

Dr. Indrajit Bandyopadhyay



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EDUCATIONAL QUALIFICATION

Degree	Details
Ph.D.	Theoretical Chemistry, Indian Institute of Technology (IIT), Kanpur, India, 2000. Thesis: "Ground State Vibrational Analysis of Some Aromatic Hydrocarbons and Heterocycles - Ab initio Study" Thesis Advisor: Professor S. Manogaran
M.Sc.	Chemistry (Physical Chemistry Specialization), The University of Burdwan, West Bengal, India, 1990
B.Sc.	Physical, Inorganic, Organic Chemistry (major), Physics and Mathematics (minor), The University of Burdwan, West Bengal, India, 1988

EMPLOYMENT

Period	Position & Institution / Advisor
March 09, 2024-Present	Associate Professor, Dream Institute of Technology, Kolkata
Feb, 2019 – June, 20	Guest Faculty, Department of Chemical Engineering, IIT Delhi, India
August 01, 2017 – June, 2018	Assistant Professor, Department of Chemistry, Vivek College, Bijnor, UP
February 08, 2016 – June 15, 2017	Postdoctoral Fellow, Centre of Polymer Science and Engineering, IIT Delhi, India. <i>Advisors: Professor A. Ghosh and Professor S. K. Pattanayek</i>
July 25, 2014 – May 16, 2015	Assistant Professor in Chemistry, GLA University, Mathura, U.P.
July 15, 2013 – July 12, 2014	Assistant Professor in Chemistry, Sanskriti Institute of Management and Technology, Mathura, U.P.
01 August, 2011 – 13 June, 2013	Assistant Professor in Chemistry, Dream Institute of Technology, Kolkata, WB, India
March – May, 2011	Guest Lecturer in B.Sc. Chemistry Honours Course, Khalisani Mahavidyalaya (College), Chandannagore, Hooghly, WB, India
February – June, 2011	Guest Lecturer in M.Sc. Chemistry Course, Vivekananda Mahavidyalaya (College), Burdwan, WB, India
August, 2009 – January, 2011	Researcher, Department of Geography, Kansas State University, Manhattan, KS, USA. <i>Advisor: Professor B. K. Paul</i>
February, 2008 – May, 2009	Postdoctoral Research Scholar, Department of Chemistry, Kansas State University, Manhattan, KS, USA. <i>Advisor: Professor C. M. Aikens</i>
August, 2007 – October, 2007	Postdoctoral Research Associate, Department of Chemistry, Indiana University, Bloomington, IN, USA.

Period	Position & Institution / Advisor
	<i>Advisor: Professor A. Flood</i>
February, 2006 – July, 2007	Postdoctoral Research Associate, Department of Chemistry, Indiana University, Bloomington, IN, USA. <i>Advisor: Professor K. Raghavachari</i>
November, 2004 – January, 2006	Temporary Research Scientist, Department of Chemistry, KAIST, Daejeon, Korea. <i>Advisor: Professor Yoon Sup Lee</i>
January, 2000 – September, 2004	Postdoctoral Fellow, Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang 790-784, Korea. <i>Advisor: Professor K. S. Kim</i>
August – September, 1998	Project Assistant, Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science (IISc), Bangalore, India. <i>Advisor: Professor Biman Bagchi</i>
August 1991 – July, 1992	West Bengal State-Funded Project Fellow, Department of Chemistry, The University of Burdwan, West Bengal, India. <i>Advisor: Professor M. Banerjee</i>

AWARDS / FELLOWSHIPS

- Graduate Student Fellowship through All-India GATE Examination 1992-1999.
- Ruplal Nandy Memorial Scholarship, 1981.

TEACHING EXPERIENCE

- C Language Instructor at Software Training Center, I. I. T. Kanpur, India, August, 1999.
- Teaching Assistant (TA) from 1993-1999 at I.I.T. Kanpur, India in the courses:
 - General Chemistry course (CHM101)
 - Postgraduate (M.Sc.) Physical Chemistry Lab course (CHM 423)
- Taught Chemistry for B.Sc. (Chemistry Honours) and for M. Sc. Chemistry.
- Taught Engineering Chemistry and Environmental Science and Engineering (B. Tech 1st and 2nd Year), Chemical Process Calculations (for chemical engineering and food

technology) at Sanskriti Institute of Management and Technology.

- Taught Inorganic, Organic and Physical Chemistry for B.Sc. Biotechnology.
- Teaching engineering chemistry theory and lab course, and environmental studies at GLA university.

ASSOCIATE EDITOR

Main Group Chemistry (IOS Press)

MEMBERSHIP IN PROFESSIONAL ORGANIZATION

American Chemical Society Membership (2008-2011), Member number: 2441961
(26/5/08-25/5/11)

MENTORSHIP

Supervised two M.Sc. Term papers on 'Spintronics Materials' and 'Core-Shell Nanoparticles'

COMPUTER SKILLS

Operating Systems	Unix and Linux (Platforms: Supercomputers, Compute Servers, Workstations and Computer Clusters), Windows
Computer Softwares	Fortran90, C, C++, Java, Python, Perl, XML, Parallel Programming, MySQL
Molecular Modeling Softwares	Gaussian, GAMESS, Amber, SAPT, VASP, MM, AcesII, Turbomole, Mopac, Molpro, ADF, Normal Coordinate Analysis Programs
Web Design	Webpage developing experience

PRESENTATIONS / WORKSHOPS

1. **I. Bandyopadhyay**, Talk "Annotation of Hessian Fly Genome: Evidence Based Maker Predictions and Other Gene Prediction Tools", National Conference on Advanced Computing and Information Technology (NCACIT-2014), Sanskriti Institute of Management and Technology, Chhata, Mathura (U.P.), February 8-9, 2014.
2. **I. Bandyopadhyay**, Talk "Structure and Stability of $(\text{TiO}_2)_n$ ($\text{SiO}_2)_n$, $\text{Ti}_m\text{Si}_{n-m}\text{O}_{2n}$ Clusters", KU-KSU Physical Chemistry Symposium, Department of Chemistry, Kansas State University, Manhattan, Kansas, November 1, 2008.
3. **I. Bandyopadhyay**, Talk "Computational Modeling of VX nerve agent model system and

surface chemical reactions", Department of Chemistry, Kansas State University, September 16, 2008.

4. **I. Bandyopadhyay**, Talk "Computational Modeling of VX nerve agent model system and surface chemical reactions", Department of Chemistry, University of Illinois, Urbana-Champaign (UIUC), November 28, 2007.
5. **I. Bandyopadhyay** and K. Raghavachari, Poster "In-rich Surface Growth on P-rich InP(001) (2×1) Surface: Structural and Mechanistic Study", Mid-West Theoretical Chemistry Conference (MWTCC)-07, Bloomington, Indiana, June 28-30, 2007.
6. **I. Bandyopadhyay** and K. S. Kim, Poster "Highly Stereospecific Epimerization of α -amino acids: Conducted Tour Mechanism", Theory and Applications of Computational Chemistry (TACC), Kyungju, Korea, February 14-20, 2004.
7. **I. Bandyopadhyay** and K. S. Kim, Poster "Molecular Recognition of Fluoride Anion: Benzene-Based Tripodal Imidazolium Receptor", 10th Korea-Japan Joint Symposium on Theoretical/Computational Chemistry, POSTECH, Pohang, Korea, January 12-13, 2003.
8. **I. Bandyopadhyay** and S. Manogaran, Poster "Vibrational Spectra of Corannulene", XII International Conference in Computers in Chemical Research and Education (ICCCRE), Pune, India, January 5-9, 1998.

PUBLICATIONS

1. **I. Bandyopadhyay** and C. M. Aikens, Structure and Stability of $(\text{TiO}_2)_n$, $(\text{SiO}_2)_n$ and Mixed $\text{Ti}_m\text{Si}_m\text{O}_{2n}$ ($n=2-5$, $m=1-(n-1)$) Clusters, *J. Phys. Chem. A*, 115 (2011), 868-879.
2. **I. Bandyopadhyay**, K. Raghavachari and Amar Flood, Strong C-H $\cdots$ Halide Hydrogen Bonds from 1,2,3-Triazoles Quantified Using Pre-Organized and Shape-Persistent Triazolophanes, *ChemPhysChem*, 10 (2009), 2535.
3. **I. Bandyopadhyay** and K. Raghavachari, In-rich Surface Growth on P-rich InP(001) (2×1) Surface: Structural and Mechanistic Study, *J. Phys. Chem. C*, 112 (2008), 6022.
4. **I. Bandyopadhyay**, M. J. Kim, Y. S. Lee, D. G. Churchill, Favorable Pendant-Amino Metal Chelation in VX Nerve Agent Model Systems, *J. Phys. Chem. A*, 110 (2006), 3655-3661.
5. N. J. Singh, A. C. Olleta, M. Park, H.-B. Yi, **I. Bandyopadhyay**, H. M. Lee, P. Tarakeshwar, K. S. Kim, Study of Interactions of Various Ionic Species with Solvents Towards the Design of Receptors, *Theor. Chem. Acc.* 115 (2006), 127-135.
6. **I. Bandyopadhyay**, H. M. Lee, K. S. Kim, Phenol vs Water Molecule Interacting with Various Molecules: π -type, σ -type, and n -type Hydrogen Bonds, Interaction Energies and Their Energy Components, *J. Phys. Chem. A*, 109 (2005), 1720-1728.
7. **I. Bandyopadhyay**, K.-H. Oh, S. Lee, S. J. Cho, S. B. Kim, Rotational Isomerism about Acyl-Oxygen Bond in Two Envelope Conformations and Vibrational Spectral Analysis of Cyclopentyl Acetate: A Combined Theoretical and Experimental Study, *J. Mol. Struct. (Theochem)*, 680 (2004), 211-217.

8. **I. Bandyopadhyay**, H. M. Lee, P. Tarakeshwar, C. Cui, K. S. Oh, J. Chin, and K. S. Kim, Highly Stereospecific Epimerization of α -amino acids: Conducted Tour Mechanism, *J. Org. Chem. (Note)* 68 (2003) 6571-6575.
9. **I. Bandyopadhyay**, Structure, Modified Scaled Quantum Mechanical Force Field and A Priori Prediction of Vibrational Spectra and their Assignment and Exponential Scaling of Frequencies of Triphenylene, *Bull. Kor. Chem. Soc.* 24 (2003) 717-722.
10. S. Yun, H. Ihm, H. G. Kim, C.-W. Lee, **I. Bandyopadhyay**, K. S. Oh, Y. J. Gong, J. W. Lee, J. Yoon, H. C. Lee, and K. S. Kim, Molecular Recognition of Fluoride Anion: Benzene-Based Tripodal Imidazolium Receptor, *J. Org. Chem.* 68 (2003) 2467-2470.
11. How Different is Azulene from Tropylium Cation and Cyclopentadienyl Anion? A Force Field and Vibrational Study, **I. Bandyopadhyay**, *J. Mol. Struct. (Theochem)*, 618 (2002) 59-64.
12. **I. Bandyopadhyay**, Vaibhav Tewari, Shruti Maheshwari and S. Manogaran, Ground State Vibrational Spectra of Corannulene: A theoretical study, *J. Mol. Struct. (Theochem)*, 538 (2001) 51-58.
13. **I. Bandyopadhyay** and S. Manogaran, Force Field and Assignment of the Vibrational Spectra of Quinoline and Isoquinoline - An Ab Initio Study, *Indian J. Chem.* 39A (2000) 189-195.
14. **I. Bandyopadhyay** and S. Manogaran, Force Fields and Assignments of the Vibrational Spectra of Acridine and Phenazine - An Ab Initio Study, *J. Mol. Struct. (Theochem)*, 507 (2000) 217-227.
15. **I. Bandyopadhyay** and S. Manogaran, Force Field and Assignment of the Vibrational Spectra of Phenanthrene - An Ab Initio Study, *J. Mol. Struct. (Theochem)* 496 (2000), 107-119.
16. **I. Bandyopadhyay** and S. Manogaran, Ground State Vibrations of Tropylium Cation: An Ab Initio Study, *J. Mol. Struct. (Theochem)*, 432 (1998), 33-39.

REFERENCES

Available upon request.