



## DR. AMBRISH KUMAR SRIVASTAVA

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Google Scholar: <http://scholar.google.co.in/citations?user=XTcgp1EAAA>

ResearchGate: [https://www.researchgate.net/profile/Amrish\\_K\\_Srivastava](https://www.researchgate.net/profile/Amrish_K_Srivastava)

### **Academic and other qualifications:**

- Ph. D. (PHYSICS)- 2017, From University of Lucknow
- CSIR-NET (JRF)- All India Rank 18 held in June 2011
- GATE-2011: All India Rank 134 organized by Ministry of Human Resource and Development, Government of India in Feb. 2011
- JEST-2011: All India Rank 138 organized by Department of Atomic Energy, Government of India in Feb. 2011
- M. Sc. (PHYSICS) -2010, From University of Lucknow with 73.75%
- B. Sc. (PSM) -2008, From University of Lucknow with 66.22%
- Intermediate -2005, From S.S. Inter College affiliated to U.P. Board with 76.60%
- High School -2003, From S.S. Inter College affiliated to U.P. Board with 67.16%

### **Awards/Positions:**

- NASI- Young Scientist Platinum Jubilee Award 2022 by National Academy of Sciences, India (NASI) in Chemical Sciences.
- Assistant Professor at Department of Physics, D D U Gorakhpur University, Gorakhpur 273009, India (July 2018 to date)
- Assistant Professor at P.G. Department of Physics, Veer Kunwar Singh University, Ara 802301, India (September 2017 to June 2018)
- National Post Doctoral Fellow (NPDF) of SERB in Department of Physics, D D U Gorakhpur University, Gorakhpur 273009, India (May 2017 to August 2017)
- Senior Research Fellow (SRF) of CSIR in Department of Physics, University of Lucknow (August 2014 to March 2017)
- Junior Research Fellow (JRF) of CSIR in Department of Physics, University of Lucknow (August 2012 to July 2014)

### **Research Projects:**

1. In Silico Investigation on the Hydrogen Storage by Superalkalis and its Implications (29.5 lakhs) by SERB in May, 2023: Ongoing

2. Superatoms as Building Blocks of Novel Materials for Various Applications: A Computational Approach (Rs. 1000000/-) by UGC in 2020: Completed
3. Computational Exploration of Superatomic Clusters and Their Potential Applications in a Variety of Fields (Rs. 1070000/-) by SERB in 2017: Completed

#### Current Research Interests:

Theoretical & Computational Chemistry  
Atomic & Superatomic Clusters  
Nanostructures & Cluster Assembled Materials  
Biophysics

#### Professional Activities/Memberships:

- Associate Editor of *Frontiers in Physics*, section: Chemical Physics & Physical Chemistry
- Editorial Board of *Current Chinese Science* and *Journal of Computational Methods in Molecular Design*
- Life Member of The Indian Science Congress Association
- Life Member of The Indian Chemical Society
- Affiliate Member of Royal Society of Chemistry
- Society Affiliate of American Chemical Society
- Life Member of the Materials Research Society of India
- Organizing Secretary, International Conference on Futuristic Materials, 18-20 December 2020
- Coordinator: Online Workshop on Computer-Aided Drug Design using BIOVIA Discovery Studio, 13 & 14 August 2020
- Organizer, 1st Virtual Conference on Scientific Research and Advances (VCSRA-2018) during 20-25 February 2018.

#### Research Achievements:

- Total number of published research papers: 125
  - Total number of published books: 05 + 01 (In Press)
  - Total number of citations > 1700
  - h-Index: 24
  - i10-Index: 56
- (Sources: Google Scholar, ResearchGate, Web of Science, Scopus)

#### List of SCI Publications

1. HCF<sub>4-n</sub>(SO<sub>3</sub>)<sub>n</sub> (n=1-4): Designing a new series of organic superacids, J. K. Tripathi, N. Misra and A. K. Srivastava, *Modern Physics Letters B* <https://doi.org/10.1142/S021798492342006X>
2. Boronyl-Based Polycyclic Superhalogens, A. K. Srivastava, *The Journal of Physical Chemistry A* 127 (2023) 10406-10411.
3. Docking and MM study of non-structural protein (NS5) of Japanese Encephalitis Virus (JEV) with some derivatives of adenosyl, R.K. Tiwari, V. Pandey, H. Srivastava, A. K. Srivastava and V. Pandey, *Frontiers in Chemistry* 11 (2023) 1258764.
4. A Simple Strategy to Design Polycyclic Superhalogens, A. K. Srivastava, *The Journal of Physical Chemistry A* 127 (2023) 4867-4872.
5. Recent progress on the design and applications of superhalogens, A. K. Srivastava, *Chemical Communications* 59 (2023) 5943-5960. [INVITED HIGHLIGHTS]
6. Influence of electric field on the electro-optical and electronic properties of 4-n-alkoxy-4-cyanobiphenyl liquid crystal series: An application of DFT, A. K. Pandey, A. Kumar, A. K. Srivastava, V. Singh, K. K. Pandey, A. Dwivedi, M. S. Chauhan, D. Sharma, *Pramana* 97 (2023) 93.
7. Molecular Dynamics and Quantum Chemical Studies on Piperine, a Naturally Occurring Alkaloid, A. K. Srivastava, A. Kumar, H. Srivastava, S. Pandey, N. Kumar, G. Brahmachari, N. Misra, *Polycyclic Aromatic Compounds* <https://doi.org/10.1080/10406638.2023.2237631>.

8. BO<sub>2</sub> substituted novel alkyl biphenyl liquid crystalline series: dependence of geometrical and electronic properties on the alkyl chain length, A. Kumar, [A. K. Srivastava\\*](#), D. Sharma, S. N. Tiwari, N. Misra, *Theoretical Chemistry Accounts* 142 (2023) 17.
9. Editorial: Superhalogens & superalkalis: Exploration of structure, properties and applications, [A. K. Srivastava\\*](#), I. Anusiewicz, S. Velickovic, W.-M. Sun, G. L. Gutsev, *Frontiers in Chemistry* 10 (2022) 1075487.
10. The role of herbal plants in the inhibition of SARS-CoV-2 main protease: A computational approach, [A. K. Srivastava](#), A. Kumar, H. Srivastava, N. Misra, *Journal of the Indian Chemical Society* 99 (2022) 100640.
11. CF<sub>4-n</sub>(SO<sub>3</sub>)<sub>n</sub> (n = 1–4): a new series of organic superhalogens, J.K. Tripathi, [A. K. Srivastava\\*](#), *Molecular Physics* 120(2022) e2123748.
12. Superalkalis for the Activation of Carbon Dioxide: A Review, H. Srivastava, [A. K. Srivastava\\*](#), *Frontiers in Physics* 10(2022) 870205. [REVIEW ARTICLE]
13. Role of central core and methyl substitutions in XH<sub>4-x</sub>(CH<sub>3</sub>)<sub>x</sub> (X = N, P, As; x = 0–4) superalkalis: an ab initio study, H. Srivastava, [A. K. Srivastava\\*](#), *Structural Chemistry* 34 (2023) 617-623.
14. M(BO)<sub>k</sub>+1<sup>-</sup> Anions: Novel Superhalogens Based on Boronyl Ligands, [A. K. Srivastava](#), *The Journal of Physical Chemistry A* 126 (2022) 515-520.
15. Spectroscopic and Structural Investigations on Novel 6-Amino-3-Phenyl-4-(Pyridin-4-yl)-2,4-Dihydropyrano[2,3-c] Pyrazole-5-Carbonitrile by FT-IR, NMR, Docking, and DFT Methods, R. Kumar, A. Kumar, [A. K. Srivastava](#), G. Brahmachari, N. Misra, *Polycyclic Aromatic Compounds* 42 (2022) 2288-2304.
16. Electronic structures and properties of small (BCN)<sub>x</sub> (x = 1–5) clusters and (BCN)<sub>12</sub> nanotube, A. Kumar, R. Kumar, N. Misra, H. Srivastava, J. K. Tripathi, [A. K. Srivastava\\*](#), *Pramana* 96 (2022) 12.
17. X(CH<sub>3</sub>)<sub>k+1</sub><sup>+</sup> superalkali cations (X = F, O and N) with methyl ligands, [A. K. Srivastava\\*](#), H. Srivastava, A. Tiwari, N. Misra, *Chemical Physics Letters* 790 (2022) 139352.
18. On the surface interaction of C<sub>60</sub> with superalkalis: a computational approach [A. K. Srivastava](#), *Molecular Physics* (2021) e1999519
19. Prediction of Novel Liquid Crystalline Molecule Based on BO<sub>2</sub> Superhalogen, [A. K. Srivastava](#), *Journal of Molecular Liquids* 344 (2021) 117968
20. Editorial: Atomic Clusters: Theory & Experiments, [A. K. Srivastava\\*](#), I. Anusiewicz, S. Velickovic, W.-M. Sun, N. Misra, *Frontiers in Chemistry* 9 (2021) 795113
21. Lithiated Graphene Quantum Dot and its Nonlinear Optical Properties Modulated by a Single Alkali Atom: A Theoretical Perspective, [A. K. Srivastava](#), *Inorganic Chemistry* 60 (2021) 3131-3138.
22. Superhalogens as Building Blocks of Ionic Liquids, [A. K. Srivastava\\*](#), A. Kumar, N. Misra, *The Journal of Physical Chemistry A* 125 (2021) 2146-2153. [INVITED ARTICLE]
23. 1-Alkyl-3-methylimidazolium belong to superalkalis, [A. K. Srivastava](#), *Chemical Physics Letters* 778 (2021) 138770.
24. Ionization of NO by superhalogens: DFT and QTAIM approaches, [A. K. Srivastava](#) *Main Group Chemistry* 20 (2021) 33-40.
25. DFT and QTAIM studies on the reduction of carbon monoxide by superalkalis, [A. K. Srivastava](#) *Journal of Molecular Graphics and Modelling* 102 (2021) 107765.
26. External electric field modulated second-order nonlinear optical response and visible transparency in hexalithiobenzene, [A. K. Srivastava](#), *Journal of Molecular Modeling* 27 (2021) 19.
27. Ab initio investigations on the interaction of CO<sub>2</sub> and non-metallic superalkalis: structure, stability and electronic properties, R. Kumar, A. Kumar, [A. K. Srivastava](#), N. Misra, *Molecular Physics* 119 (2021) e1841311.
28. Structural and electronic properties of 2D-activated carbon sheet, R. Kumar, A. Kumar, B. K. Rao, [A. K. Srivastava](#), M. L. Verma, N. Misra, *Carbon Letters* 31 (2021) 483-488.
29. Structures and Electronic Properties of Small Al<sub>n</sub>Se<sub>n</sub> (n = 1–5) Clusters, D.V. Shukla, [A. K. Srivastava](#), N. Misra, *Proceedings of National Academy of Science, India, Section A Physical Sciences* 91 (2021) 181-188.
30. Ab initio investigations on bimetallic mononuclear superalkali clusters, [A. K. Srivastava](#), *Chemical Physics Letters* 759 (2020) 138049.
31. Superalkali behavior of ammonium (NH<sub>4</sub><sup>+</sup>) and hydronium (OH<sub>3</sub><sup>+</sup>) cations: a computational analysis, [A. K. Srivastava\\*](#), N. Misra, S. N. Tiwari, *SN Applied Sciences* 2 (2020) 307.
32. FT-IR, UV-visible, and NMR Spectral Analyses, Molecular Structure, and Properties of Nevadensin Revealed by Density Functional Theory and Molecular Docking, A. Kumar, [A. K.](#)

- Srivastava, S. K. Gangwar, N. Misra, G. Brahmachari, A. Mondal, S. Mondal, *Polycyclic Aromatic Compounds* 40 (2020) 540-552.
33. Enormously high second-order nonlinear optical response of single alkali atom decorated hexalithiobenzene, A. K. Srivastava, *Journal of Molecular Liquids* 298 (2020) 112187.
  34.  $MC_6Li_6$  (M = Li, Na and K): a new series of aromatic superalkalis, A. K. Srivastava, *Molecular Physics* 118 (2020) e1730991.
  35.  $C_xH_{4x+1}^+$  (x = 1–5): a unique series of organic superalkali cations, A. K. Srivastava, *Molecular Physics* 118 (2020) e1615648.
  36.  $BH_x^+$  (x=1–6) clusters: In the quest for superalkali cation with B-core and H-ligands, A. K. Srivastava, *Chemical Physics* 524 (2019) 118-123.
  37. Ab initio investigations on non-metallic chain-shaped  $F_nH_{n+1}^+$  series of superalkali cations, A. K. Srivastava, *Chemical Physics Letters* 721 (2019) 7-11.
  38. In-silico investigation of optical, thermal and electronic properties for 4-n-alkoxy benzoic acid series (nOBA; n = 1–8), D. Sharma, A. K. Srivastava, S. N. Tiwari, *Journal of Molecular Liquids* 294 (2019) 111672.
  39. Evolution of Anisotropy, First Order Hyperpolarizability and Electronic Parameters in p-Alkyl-p'-Cynobiphenyl Series of Liquid Crystals: Odd-Even Effect Revisited, A. Kumar, A. K. Srivastava, S. N. Tiwari, N. Misra, D. Sharma, *Molecular Crystals and Liquid Crystals*, 681 (2019) 23-31.
  40. Quantum chemical and molecular docking studies on two potential hepatitis C virus inhibitors, G. Tiwari, A. K. Srivastava, R. Kumar, A. Kumar, *Main Group Chemistry* 18 (2019) 107-121.
  41.  $O_xH_{2x+1}^+$  clusters: A new series of non-metallic superalkali cations by trapping  $H_3O^+$  into water, A. K. Srivastava, *Journal of Molecular Graphics and Modelling* 88 (2019) 292-298.
  42.  $CO_2$ -activation and enhanced capture by  $C_6Li_6$ : A density functional approach, A. K. Srivastava, *International Journal of Quantum Chemistry* 119 (2019) e25904. [FEATURED ON COVER PAGE]
  43. Design of the  $N_nH_{3n+1}^+$  series of "non-metallic" superalkali cations, A. K. Srivastava, *New Journal of Chemistry* 43 (2019) 4959-4964.
  44.  $C_{60}$  as Electron Acceptor and Donor: A Comparative DFT Study of  $Li@C_{60}$  and  $F@C_{60}$ , A. K. Srivastava, S. K. Pandey, A. K. Pandey, N. Misra, *Australian Journal of Chemistry* 71 (2018) 953-956.
  45. Organic superalkalis with closed-shell structure and aromaticity, A. K. Srivastava, *Molecular Physics* 116 (2018) 1642-1649.
  46. Reduction of nitrogen oxides (NO<sub>x</sub>) by superalkalis, A. K. Srivastava, *Chemical Physics Letters* 695 (2018) 205-210
  47. Stigmasterol from the flowers of *Peltophorum pterocarpum* (DC.) Backer ex K. Heyne (Fabaceae) — Isolation, spectral properties and quantum chemical studies, G. Brahmachari, S. Majhi, B. Mandal, M. Mandal, A. Kumar, A. K. Srivastava, R. B. Singh, N. Misra, *Journal of Indian Chemical Society* 95 (2018) 1231-1244.
  48. Single- and double-electron reductions of  $CO_2$  by using superalkalis: An ab initio study, A. K. Srivastava, *International Journal of Quantum Chemistry* 118 (2018) e25598.
  49. A computational study on semiconducting  $Si_{60}$ ,  $Si_{59}Al$  and  $Si_{59}P$  nanocages, A. K. Srivastava, S. K. Pandey, N. Misra, *Chemical Physics Letters* 691 (2018) 82-86.
  50. Alkalized Broazine: A simple recipe to design closed shell superalkalis, A. K. Srivastava\*, S. N. Tiwari, N. Misra, *International Journal of Quantum Chemistry* 118 (2018) e25507.
  51. DFT Study on Planar  $(CaO)_n$  Rings (n = 1–5) and Their Hydrogen Storage Behavior: Ca–O Versus Mg–O Clusters, A. K. Srivastava, N. Misra, S. K. Pandey, *Journal of Cluster Science* 29 (2018) 57-65.
  52. Application of superhalogens in the design of organic superconductors, A. K. Srivastava\*, A. Kumar, S. N. Tiwari, N. Misra, *New Journal of Chemistry* 41 (2017) 14847-14850.
  53. Structure, Electronic Properties and Electronic Excitation Analyses of  $Si_{60}$ - $Si_{60}$  Dimer and  $AlSi_{59}$ - $Si_{59}P$  Complex, A. K. Srivastava, S. K. Pandey, N. Misra, *Current Applied Physics* 17 (2017) 1376-1381.
  54. Superalkali@ $C_{60}$ -Superhalogen: Structure and Nonlinear Optical Properties of a New Class of Endofullerene Complexes, A. K. Srivastava, A. Kumar, N. Misra, *Chemical Physics Letters* 682 (2017) 20-25.
  55. Superhalogen as building blocks of a new series of superacids, A. K. Srivastava, A. Kumar, N. Misra, *New Journal of Chemistry* 41 (2017) 5445-5449.
  56. Functionalization of benzene by superhalogens, A. K. Srivastava, A. Kumar, N. Misra, *Chemical Physics Letters* 671 (2017) 44-48.
  57. A path to design stronger superacids by using superhalogens, A. K. Srivastava, A. Kumar, N. Misra, *Journal of Fluorine Chemistry* 197 (2017) 59-62

58. Competition between alkali characteristics and nonlinear optical properties in  $OLi_3$ -M- $Li_3O$  (M=Li, Na, and K) complexes, [A. K. Srivastava](#), N. Misra, *International Journal of Quantum Chemistry* 117 (2017) 208-212.
59. Density functional study on the evolution of superhalogen properties in  $VO_n$  ( $n = 1-5$ ) species, D.V. Shukla, [A. K. Srivastava](#), N. Misra, *Main Group Chemistry* 16 (2017) 141-150.
60. Spectral (FT-IR, NMR) Analyses, Molecular Structures, and Chemical Bonding of Two Hexahydroacridine-1,8(2H,5H)-dione Derivatives: A Comparative Quantum Chemical Study, D. V. Shukla, A. Kumar, [A. K. Srivastava](#), N. Misra, G. Brahmachari, *Polycyclic Aromatic Compounds* 37 (2017) 426-441.
61. Molecular Structures, Vibrational Spectra, Electronic Properties, and Molecular Docking of Two Pyrazoline Derivatives Containing 1-Carboxamide and 1-Carbothioamide: A Comparative Study, A. Kumar, A. Dwivedi, [A. K. Srivastava](#), N. Misra, B. Narayana, S. Samshuddin, B. K. Sarojini, *Polycyclic Aromatic Compounds* 37 (2017) 267-279.
62. Experimental and quantum chemical studies on poriferasterol - A natural phytosterol isolated from *Cassia sophera* Linn. (Caesalpinaceae), G. Brahmachari, A. Mondal, N. Nayek, A. Kumar, [A. K. Srivastava](#), N. Misra, *Journal of Molecular Structure* 1143 (2017) 184-191.
63.  $(CH_3Br \cdots NH_3)@C_{60}$ : The effect of nanoconfinement on halogen bonding, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Chemical Physics Letters* 662 (2016) 240-243.
64. Structure and Properties of  $Li@C_{60}$ - $PF_6$  Endofullerene Complex, [A. K. Srivastava](#), A. Kumar, N. Misra, *Physica E* 84 (2016) 524-529.
65. Designing New Electrolytes for Lithium Ion Batteries Using Superhalogen Anions, [A. K. Srivastava](#), N. Misra, *Polyhedron* 117 (2016) 422-426.
66. Prediction of superalkali@ $C_{60}$  endofullerenes, their enhanced stability and interesting properties, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Chemical Physics Letters* 655-656 (2016) 71-75.
67. Can boron nitride analog of carbon nanoneedle exist?, [A. K. Srivastava](#), N. Misra, *Main Group Chemistry* 15 (2016) 191-196.
68. The aromaticity and electronic properties of monosubstituted benzene, borazine and diazadiborane rings: an ab initio MP2 study, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Theoretical Chemistry Accounts* 135 (2016) 158.
69. Superhalogens as building blocks of complex hydrides for hydrogen storage, [A. K. Srivastava](#), N. Misra, *Electrochemistry Communications* 68 (2016) 99-103.
70. Hydrogenated superalkalis and their possible applications, [A. K. Srivastava](#), N. Misra, *Journal of Molecular Modelling* 22 (2016) 122.
71.  $BO_2$ -functionalized  $B_3N_3C_{54}$  Heterofullerene as a Possible Candidate for Molecular Spintronics and Nonlinear Optics, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Materials Research Express* 3 (2016) 045008.
72. Encapsulation of lawrencium into  $C_{60}$  fullerene:  $Lr@C_{60}$  versus  $Li@C_{60}$ , [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Materials Chemistry and Physics* 177 (2016) 437-441.
73. Spectroscopic analyses, intra-molecular interaction, chemical reactivity and molecular docking of imerubrine into bradykinin receptor, [A. K. Srivastava](#), A. Kumar, S. K. Pandey, N. Misra, *Medicinal Chemistry Research* 25 (2016) 2832-2841
74. Remarkable NLO Responses of Hyperalkalized Species: Size Effect and Atomic Number Dependence, [A. K. Srivastava](#), N. Misra, *New Journal of Chemistry* 40 (2016) 5467-5472
75.  $OLi_3O^-$  anion: designing the strongest base to date using  $OLi_3$  superalkali, [A. K. Srivastava](#), N. Misra, *Chemical Physics Letters* 648 (2016) 152-155. [CITED IN WIKIPEDIA]
76. Stability versus aromaticity in mono-hydroxylated borazine, 1,2-azaborine and 1,3,2,4-diazadiborane, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Molecular Physics* 114 (2016) 1763-1770.
77. Synthesis, spectroscopic characterization and crystallographic behavior of a biologically relevant novel indole-fused heterocyclic compound - Experimental and theoretical (DFT) studies, S. Sharma, G. Brahmachari, B. Banerjee, K. Nurjamal, A. Kumar, [A. K. Srivastava](#), N. Misra, S. K. Pandey, Rajnikant, V. K. Gupta, *Journal of Molecular Structure* 1118 (2016) 344-355.
78. Visible Light Assisted Photocatalytic [3 + 2] Azide-Alkyne "Click" Reaction for the Synthesis of 1,4-Substituted 1,2,3-Triazoles Using a Novel Bimetallic Ru-Mn Complex, P. Kumar, C. Joshi, [A. K. Srivastava](#), P. Gupta, R. Boukherroub, S. L. Jain, *ACS Sustainable Chemistry & Engineering* 4 (2016) 69-75.
79. 3,5,7-Trimethoxyphenanthrene-1,4-dione: a new biologically relevant natural phenanthrenequinone derivative from *Dioscorea prazeri* and studies on its single X-ray crystallographic behavior, molecular docking and other physicochemical properties, G. Brahmachari, S. Das, M. Biswas, A. Kumar, [A. K. Srivastava](#), N. Misra, *RSC Advances* 6 (2016) 7317-7329.

80.  $M_2X$  ( $M = \text{Li, Na}$ ;  $X = \text{F, Cl}$ ): the smallest superalkali clusters with significant NLO responses and electronegativity characteristics, [A. K. Srivastava](#), N. Misra, *Molecular Simulation* 42 (2016) 981-985.
81. Quantum chemical studies on cocsuline using density functional theory and its docking into dihydrofolate reductase receptor, [A. K. Srivastava](#), A. Kumar, N. Misra, *Main Group Chemistry* 15 (2016) 97-106.
82. Synthesis, spectral (FT-IR, UV-visible, NMR) features, biological activity prediction and theoretical studies of 4-Amino-3-(4-hydroxybenzyl)-1H-1,2,4-triazole-5(4H)-thione and its tautomer, [A. K. Srivastava](#), A. Kumar, N. Misra, P. S. Manjula, B. K. Sarojini, B. Narayana, *Journal of Molecular Structure* 1107 (2016) 137-144.
83. *Ab initio* investigations on planar  $(\text{MgO})_n$  clusters ( $n = 1-5$ ) and their hydrogen adsorption behavior, [A. K. Srivastava](#), N. Misra, *Molecular Simulation* 42 (2016) 208-214.
84. Superbases and superacids form supersalts, [A. K. Srivastava](#), N. Misra, *Chemical Physics Letters* 644 (2016) 1-4.
85. Structural, electronic properties, hydrogen bonding analyses and biological activity of two multiple myeloma drugs: Lenalidomide and Pomalidomide, [A. K. Srivastava](#), A. K. Pandey, S. Pandey, N. Misra, *Polycyclic Aromatic Compounds* 36 (2016) 452-466.
86. Structures and Basicity of  $\text{Li}_n\text{OH}$  ( $n=1-5$ ) Species, [A. K. Srivastava](#), N. Misra, *International Journal of Quantum Chemistry* 116 (2016) 524-528.
87. Structure, energetics, spectral and electronic properties of  $\text{B}_3\text{N}_3\text{C}_5\text{H}_4$  heterofullerene, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Journal of Nanostructure in Chemistry* 6 (2016) 103-109.
88. Hydrogenated superhalogens behave as superacids, [A. K. Srivastava](#), N. Misra, *Polyhedron* 102 (2015) 711-714.
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90. Quantum chemical investigation on structures and energetics of Tungsten Fluoride ( $\text{WF}_n$ )<sup>q</sup> species ( $q = 0, \pm 1$ ;  $n < 6$ ), [A. K. Srivastava](#), A. K. Pandey, N. Misra, *Journal of Chemical Sciences* 127 (2015) 1853-1858.
91. Nonlinear optical behavior of  $\text{Li}_n\text{F}$  ( $n=2-5$ ) superalkali clusters, [A. K. Srivastava](#), N. Misra, *Journal of Molecular Modelling* 21 (2015) 305.
92. *Ab initio* investigations on the gas phase basicity and nonlinear optical properties of  $\text{FLi}_n\text{OH}$  species ( $n = 2-5$ ), [A. K. Srivastava](#), N. Misra, *RSC Advances* 5 (2015) 74206-74211.
93. Gold oxyfluorides,  $\text{Au}(\text{OF})_n$  ( $n = 1-6$ ): novel superhalogens with oxyfluoride ligands, [A. K. Srivastava](#), N. Misra, *New Journal of Chemistry* 39 (2015) 9543-9549.
94. Superhalogen properties of  $\text{CoO}_n$  ( $n \geq 3$ ) species revealed by density functional theory, [A. K. Srivastava](#), N. Misra, *Theoretical Chemistry Accounts* 134 (2015) 93.
95. Superalkali-hydroxides as strong bases and superbases, [A. K. Srivastava](#), N. Misra, *New Journal of Chemistry* 39 (2015) 6787-6790.
96. Heterocyclic  $\text{C}_2\text{B}_2\text{N}_2\text{H}_6$  versus homocyclic  $\text{C}_6\text{H}_6$ , [A. K. Srivastava](#), N. Misra, *Main Group Chemistry* 14 (2015) 369-375.
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125. First principle investigations on the superhalogen behavior of RuO<sub>n</sub> (n = 1 to 5) species, A. K. Srivastava, N. Misra, *European Physical Journal D* 68 (2014) 309.

#### List of Publications in Conference Proceedings:

1. Effect of Methyl Substitutions on the Ionization Energy of OH<sub>3</sub>–n(CH<sub>3</sub>)<sub>n</sub><sup>+</sup>, H. Srivastava, J. K. Tripathi, A. K. Srivastava, *Springer Proceedings in Materials*, 27 (2023) 235–240.
2. Structural, spectroscopic analysis of two hexahydroacridine-1,8(2H,5H)-dione derivatives and identification of drug like properties: Experimental and computational study, R. Kumar, A. Kumar, A. K. Srivastava, G. Brahmachari, G. Tiwari, N. Misra, *Materials Today: Proceedings* 29 (2020) 1050-1054.

3. Computational study on CH<sub>3</sub>-functionalized Tetraphenyl-1,4-phenylenediamine: A hole-transporting material for OLED devices, A. Tiwari, B. Kumar, [A. K. Srivastava](#), *Materials Today: Proceedings* 29 (2020) 772-775.
4. Computational study on 8-quinolinolatoalkali, an electron transporting material for OLED devices, A. Tiwari, B. Kumar, [A. K. Srivastava](#), *AIP Conference Proceedings* 2220 (2020) 040019.
5. Structures and electronic properties of TiFn (n= 1–5) species, [A. K. Srivastava](#), S. Pandey, N. Misra, *AIP Conference Proceedings* 2220 (2020) 130011.
6. DFT Studies on AlSe Nano Clusters, D. V. Shukla, A. Kumar, [A. K. Srivastava](#), N. Misra, *Materials Today: Proceedings* 5 (2018) 9187–9190
7. Quantum bound states with interaction potential having linear combination of exponential functions and its possible applications, V. K. Shukla, [A. K. Srivastava](#), *Materials Today: Proceedings* 5 (2018) 9094–9101.
8. Nonlinear Optical Property of 2-Amino-4-(4-fluorophenyl)-7-methyl-5-oxo-4,5-dihydropyrano[4,3-b]pyran-3-carbonitrile- DFT Approach, A. Kumar, [A. K. Srivastava](#), G. Brahmachari, N. Misra, *Bulletin of Laser and Spectroscopy Society of India* 22 (2016) 124-128.

### Books Authored/Edited:

1. Computational Studies: From Molecules to Materials  
Editor: [A. K. Srivastava](#)  
Publisher: Taylor & Francis/CRC Press, United Kingdom (IN PRESS)  
ISBN: 9781032528540
2. Superhalogens and Superalkalis: Bonding, Reactivity, Dynamics and Applications  
Editors: P. K. Chattaraj, [A. K. Srivastava](#)  
Publisher: Taylor & Francis/CRC Press, United Kingdom (2024)  
ISBN: 9781032466231
3. Superhalogens: Properties and Applications  
Author: [A. K. Srivastava](#)  
Publisher: Springer Nature, Switzerland (2023)  
ISBN: 9783031375705
4. Superhalogens & Superalkalis: Exploration of Structure, Properties and Applications (e-Book)  
Editors: [A. K. Srivastava](#), I. Anusiewicz, S. Velickovic, W.-M. Sun, G. L. Gutsev.  
Publisher: Frontiers Media SA, Laussane (2022)  
ISBN: 9782832508930
5. DFT Based Studies on Bioactive Molecules  
Authors: [A. K. Srivastava](#), N. Misra  
Publisher: Bentham Science Publishers Ltd., Singapore (2021)  
ISBN: 9789814998369
6. Atomic Clusters: Theory & Experiments (e-Book)  
Editors: [A. K. Srivastava](#), I. Anusiewicz, S. Velickovic, W.-M. Sun, N. Misra  
Publisher: Frontiers Media SA, Laussane (2021)  
ISBN: 9782889719204

### Chapters in Books:

1. Superhalogens-Based Superacids, in *Superhalogens and Superalkalis: Bonding, Reactivity, Dynamics and Applications*, Edited by P. K. Chattaraj, [A. K. Srivastava](#), (2024) 246-258.  
Authors: J. Tripathi, [A. K. Srivastava](#)  
Publisher: Taylor & Francis/CRC Press, United Kingdom  
ISBN: 9781032466231
2. Superalkalis in the Design of Strong Bases and Superbases, in *Superhalogens and Superalkalis: Bonding, Reactivity, Dynamics and Applications*, Edited by P. K. Chattaraj, [A. K. Srivastava](#), 2024 198-210.  
Authors: H. Srivastava, [A. K. Srivastava](#)



- Publisher: Taylor & Francis/CRC Press, United Kingdom  
ISBN: 9781032466231
3. Spectroscopic signatures of some organic compounds: Theory meets experiment, in *Computational Studies: From Molecules to Materials*, Edited by A. K. Srivastava, Authors: A. Kumar, A. K. Srivastava, R. Kumar, N. Misra  
Publisher: Taylor & Francis/CRC Press, United Kingdom  
ISBN: 9781032528540
  4. Superhalogen properties of some transition metal oxides, in *Superhalogens and Superalkalis: Bonding, Reactivity, Dynamics and Applications*, Edited by P. K. Chattaraj, A. K. Srivastava, (2024) 40-54.  
Authors: A. Kumar, A. K. Srivastava, N. Misra  
Publisher: Taylor & Francis/CRC Press, United Kingdom  
ISBN: 9781032466231
  5. Quantum Chemical Study on Pure and Silicon-Doped Activated Carbon Sheets, in *Computational Studies: From Molecules to Materials*, Edited by A. K. Srivastava, IN PRESS  
Authors: R. Kumar, A. Kumar, A. K. Srivastava, N. Misra  
Publisher: Taylor & Francis/CRC Press, United Kingdom  
ISBN: 9781032528540
  6. Structures, reactivity, and properties of low ionization energy species doped fullerenes and their complexes with superhalogen in *Atomic Clusters with Unusual Structure, Bonding and Reactivity*, Edited by P. K. Chattaraj, S. Pan and G. Merino (2023) 173-183.  
Authors: A. Kumar, A. K. Srivastava\*, G. Tiwari, N. Misra.  
Publisher: Elsevier, Netherlands  
ISBN: 9780128229439

#### **Invited Talks/Special Recognitions/Other Activities:**

1. Included in the list of Top 2% of world scientists for a single year category published by researchers at Stanford University.
2. Evaluator of science projects in 27<sup>th</sup> State-Level National Children's Science Congress organized by Council of Science & Technology, Uttar Pradesh, India during 04-06 December, 2019.
3. One of my research papers has been selected as Cover Image (URL link to the cover page: <https://onlinelibrary.wiley.com/doi/10.1002/qua.26049>) for International Journal of Quantum Chemistry (Volume: 119 & Issue: 20 of the Year 2019)
4. One of my research articles has been cited on a Wikipedia (page: <https://en.wikipedia.org/wiki/Borazine>).
5. Invited Talk "Superhalogens in Energy Storage Materials" in One Day National Webinar on Energy Crisis: Long Term Solutions jointly organized by S.S. College, Shahjahanpur & L.B.S. Degree College, Gonda (8 Nov. 2020)
6. Invited Talk "In Silico Methods of Drug Design for COVID-19" in National E-Conference on Interdisciplinary Research in Science and Technology organized by Amiruddaula Islamia Degree College, Lucknow (30 & 31 May 2020)
7. Invited Talk "In Silico Approaches to Combat COVID-19" in Leveraging Science and Technology to Combat COVID-19 organized by D.D.U. Gorakhpur University, Gorakhpur (23 & 24 May 2020)
8. Invited Talk "Superhalogens: The Clusters with High Electron Affinity" in National Conference on Advances in Materials Science organized by Marwar Business School, Gorakhpur (21 & 22 Feb. 2019)
9. Invited Talk "Superhalogens: A Special Class of Superatoms" in National Conference on Soft Matter organized by D.D. U. Gorakhpur University, Gorakhpur (27 & 28 March 2018)