

CURRICULUM VITAE

SOURAB SINHA

ACADEMIC PROFILE:

Standard	Year	Subjects
10 th	2003	Eng, Sc, S.St, Mat, Hindi
12 th	2005	Eng, Phy, Chem, Mat, Bio, Agri
B. Sc.	2009	Chem (Hons.), Phy, Mat, Eng
M. Sc.	2011	Chem (Hons.)

** CBSE = Central Board of Secondary Education, Eng = English, Sc = Science, S.St = Social Studies, Mat = Mathematics, Phy = Physics, Chem = Chemistry, Bio = Biology, Agri = Agriculture, Hons = Honors

Special Papers include: Organic, Inorganic, Physical and Quantum Chemistry, Biochemistry, Spectroscopy, Instrumentation, Computational Chemistry and Analytical Chemistry.

Master Degree Specialization: Physical Chemistry

LANGUAGES:

Read, Write & Speak (Fluently): English and Hindi

RESEARCH EXPERIENCE:

1. Did a Project under the supervision of Dr. Ramamoorthy Bhoomishankar, Indian Institute of Technology, Guwahati, Assam, India, on the project entitled “*Preparation of Phosponium ligands, their metallization and characterization*” on June-August 2010.
2. Did a project under Prof. Abani Kumar Misra, Department of Chemistry, Gauhati University, Assam, India, entitled “*Analysis of Drinking Water Quality of Guwahati City*” in partial fulfillment of M.Sc. Degree, 2010-11.
3. Completed Ph.D. research work, under the supervision of Dr. Pradip Kr. Bhattacharya, Department of Chemistry, Arya Vidyapeeth College, Gauhati University, Assam, India, on the project entitled, “*Mechanistic Study on DNA Alkylation by Nitrogen Mustard: A DFT Study*”, since May 2012 – August 2017.

4. Was selected as assistant researcher for the projects entitled “*BTX destruction in Claus Process: A DFT study*” and “*Role of resonantly stabilized radical in the growth of PAH*” under the supervision of Abhijeet Raj, Ahmed S. AlShoaibi, Saeed M. Alhassan, Department of Chemical Engineering, The Petroleum Institute, Khalifa University, Abu Dhabi, UAE, September 2013 – November 2016.

5. Worked as a Postdoctoral Fellow on projects based on “*Theoretical study of surface chemistry*” under the supervision of Prof. Zoltan Konya, Department of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary, since October 2017.

RESEARCH INTEREST:

1. **Density Functional Theory:** Analyzing the electronic structure (principally the ground and transition state) of many-body systems.
2. **Density Functional Reactivity Theory:** Analyzing the chemical and physical properties of many body systems at molecular level.
3. **Time-Dependent Density Functional Theory:** Analyzing the excited state chemistry.
4. **Polarizable Continuum Model:** Analyzing chemical and physical properties in solvent phase.
5. **Intrinsic Reaction Coordinates and Potential Energy Surface** scan.
6. Theoretical investigation of **IR, UV-Vis** and **NMR** spectra.
7. Plane wave DFT calculations.

SOFTWARE:

1. **Gaussian 09:** For Quantum and Molecular Mechanics calculations. Trained in analyzing the output results obtained from G09 calculations required for various chemical and physical studies of molecules in both Windows and LINUX. Analyzing optimized geometries of ground, excited and transition state structures to verifying their modes of vibration via frequency calculation. A good knowledge of G09 keywords and solution of the errors.
2. **Vienna Ab initio Simulation Package (VASP)** for plane wave DFT calculations.
3. **Materials Studio:** From building structures to running calculations for Dmol and DFT calculations.
4. **Quantum Espresso** for plane wave DFT calculations.
5. **ChemKin** for kinetic simulation and mechanism analysis.
6. **Gauss View, Chemcraft, VESTA, Avogadro:** From building complex structures to inspecting input, output and check point Gaussian files. For analyzing HOMO, LUMO, ESP, Vector displacement, plotting IR, NMR, UV spectra, IRC paths, geometry optimization, etc.
7. **Mnova**, the latest Nuclear Magnetic Resonance (NMR), Liquid Chromatography (LC)/Gas Chromatography (GC)/Mass Spectroscopy (MS) and UV-Visible data processing, visualization, simulation, prediction, presentation and analysis software package.

8. **ChemOffice Professional**, the gold standard for chemical drawing and research publications.
9. **Signals Notebook**, web based electronic lab notebook.
10. Basic computer software such as word, excel, power point, photo editor and many more in both Windows and LINUX.

PUBLICATIONS:

Journal Papers:

1. **Sourab Sinha** and Pradip Kr. Bhattacharyya, Variation of reactivity of aziridinium ion during alkylation, *Molecular Physics*, 112, 2014, 14-21.
2. **Sourab Sinha**, Babul Neog, Nabajit Sarmah and Pradip Kr. Bhattacharyya, Effect of guanine alkylation on Keto-enol tautomerism: A DFT study, *Journal of Indian Chemical Society*, 91, 2014, 679-687.
3. **Sourab Sinha**, Pradip Kr. Bhattacharyya, Alkylation of guanine by formononetin nitrogen mustard derivatives: A DFT study, *Computational and Theoretical Chemistry*, 1027, 2014, 135–141.
4. **Sourab Sinha**, Abhijeet Raj, Ahmed S. AlShoaibi, Saeed M. Alhassan, Suk Ho Chung, Benzene Destruction in Claus Process by Sulfur Dioxide: A Reaction Kinetics Study, *Industrial and Engineering Chemistry Research*, 53, 2014, 10608–10617.
5. **Sourab Sinha**, Abhijeet Raj, Ahmed S. AlShoaibi, Saeed M. Alhassan, Suk Ho Chung, Toluene Destruction in the Claus Process by Sulfur Dioxide: A Reaction Kinetics Study, *Industrial and Engineering Chemistry Research*, 53, 2014, 16293–16308.
6. **Sourab Sinha**, Abhijeet Raj, Ahmed S. Al Shoaibi, and Suk Ho Chung, Reaction mechanism for *m*-xylene oxidation in the Claus process by sulfurdioxide, *The Journal of Physical Chemistry A*, 2015, 119, 9889-9900.
7. **Sourab Sinha** and Abhijeet Raj, Polycyclic aromatic hydrocarbon (PAH) formation from benzyl radicals: a reaction kinetics study, *Physical Chemistry Chemical Physics*, 18, 2016, 8120-8131.
8. **Sourab Sinha**, Ramees K. Rahman and Abhijeet Raj, On the role of resonantly stabilized radicals in polycyclic aromatic hydrocarbon (PAH) formation: Pyrene and fluoranthene formation from benzyl-indenyl addition, *Physical Chemistry Chemical Physics*, 19, 2017, 19262-19278.
9. **Sourab Sinha** and Pradip Kr. Bhattacharyya, Understanding the influence of external perturbation on aziridinium ion formation, *Molecular Physics*, 116, 2018, 29-43.
10. **Sourab Sinha** and Abhijeet Raj, Reaction mechanism and modeling study for the oxidation by SO₂ of *o*-xylene and *p*-xylene in Claus process, *International Journal of Quantum Chemistry*, 118, 2018, e25583.
11. Bapan Saha, **Sourab Sinha**, Himakshi Sharma, Pradip Kr. Bhattacharyya, On the formation of polymeric housene molecules of group 15 elements (N, P, As and Sb): A DFT study, *The Journal of*

Physical Chemistry A, 122, 2018, 6780-6788.

12. Kundan Baruah, **Sourab Sinha**, Swapnali Hazarika, Pradip Kr. Bhattacharyya, QM/MM Studies on Cyclodextrin-Alcohol Interaction, Journal of Macromolecular Science, Part A, 52, 2015, 64-68.

13. Babul Neog, **Sourab Sinha** and Pradip Kr. Bhattacharyya, Alkylation of DNA by nitrogen mustard: A DFT study, Computational and Theoretical Chemistry, 1018, 2013, 19–25.

14. J. Sarma, **Sourab Sinha**, N. Sarmah, S. K. Purkayastha, P. Sarkar, P. K. Bhattacharyya, DFRT studies of amide-coupled benzoic nitrogen mustard derivatives, Journal of Indian Chemical Society, 91, 2014, 2211-2216.

15. Rupam J. Sarma, Arup Kr. Deka, **Sourab Sinha** and Pradip Kr. Bhattacharyya, Coordination of bromide anions and organic bromine to tryptophan ligands, Journal of Molecular Structure, 1052, 2013, 197–203.

16. Rajib kumar Debnath, Apurba Kalita, **Sourab Sinha**, Pradip Kr. Bhattacharyya, Biplab Mondal, Jatindra Nath Ganguly, Solvent dependent disproportionation of Cu(II) complexes of N₂O₂-type ligands: Direct evidence of formation of phenoxy radical: An experimental and computational study, Asian Journal of Chemistry, 27, 2015, 4490-4500.

17. Babul Neog, Nabajit Sarmah, **Sourab Sinha** and Pradip Kr. Bhattacharyya, Density functional based reactivity studies on aziridinium ion intermediates, Journal of Indian Chemical Society, 90, (2013) 2231-2236.

18. Kusum K. Bania, Ankur Kanti Guha, Pradip Kr. Bhattacharyya, **Sourab Sinha**, Effect of substituent and solvent on cation– π interactions in benzene and borazine: a computational study, Dalton Transactions, 43, 2014, 1769-1784.

19. Evgenia Georganta, Ramees K. Rahman, Abhijeet Raj and **Sourab Sinha**, Growth of polycyclic aromatic hydrocarbons (PAHs) by methyl radicals: Pyrene formation from phenanthrene, Combustion and Flame, 185, 2017, 129-141.

Conference Papers:

1. **Sourab Sinha**, Abhijeet Raj, Reaction Mechanism for the Oxidation of Aromatic Contaminants Present in Feed Gas to Claus Process, Energy Procedia, 66, 2015, 61-64.

2. **Sourab Sinha**, Abhijeet Raj, Destruction of H₂S Contaminants (Benzene, Toluene and Xylenes) by Sulphur Dioxide in Claus Process, ADIPEC 2014, Paper no: SPE 172080.

Books/Chapters:

1. Pradip Kr. Bhattacharyya, **Sourab Sinha**, Nabajit Sarmah, Bhabesh Chandra Deka, “Density Functional Studies of Bis-alkylating Nitrogn Mustards” in: Frontiers in Computational Chemistry (Volume 2), ed. Zaheer Ul-Haq and Jeffry D. Madura, Bentham e-books, 2015, eISBN: 978-1-60805-978-2.

WORKING/WORKED AS:

1. Ph.D. Research Scholar, Department of Chemistry, Gauhati University, Assam, India.
2. Assistant Researcher, Department of Chemical Engineering, The Petroleum Institute, Khalifa University, Abu Dhabi, UAE (3 years).
3. Postdoctoral Researcher, Department of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary (1 year).
4. Technical Consultant at Scube Scientific Software Solution, New Delhi, India.

TEACHING EXPERIENCE:

During my PhD period, I have worked as a Teaching Assistant which included theoretical and practical classes. During this period, many Graduate and Undergraduate students (both in India and UAE) have worked under my supervision and successfully performed their thesis research which ended up in publications in prestigious scientific journals.

OTHER ACTIVITIES:

Sports: Cricket, Football, Badminton, Table Tennis.

Badminton champion 2013-2014, Runners up 2015 in Inter-University Sports League (ADISL).

Awarded best athlete of the year 2015 in Abu Dhabi, ADISL.

Awarded best oral and poster presentation in many scientific conferences.