, **2013**.

34. Oral Presentation in IISER Pune-Glasgow University symposium on Structure and Dynamics on “Mimicking trimeric interactions in the aromatic side chains of proteins: A gas phase study of indole...(pyrrole)<sub>2</sub> heterotrimer” organized by IISER Pune during December 10-12, **2012**.
35. Attended full agenda of ACS (American Chemical Society) on Campus event at National Chemical Laboratory, Pune on Oct. 10, **2012**.
36. Poster Presentation in Mini-Symposium on Spectroscopy and Dynamics in Chemistry on “Mimicking trimeric interactions in the aromatic side chains of the proteins: A gas phase study of indole...(pyrrole)<sub>2</sub> heterotrimer” organized by IISER Pune on 20th April, **2012**.
37. Poster Presentation in 9th meeting of Spectroscopy and Dynamics of Molecules and Clusters on “Direct evidence for the cyclic asymmetric structure of indole...(pyrrole)<sub>2</sub> trimer in a supersonic jet” organized in Eagleton Golf Resort, Bangalore on February 17-19, **2012**.
38. Poster Presentation in Zonal meeting of Chemical Research Society of India on “Competition between hydrogen-bonding and dispersion interactions in indole...pyridine dimer and (indole)<sub>2</sub>...pyridine trimer studied in a supersonic jet.” organized by National Chemical Laboratory, Pune during May 13-14, **2011**.
39. Poster Presentation in 8th meeting of Spectroscopy and Dynamics of Molecules and Clusters (SDMC) on “Conformational studies of mixed dimer of 7-azaindole and 2-fluoropyridine in a supersonic jet.” organized in Corbett river view retreat, Nainital, Uttarakhand during Feb 18-20, **2011**.
40. Poster Presentation in RSC West India Ph.D. Students Symposium on “Conformational studies of mixed dimer of indole and pyridine in supersonic jet using laser based spectroscopic techniques.” organized by University of Goa, Goa during September 03-04, **2010**.
41. **Graduate Seminar** on 2D-IR spectroscopy: Principle and applications in IISER Pune on August 03, **2010**.

#### **Administrative Work:**

1. Member, Internal Quality Assurance Cell (IQAC), Magadh University, Bodh Gaya (March **2021** – Till Date)
2. Member, जन संचार समूह, Magadh University, Bodh Gaya (March **2021** – Till Date)
3. Nodal Officer, Anugrah Memorial College, Gaya (Jan **2018** – Dec 2019)
4. IQAC Coordinator, A. M. College, Gaya (March 23, **2019** – Dec 2019)
5. SWAYAM Mentor, MOOCs (Massive Open Online Courses), A. M. College, Gaya (May 05, **2018**-Dec 2019).
6. Coordinator, ICT Cell, A. M. College, Gaya (March 23, **2019** – Dec 2019)
7. Member, Development and Building Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
8. Member, Purchase Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
9. Member, Examination Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
10. Member, Proctorial Board, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
11. Member, Academic and Research Board, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
12. Member, Attendance and Time-table Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)

13. Member, Alumni Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
14. Member, Stipend and Scholarship Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
15. Member, Clean and Green Committee, A. M. College, Gaya, (March 23, **2019** – Dec 2019)
16. Member, Student Union Election Committee, A. M. College, Gaya (March 10-17, **2018**)
17. Member, NAAC team, A. M. College, Gaya (Jan **2018** – Dec 2019)
18. Deputy Examination Controller, A. M. College, Gaya. (April 28, **2018**-Dec 2019).
19. Volunteer, 1st Indo-US Research Fellowship Conclave at IISER Pune (December 10-12, **2012**).

**Extracurricular activities:**

**2007-2008: 1st Prize** in Double's Table-Tennis in ANNUAL GAMES & SPORTS at Faculty of Science, Banaras Hindu University (BHU), Varanasi, India.

**2007-2008: 2nd Prize** in Singles Table-Tennis in ANNUAL GAMES & SPORTS at Faculty of Science, Banaras Hindu University (BHU), Varanasi, India.

**Computational Skills:**

Programming Softwares: LabVIEW, Mathcad, Mathematica, C++, Python, Fortran, Java, Scala.

Computational Softwares: Gaussian, NWChem, Q-chem, GAMESS (USA), GROMACS, AIM 2000.

Others: 3D CAD software: Autodesk inventor. Html/Web page designing