***Dr. Ajeet Singh,*** Department of Chemistry, Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research, V. B. S. Purvanchal University, Jaunpur-222003, U. P., India,

Phone: (+91)8808494988(Mobile)
Email: ajeetmolecule@gmail.com

## Education

| | | |
|---|---|---|
| Ph.D. | **CSIR**-Central Salt & Marine Chemicals Research Institute, Bhavnagar Gujarat/ University of Bhavnagar, India<br>*Supervisor*: Dr. Bishwajit Ganguly (Scientist-F) | 2011 |
| M.Sc. | Department of Chemistry, University of Allahabad, India | 2003 |
| B.Sc. | Department of Chemistry and Botany, University of Allahabad, India | 2000 |

**Title of Ph.D. Thesis**: Molecular Modeling/Computational Studies towards Understanding the Morphology of Ionic Solids and to Design Novel Molecular Systems of Varying Reactivities

## Academic Appointment:

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|---|---|---|---|
| Department of Chemistry, Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research, V. B. S. Purvanchal University, Jaunpur-222003, U. P., India, | Assistant Professor | September 2018 | Till date |

## Research Appointments:

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|---|---|---|
| DST-SERB Fast track, Young Scientist | Department of Physics, MNNIT Allahabad, Prayagraj, India | July 2015 to July 2018 (Completed) |
| Postdoctoral Associate | Division of Advanced Materials Science, POSTECH, South Korea<br>*Advisor*: Prof. H. M. Jang | Sept.-2014. to July. 2015 (Completed) |

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|---|---|---|
| Postdoctoral Associate | Department of Chemistry, University of Allahabad, India<br>*Advisor*: Prof. A. K. Srivastava | July 2011-July 2014 (Completed) |
| Postdoctoral Associate | Department of Chemistry, Kyung Hee University, South Korea<br>*Advisor*: Prof. Minserk Cheong | Oct. 2010 – Feb. 2011 (Completed) |

## Awards

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|---|---|---|---|
| 1. | Best oral presentation award in "XXII-Gujarat science congress, | Bhavnagar University | 2008 |
| 2. | 2009 Young scientist award | Bioved Research Society, India | 2009 |
| 3. | Dr. D. S Kothari Post-doctoral fellowship | UGC, Govt. of India | 2011 |
| 4. | 2012 Best academic excellence award | United group of institutions, India | 2012 |
| 5 | Best oral presentation award (Allahabad Chapter) | Indian Science Congress Association | 2013 |

**Foreign Visit:**

| Sr. No. | Country Visited |
|---|---|
| 1. | South Korea |
| 2. | Czech Republic |

## Project grant

1. A major research project was executed and it was funded by DST-SERB New Delhi. The total cost of project was 3220000.00 (Year: **July 2014-July 2018**).

2. Got approval ( Ref. No.: CRG/2019/001032 dated **14 Dec. 2020**) for funding a core research grant (CRG) from DST-SERB New Delhi and proposed project cost will be 5564000/- (Fifty-fives Lakh Sixty-four Thousand).

**Research Experience**

1. Well versed with computational methods and techniques, for example: HF, DFT, TD-DFT, MP2, MP3, CCSD(T), IPCM (isodensity polarizable continuum model), the conductor-like screening model (COSMO), the solution model GB/SA (GB: generalized Born; SA: surface area), the Poisson-Boltzmann continuum solvent model for computing solvation energies, Molecular Mechanics, Molecular Dynamics.

**Research Publications, Patent and Conferences:**

**(a) Research Articles in Peer Reviewed Journals**

(1) **Ajeet Singh**, Shampa Chakraborty and Bishwajit Ganguly, $C_2$-Chiral Substituted *cis*-1,3,5,7-Tetraazadecalins as Proton Sponges: A Computational Study; ***E. J. Org. Chem.***, 2006, 4938. *Impact Factor: 3.096*

(2) **Ajeet Singh**, Shampa Chakraborty and Bishwajit Ganguly, Computational Study of Urea and Its Homologue Glycinamide: Conformations, Rotational Barriers and Relative Interactions with Sodium Chloride; ***Langmuir***, 2007, *23*, 5406. *Impact Factor: 3.898*

(3) **Ajeet Singh** and Bishwajit Ganguly, DFT Studies towards the Design and Discovery of a Versatile Cage-Functionalized Proton Sponge; ***E. J. Org. Chem.***, 2007, 420. *Impact Factor: 3.096*

(4) **Ajeet Singh** and Bishwajit Ganguly, Rational Design and First-Principles Studies toward the Remote Substituent Effects on a Novel Tetracyclic Proton Sponge; ***J. Phys. Chem. A***, 2007, *111*, 6468. *Impact Factor: 2.899*

(5) **Ajeet Singh** and Bishwajit Ganguly, Probing the Influence of Solvent Effect on 1,3-diazacyclohexane System; ***J. Phys. Chem. A,*** 2007, *111*, 9884. *Impact Factor: 2.899*

(6) **Ajeet Singh**, Shampa Chakraborty and Bishwajit Ganguly, Conformational Analysis and the Binding Sites of Nitrilotriacetamide: A Computational Study; ***Int. J. Quant. Chem.***, 107, *1430*. **2007**, *Impact Factor: 2.92*

(7) D. Amilan Jose, **Ajeet singh**, Bishwajit Ganguly and Amitava Das, Density Functional Study towards the Preferential Binding of Anions to Urea and Thiourea Molecules; ***Tetrahedron lett.***, 2007, *48*, 3698. *Impact Factor: 2.66*

(8) **Ajeet Singh** and Bishwajit Ganguly, Strategic Design of a Small and Versatile Bicyclic Organic Superbase: A Density Functional Study; ***New J. Chem.***, 2008, *32*, 210. *Impact Factor: 3.006*

(9) **Ajeet Singh** and Bishwajit Ganguly, DFT Study of Urea Interaction with Potassium Chloride Surfaces; ***Mol. Simul.***, 2008, *38*, 973. *Impact Factor: 1.42*

(10) Bishwajit Ganguly, **Ajeet Singh**, Nikola Basarić, Marija Matković and Kata Mlinarić-Majerski, Conformational Analysis of 2-(1-adamantyl)-3-hydroxybutyric acid by Computational Studies and $^{1}$H NMR spectroscopy and Computational Studies; ***J. Mol. Struct.***, 2008, *888*, 238. *Impact Factor: 1.551*

(11) **Ajeet Singh**, Manoj K. Kesharwani and Bishwajit Ganguly, Influence of Formamide on the Crystal Habit of LiF, NaCl, and KI: A DFT and Aqueous Solvent Model Study; ***Cryst. Growth Des.***, 2009, *9*, 77. *Impact Factor: 4.162*

(12) **Ajeet Singh** and Bishwajit Ganguly, DFT Studies on a New Class of Cage Functionalized Organic Superbases; ***New J. Chem.***, 2009, *33*, 583. *Impact Factor: 3.006*

(13) **Ajeet Singh**, T. Selvamani, Indrajit Mukhopadhyay and Bishwajit Ganguly, Morphology of Potassium Chloride in Aqueous Solution and in Formamide Solution: An Experimental and Computational Investigation; ***Can. J. Chem.***, 2009, *87*, 514. *Impact Factor: 1.423*

(14) **Ajeet Singh**, Anik Sen and Bishwajit Ganguly, First Principle Study towards the Influence of $Cd^{2+}$ on the Morphology of Sodium Chloride; ***J. Mol. Graphics Modell.***, 2010, *28*, 413. *Impact Factor: 2.169*

(15) **Ajeet Singh**, Moorthy Suresh and Bishwajit Ganguly, Probing the Influence of Electronic Effects of Organic Additives on the Morphology of Sodium Chloride Crystals: A Combined Experimental and Computational Study; ***CrystEngComm***, 2010, *12*, 4168. *Impact Factor: 4.183*

(16) Bishwajit Ganguly, Manoj K. Kesharwani, Nikola Basarić, Marija Matković, **Ajeet Singh** and Kata Mlinarić-Majerski, Hydrolysis and Retro-Aldol Cleavage of Ethyl *threo*-2-(1-adamantyl)-3 hydroxybutyrate: Competing Reactions; ***J. Phys. Org. Chem.,*** 2011, *24*, 578 (on web). *Impact Factor: 1.602*

(17) **Ajeet Singh**, Anik Sen and Bishwajit Ganguly, Probing the Influence of Solvent Effect on 1,4-diazacyclohexane System; ***J. Mol. Struct.***, 2010, *984*, *294*. *Impact Factor: 1.551*

(18) Md Abdul Shafeeuulla Khan, **Ajeet Singh**, Soumya Haldar, Bishwajit Ganguly, Can Nitrilotriacetic Acid (NTA) Act as a Habit Modifier for Rock Salt Crystals? An Answer from Computational and Experimental Studies; ***Cryst. Growth Des.***, 2011, 111, 1675. *Impact Factor: 4.162.*

(19) R. Lo, A. Ballabh, **Ajeet Singh**, P. Dastidar, B Ganguly, Probing the –C=O…Br–Br halogen bonding in X-ray crystal structures with *ab initio* calculations ***CrystEngComm*** 2012, 14 1833, *Impact Factor: 4.183.*

(20) R. Lo, **Ajeet Singh**, Manoj K. Kesharwani and Bishwajit Ganguly, Rational Design on a new class of polycyclic organic bases bearing two superbasic sites and their applications in $CO_2$ capture and activation process, ***ChemComm***, 2012 , *48*, 5865, *Impact Factor: 6.169*.

(21) AmritaDwivedi, A. K. Srivastava, **Ajeet Singh***, Molecular modeling of pyridine derivatives for COX-2 inhibitors: quantitative structure–activity relationship study, ***Medicinal Chemistry Research***, 2014, *23*, 1865 *Impact Factor: 1.25.*

(22) Amrita Dwivedi, A. K. Srivastava, **Ajeet Singh*,** *In silico* molecular modeling and prediction of activity of substituted tetrahydropyrans as COX-2 inhibitor; **2014**, ***Med.Chem.Res.*** **2015,** *24*, 714, *Impact Factor: 1.25*.

(23) Anik Sen, Bishwajit Ganguly, **Ajeet Singh**, Sunirmal Barik, Revealing the Parameters to Design the Habit Modifiers for Rock-salt Crystals: Empirical to Rational Approach, ***Canadian Journal of Chemistry,*** **2015,** *93*, 1219, *Impact Factor: 1.24.*

(24) Amrita Dwivedi, **Ajeet Singh**, A. Tripathi, A. K. Srivastava, Hansch analysis of dihydro-pyrazolyl-thiazolinone derivatives as potential COX-2 inhibitors, *J. Indian Chem. Soc.*, **2015**, 92, 1747, *Impact Factor:* 0.145.

(25) Snehasis Bhunia, **Ajeet Singh**, A. K Ojha, Un-catalyzed peptide bond formation between two monomers of glycine, alanine, serine, threonine, and aspartic acid in gas phase: a density functional theory study, ***Eur. Phys. J. D,*** **2016**, *70*, 106, *Impact Factor: 1.22*.

(26) Rahul Kaushik, **Ajeet Singh**, Amrita Ghosh and D. Amilan Jose, Selective Colorimetric Sensor for the Detection of $Hg^{2+}$ and $H_2S$ in Aqueous Medium and Waste Water Samples, ***Chemistry Select***, **2016**, 1,1533-1540, *Impact Factor:1.505.*

(27) Neetu Sharma, Amrita Dwivedi, AK Srivastava, **Ajeet Singh*,** QSAR modeling of HIV-1 reverse transcriptase inhibitor of aryluracil derivatives using *ab initio* and empirical calculations, ***Indian J. Chem. Sect. B,*** **2016**, 55B, 752, *Impact Factor:* 0.353.

(28) Amrita Dwivedi, **Ajeet Singh*,** Arun Kumar, Quantitative Structure-Activity Relationship Based Modeling of Substituted Indole Schiff Bases as Inhibitor of COX-2, ***Journal of Saudi Chemical Society,*** **2016,** *20*, S457 *Impact Factor: 2.22*.

(29) Rahul Kaushik, Amrita Ghosh, **Ajeet Singh**, Prachi Gupta, Ashwani Mittal, D Amilan Jose, Selective detection of cyanide in water and biological samples by an off-the-shelf compound, ***ACS Sens.,*** **2016**, *1*, 1265–1271, *Impact Factor:5.62*.

(30) Snehasis Bhunia, **Ajeet Singh**, A. K Ojha, Investigation of the encapsulation of metal cations ($Cu^{2+}$, $Zn^{2+}$, $Ca^{2+}$ and $Ba^{2+}$) by the dipeptide Phe–Phe using natural bond orbital theory and molecular dynamics simulation, ***Journal of molecular modeling,*** **2017**, 23, 88. *Impact Factor: 1.221*.

(31) B. Ahmed, A. K. Ojha, **Ajeet Singh,** F Hirsch, I Fischer, D Patrice, A Materny, Well-controlled in-situ growth of 2D $WO_3$ rectangular sheets on reduced graphene oxide with strong photocatalytic and antibacterial properties, ***Journal of Hazardous Materials,*** **2018**, *347*, 266–278, *Impact Factor: 6.221*.

(32) **Ajeet Singh*,** Animesh K. Ojha, Hyun Myung Jang, Strategic design and utilization of molecular flexibility for straddling the application of organic superbases: a DFT study, ***ChemistrySelect,*** **2018**, *3*, 837–842, *Impact Factor:1.505*.

(33) Sachin Kumar, Bilal Ahmed, Arvind Singh, **Ajeet Singh**, Animesh K Ojha, Experimental and Theoretical Investigations of Unusual Enhancement of Room Temperature Ferromagnetism in Nickel-Cobalt Codoped $CeO_2$ Nanostructures, ***Journal of Magnetism and Magnetic Materials,*** **2018**, *465*, 756, *Impact Factor: 2.683*

(34) Arvind Singh, Bilal Ahmed, **Ajeet Singh**, Animesh K Ojha, Photodegradation of phenanthrene catalyzed by rGO sheets and disk like structures synthesized using sugar cane juice as a reducing agent, ***Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy,*** **2018**, *204*, 603, *Impact Factor: 2.931*.

(35) Rahul Kaushik, Amrit Ghosh, **Ajeet Singh,** D. Amilan Jose, Colorimetric sensor for the detection of $H_2S$ and its application in molecular half-subtractor, ***Analytica Chimica Acta***, **2018**, *1040*, 177, *Impact Factor: 5.256*.

(36) Snehasis Bhunia, **Ajeet Singh**, A. K Ojha, Binding patterns of metal cations ($Na^+$, $K^+$, $Cu^{2+}$, and $Zn^{2+}$) with Trp-Trp di-peptide investigated by DFT, NBO, and MD simulation**,** ***Computational and Theoretical Chemistry,*** **2018**, *1141*, 7, *Impact Factor:* 1.403 .

(37) Pawan Kumar, Dheeraj Aryaa, Deepak Naina, **Ajeet Singh**, Amrita Ghosha, Dual colorimetric sensor for picric acid and pyrophosphate: Practical application for molecular logic gates, Dual colorimetric sensor for picric acid and pyrophosphate: Practical application for molecular logic gates, ***Dyes and Pigments,*** **2019**, *166*, 443, *Impact Factor:* 4.018.

(38) Aditya Kumar, **Ajeet Singh**, Animesh K. Ojha Reshuffling of Electronic Environment by Introducing $CH_3NH_2F^+$ as an Organic Cation for Enhanced Power Conversion Efficiency and Stability of the Designed Hybrid Organic–Inorganic Perovskite, **J. Phys. Chem. C, 2019**, *123*, 13385, *Impact Factor:* 4.309.

(39) Aditya Kumar, **Ajeet Singh**, Animesh K. Ojha, A new approach to predict the formation of 3D hybrid organic , inorganic perovskites ***International Journal of Quantum Chemistry,*** **2019**, *119,* 1, *Impact Factor:* 2.263.

(40) Rahul Sakla,, Ajeet Singh, Rahul Kaushik, Pawan Kumar, D. Amilan Jose, Allosteric Regulation in Carbon Monoxide (CO) Release: Anion Responsive CO-Releasing Molecule (CORM) Derived from (Terpyridine)phenol Manganese Tricarbonyl Complex with Colorimetric and Fluorescence Monitoring, ***Inorg. Chem.*** **2019**, *58*, 10761, *Impact Factor: 4.850.*

**Highlighted Article:**

(1) ***J. Phys. Chem. A***, 2007, *111,* 6468. and ***New J. Chem.***, 2008, *32*, 210**.** These works were highlighted in "Superbases for Organic Synthesis. Guanidines, Amidines, Phosphazenes and Related Organocatalysts" Book, Edited by Tsutomu Ishikawa, John Wiley & Sons, Hoboken 2009.

(2) ***New J. Chem.,*** 2008, *32*, 210; Selected for **Top 10 Hottest Articles**.

**Book and Book Chapter:**

- Density Functional Theory Study of Urea Interaction with Potassium Chloride Surfaces, Ajeet Singh, Bishwajit Ganguly; Industrial Applications of Molecular Simulations, Edited by Marc Maunier, CRC Press Taylor & Francis, 2012, Page No. 109-117 ISBN-13: 978-1-4398-6102-8 (Book Chapter).

**Patent:**

A Processor for the Preparation of Inorganic Hydrogel with Alkalihalide,
**Ajeet Singh** and Bishwajit Ganguly

**(b) Conference Proceedings:**

(1) Attended workshop cum symposium on An Approach to Analytical Instruments Commonly Used in Chemical Industries held at Department of Chemistry, University of Bhavnagar, Gujarat, India, 17 -18 September 2005.

(2) DFT Calculation on a New Class of Chiral and Achiral Proton Sponge; ***Ajeet Singh***, *Bishwajit Ganguly.* Royal Society of Chemistry-West India Section Students symposium-2006 (RSC-WIS 2006) held at the M. S. University Baroda, Vadodara on October 13 & 14, 2006, (Oral presentation).

(3) Subsituted *cis*-Azadecalins as Proton Sponge: A Density Functional study; ***Ajeet Singh*** *and Bishwajit Ganguly***.** Poster Presentation in International Symposium on Material Chemistry held at Chemistry Division, Bhabha Atomic Research Centre Mumbai. Dec. 4-8, 2006, (Poster presentation).

(4) Computational Study of Urea and Its Homologue Glycinamide: Relative Interactions with Sodium Chloride; ***Ajeet Singh*** *and Bishwajit. Ganguly*; XXII-Gujarat Science Congress, held on 9$^{th}$ March 2008 at Bhavnagar University Bhavnagar, (Oral presentation).

(5) DFT Calculation on a New Class of Chiral and Achiral Proton Sponge; ***Ajeet Singh*** *and Bishwajit Ganguly*; 5$^{th}$ All Gujarat Research Scholars Meet (AGRSM 08) held on Department of Chemistry Faculty of Science, M. S. University Baroda Vadodara on 15$^{th}$ Feb. 2008, (Oral presentation).

(6) Rational design of a new class of polycyclic organic bases bearing two superbasic sites and their applications in the $CO_2$ capture and activation process; **Ajeet Singh**, *Rabindranath Lo, and Bishwajit Ganguly, Indian Science Congress Association (Allahabad Capter),* organized by Department of Chemistry, University of Allahabad, Allahabad held during 28 Feb. 1 March 2013(Oral presentation).

(7) Strategic design and utilization of molecular flexibility for the straddling the applications of organic superbases : a DFT study, ***Ajeet Singh***, *Animesh Kumar Ojha, Hyun Myung Jang, Indian Science Congress Association (Allahabad Capter),* organized by Department of Chemistry, University of Allahabad, Allahabad held during 2 March - 4 March 2016(Oral presentation).

(8) Azaborine isomers based π-spacer in D- π -A type molecule for dye-sensitized solar cell: A computational investigation, ***Ajeet Singh***, *Animesh K. Ojha*, 8th Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC-8), 15-17 Dec. 2017 at IIT Bombay.

**(c) Invited Talk:**

**1:** Participated (Invited Talk) in International Conference on Crystal Engineering: From Molecule to Crystal, Held on March 30- 31, 2019 at NIT Raipur.
**Title:** Effect of additive onto the crystal of ionic solids: An experimental and computational study