



DR. AMBRISH KUMAR SRIVASTAVA

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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:

- Principal Investigator, UGC Start Up Grant Project [No. 30-466/BSR(2019)]
- 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. Superatoms as Building Blocks of Novel Materials for Various Applications: A Computational Approach (Rs. 1000000/-) by UGC in 2020: Ongoing
2. Computational Exploration of Superatomic Clusters and Their Potential Applications in a Variety of Fields (Rs. 1070000/-) by SERB in 2017: Completed

Current Research Interests:

Computational Materials Science
Atomic & Superatomic Clusters
Nanostructures
Biophysics

Professional Activities:

- Manager and Associate Editor of *Journal of Scientific Research and Advances* (ISSN: 2395-0226)
- Member of Editorial Board of *Journal of Computational Methods in Molecular Design* (ISSN: 2231-3176)
- Life Member of The Indian Science Congress Association
- Active Member of all major research platforms and networks, such as;
ORCID: <http://orcid.org/0000-0001-8340-856X>
ResearcherID: <http://www.researcherid.com/rid/C-4533-2015>
Google Scholar: <http://scholar.google.co.in/citations?user=XTcgp1EAAAJ>
ResearchGate: https://www.researchgate.net/profile/Ambrish_K_Srivastava
- Active Reviewer for various international journals, reviewer credits are available at: <https://publons.com/a/1281922/>

Research Achievements:

- Total number of published research papers: 98
 - Total number of communicated/accepted research papers: 3
 - Total number of citations > 800
 - h-Index: 16
 - i10-Index: 21
- (Sources: Google Scholar, ResearchGate, Web of Science, Scopus)

Selected List of Publications (As Principal/Corresponding/Single Author):

1. Superalkali behavior of ammonium (NH₄⁺) and hydronium (OH₃⁺) cations: a computational analysis, A. K. Srivastava, N. Misra, S. N. Tiwari, *SN Applied Sciences* 2 (2020) 307.
2. Enormously high second-order nonlinear optical response of single alkali atom decorated hexalithiobenzene, A. K. Srivastava, *Journal of Molecular Liquids* 298 (2020) 112187.
3. MC₆Li₆ (M = Li, Na and K): a new series of aromatic superalkalis, A. K. Srivastava, *Molecular Physics* <https://doi.org/10.1080/00268976.2020.1730991>.
4. C_xH_{4x+1}⁺ (x = 1–5): a unique series of organic superalkali cations, A. K. Srivastava, *Molecular Physics*, 118 (2020) e1615648.
5. 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.
6. Ab initio investigations on non-metallic chain-shaped FnHn+1⁺ series of superalkali cations, A. K. Srivastava, *Chemical Physics Letters* 721 (2019) 7-11.
7. OxH_{2x+1}⁺ clusters: A new series of non-metallic superalkali cations by trapping H₃O⁺ into water, A. K. Srivastava, *Journal of Molecular Graphics and Modelling* 88 (2019) 292-298.
8. CO₂-activation and enhanced capture by C₆Li₆: A density functional approach, A. K. Srivastava, *International Journal of Quantum Chemistry* 119 (2019) e25904.
9. Design of the NnH_{3n+1}⁺ series of "non-metallic" superalkali cations, A. K. Srivastava, *New Journal of Chemistry* 43 (2019) 4959-4964.
10. C₆₀ as Electron Acceptor and Donor: A Comparative DFT Study of Li@C₆₀ and F@C₆₀, A. K. Srivastava, S. K. Pandey, A. K. Pandey, N. Misra, *Australian Journal of Chemistry* 71 (2018) 953-956.
11. Organic superalkalis with closed-shell structure and aromaticity, A. K. Srivastava, *Molecular Physics* 116 (2018) 1642-1649.
12. Reduction of nitrogen oxides (NO_x) by superalkalis, A. K. Srivastava, *Chemical Physics Letters* 695 (2018) 205-210

13. Single- and double-electron reductions of CO₂ by using superalkalis: An ab initio study, [A. K. Srivastava](#), *International Journal of Quantum Chemistry* 118 (2018) e25598.
14. A computational study on semiconducting Si₆₀, Si₅₉Al and Si₅₉P nanocages, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Chemical Physics Letters* 691 (2018) 82-86.
15. 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.
16. 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.
17. 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.
18. Structure, Electronic Properties and Electronic Excitation Analyses of Si₆₀-Si₆₀ Dimer and AlSi₅₉-Si₅₉P Complex, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Current Applied Physics* 17 (2017) 1376-1381.
19. Superalkali@C₆₀-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.
20. 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.
21. Functionalization of benzene by superhalogens, [A. K. Srivastava](#), A. Kumar, N. Misra, *Chemical Physics Letters* 671 (2017) 44-48.
22. A path to design stronger superacids by using superhalogens, [A. K. Srivastava](#), A. Kumar, N. Misra, *Journal of Fluorine Chemistry* 197 (2017) 59-62.
23. Competition between alkalide characteristics and nonlinear optical properties in OLi₃-M-Li₃O (M=Li, Na, and K) complexes, [A. K. Srivastava](#), N. Misra, *International Journal of Quantum Chemistry* 117 (2017) 208-212.
24. (CH₃Br⁻---NH₃)@C₆₀: The effect of nanoconfinement on halogen bonding, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Chemical Physics Letters* 662 (2016) 240-243.
25. Structure and Properties of Li@C₆₀-PF₆ Endofullerene Complex, [A. K. Srivastava](#), A. Kumar, N. Misra, *Physica E* 84 (2016) 524-529.
26. Designing New Electrolytes for Lithium Ion Batteries Using Superhalogen Anions, [A. K. Srivastava](#), N. Misra, *Polyhedron* 117 (2016) 422-426.
27. Prediction of superalkali@C₆₀ endofullerenes, their enhanced stability and interesting properties, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Chemical Physics Letters* 655-656 (2016) 71-75.
28. Can boron nitride analog of carbon nanoneedle exist?, [A. K. Srivastava](#), N. Misra, *Main Group Chemistry* 15 (2016) 191-196.
29. 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.
30. Superhalogens as building blocks of complex hydrides for hydrogen storage, [A. K. Srivastava](#), N. Misra, *Electrochemistry Communications* 68 (2016) 99-103.
31. Hydrogenated superalkalis and their possible applications, [A. K. Srivastava](#), N. Misra, *Journal of Molecular Modelling* 22 (2016) 122.
32. BO₂-functionalized B₃N₃C₅₄ 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.
33. Encapsulation of lawrencium into C₆₀ fullerene: Lr@C₆₀ versus Li@C₆₀, [A. K. Srivastava](#), S. K. Pandey, N. Misra, *Materials Chemistry and Physics* 177 (2016) 437-441.
34. Spectroscopic analyses, intra-molecular interaction, chemical reactivity and molecular docking of ivermectin into bradykinin receptor, [A. K. Srivastava](#), A. Kumar, S. K. Pandey, N. Misra, *Medicinal Chemistry Research* 25 (2016) 2832-2841.
35. 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.
36. OLi₃O⁻ anion: designing the strongest base to date using OLi₃ superalkali, [A. K. Srivastava](#), N. Misra, *Chemical Physics Letters* 648 (2016) 152-155.
37. 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.
38. M₂X (M= Li, Na; X= F, Cl): the smallest superalkali clusters with significant NLO responses and electride characteristics, [A. K. Srivastava](#), N. Misra, *Molecular Simulation* 42 (2016) 981-985.

39. 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.
40. 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.
41. *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.
42. Superbases and superacids form supersalts, A. K. Srivastava, N. Misra, *Chemical Physics Letters* 644 (2016) 1-4.
43. 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.
44. Structures and Basicity of Li_nOH ($n=1-5$) Species, A. K. Srivastava, N. Misra, *International Journal of Quantum Chemistry* 116 (2016) 524-528.
45. Structure, energetics, spectral and electronic properties of $\text{B}_3\text{N}_3\text{C}_5$ heterofullerene, A. K. Srivastava, S. K. Pandey, N. Misra, *Journal of Nanostructure in Chemistry* 6 (2016) 103-109.
46. Hydrogenated superhalogens behave as superacids, A. K. Srivastava, N. Misra, *Polyhedron* 102 (2015) 711-714.
47. *Ab initio* prediction of novel alkalides $\text{FLi}_2\text{-M-Li}_2\text{F}$ ($\text{M} = \text{Li, Na and K}$), A. K. Srivastava, N. Misra, *Chemical Physics Letters* 639 (2015) 307-309.
48. Quantum chemical investigation on structures and energetics of Tungsten Fluoride (WF_n)^q species ($q = 0, \pm 1; n < 6$), A. K. Srivastava, A. K. Pandey, N. Misra, *Journal of Chemical Sciences* 127 (2015) 1853-1858.
49. Nonlinear optical behavior of Li_nF ($n=2-5$) superalkali clusters, A. K. Srivastava, N. Misra, *Journal of Molecular Modelling* 21 (2015) 305.
50. *Ab initio* investigations on the gas phase basicity and nonlinear optical properties of FLi_nOH species ($n = 2-5$), A. K. Srivastava, N. Misra, *RSC Advances* 5 (2015) 74206-74211.
51. 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.
52. Superhalogen properties of CoO_n ($n \geq 3$) species revealed by density functional theory, A. K. Srivastava, N. Misra, *Theoretical Chemistry Accounts* 134 (2015) 93.
53. Superalkali-hydroxides as strong bases and superbases, A. K. Srivastava, N. Misra, *New Journal of Chemistry* 39 (2015) 6787-6790.
54. Heterocyclic $\text{C}_2\text{B}_2\text{N}_2\text{H}_6$ versus homocyclic C_6H_6 , A. K. Srivastava, N. Misra, *Main Group Chemistry* 14 (2015) 369-375.
55. Tuning the oxidation state of Au and exploring new superhalogen anions, AuO_xF_y^- ($x, y = 1-4; x+y = 2-5$), A. K. Srivastava, N. Misra, *Chemical Physics Letters* 630 (2015) 106-110.
56. Structures, stability and electronic properties of novel superalkali-halogen clusters, A. K. Srivastava, N. Misra, *Journal of Molecular Modeling* 21 (2015) 147.
57. The boron-carbon-nitrogen heterocyclic rings, A. K. Srivastava, N. Misra, *Chemical Physics Letters* 625 (2015) 5-9.
58. Superhalogen properties of ReF_n ($n \geq 6$) species, A. K. Srivastava, S. K. Pandey, N. Misra, *Chemical Physics Letters* 624 (2015) 15-18.
59. Introducing carborazine as a novel heterocyclic aromatic species, A. K. Srivastava, N. Misra, *New Journal of Chemistry* 39 (2015) 2483-2488.
60. Fluorinated Ferromagnetic Metal Clusters and their Superhalogen Behaviour, A. K. Srivastava, N. Misra, *Molecular Physics* 113 (2015) 36-44.
61. FT-IR spectroscopy, intra-molecular C-H...O interactions, HOMO, LUMO, MESP analysis and biological activity of two natural products, triclisine and rufescine: DFT and QTAIM approaches, A. K. Srivastava, A. K. Pandey, S. Jain, N. Misra, *Spectrochimica Acta Part A* 136 (2015) 682-689.
62. Can Li_2F_2 cluster be formed by $\text{LiF}_2/\text{Li}_2\text{F-Li/F}$ interactions? An *ab initio* investigation, A. K. Srivastava, N. Misra, *Molecular Simulation* 41 (2015) 1278-1282.
63. *Ab initio* investigations on lithium-superhalogen (Li-X) complexes ($\text{X} = \text{LiF}_2, \text{BeF}_3, \text{BF}_4$ and PF_6): competition between s-block and p-block anions, A. K. Srivastava, N. Misra, *Molecular Physics* 113 (2015) 866-870.
64. Unusual properties of novel Li_3F_3 ring: ($\text{LiF}_2\text{-Li}_2\text{F}$) superatomic cluster or Lithium fluoride trimer, (LiF)₃?, A. K. Srivastava, N. Misra, *RSC Advances* 4 (2014) 41260-41265.
65. Structures, stabilities, electronic and magnetic properties of small Rh_xMn_y ($x + y = 2-4$) clusters, A. K. Srivastava, N. Misra, *Computational and Theoretical Chemistry* 1047 (2014) 1-5.

66. Novel planar chain like Li_7F_7 and Li_9F_9 nanostructures, A. K. Srivastava, N. Misra, *Chemical Physics Letters* 612 (2014) 302-305.
67. Unusual bonding and electron affinity of nickel group transition metal oxide clusters, A. K. Srivastava, N. Misra, *Molecular Physics* 112 (2014) 1639-1644.
68. Theoretical Investigations on the Superhalogen Properties and Interaction of PdO_n ($n = 1-5$) Species, A. K. Srivastava, N. Misra, *International Journal of Quantum Chemistry* 114 (2014) 328-332.
69. Ab Initio Investigations on the Stabilities of AuO_n^{q-} ($q = 0$ to 3; $n = 1$ to 4) Species: Superhalogen Behavior of AuO_n ($n \geq 2$) and their Interactions with an Alkali Metal, A. K. Srivastava, N. Misra, *International Journal of Quantum Chemistry* 114 (2014) 521-524.
70. A comparative theoretical study on the biological activity, chemical reactivity and coordination ability of dichloro substituted (1, 3-thiazol-2-yl) acetamides, A. K. Srivastava, N. Misra, *Canadian Journal of Chemistry* 92 (2014) 234-239.
71. Vibrational, structural and hydrogen bonding analysis of N'-[(E)-4-Hydroxybenzylidene]-2-(naphthalen-2-yloxy) acetohydrazide – combined density functional and atoms-in-molecule based studies, A. K. Srivastava, B. Narayana, B. K. Sarojini, N. Misra, *Indian Journal of Physics* 88 (2014) 547-556.
72. Theoretical investigation on the structure, stability and superhalogen properties of OsF_n ($n = 1-7$) species, A. K. Srivastava, N. Misra, *Journal of Fluorine Chemistry* 158 (2014) 65-68.
73. Superhalogen properties of ReO_n ($n = 1$ to 5) species and their interactions with an alkali metal: An *ab initio* study, A. K. Srivastava, N. Misra, *Molecular Physics* 112 (2014) 1954-1962.
74. Novel $(\text{Li}_2\text{X})^+(\text{LiX}_2)^-$ supersalts ($\text{X} = \text{F}, \text{Cl}$) with aromaticity: a journey towards the design of a new class of salts, A. K. Srivastava, N. Misra, *Molecular Physics* 112 (2014) 2621-2626.
75. Novel Li_3X_3 supersalts ($\text{X} = \text{F}, \text{Cl}, \text{Br} \ \& \ \text{I}$) and their alkalide characteristics, A. K. Srivastava, N. Misra, *New Journal of Chemistry* 38 (2014) 2890-2893.
76. The Highest Oxidation State of Au Revealed by Interactions with Successive Cl Ligands and Superhalogen Properties of AuCl_n ($n = 1-6$) Species, A. K. Srivastava, N. Misra, *International Journal of Quantum Chemistry* 114 (2014) 1513-1516.
77. Structures, stabilities and electronic properties of manganese oxyfluoride (MnO_xF_y) species ($x + y = 1-4$; $x, y = 0-4$), A. K. Srivastava, N. Misra, *Molecular Physics* 112 (2014) 2820-2826.
78. Comparative DFT study on Reactivity, Acidity and Vibrational Spectra of Halogen substituted Phenylacetic Acids, A. K. Srivastava, V. Baboo, B. Narayana, B. K. Sarojini, N. Misra, *Indian Journal of Pure and Applied Physics* 52 (2014) 507-519.
79. First principle investigations on the superhalogen behavior of RuO_n ($n = 1$ to 5) species, A. K. Srivastava, N. Misra, *European Physical Journal D* 68 (2014) 309.

List of Publications (As Co-Author):

1. Structures and Electronic Properties of Small AlnSen ($n = 1-5$) Clusters, D.V. Shukla, A. K. Srivastava, N. Misra, *Proceedings of National Academy of Science, India, Section A Physical Sciences* <https://doi.org/10.1007/s40010-019-00653-0>
2. 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.
3. 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.
4. 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.
5. 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.
6. Density functional study on the evolution of superhalogen properties in VOn ($n = 1-5$) species, D.V. Shukla, A. K. Srivastava, N. Misra, *Main Group Chemistry* 16 (2017) 141-150.
7. 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.
8. 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.

9. 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.
10. 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.
11. 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.
12. 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.
13. Synthesis, spectroscopic characterization, X-ray analysis and theoretical studies on the spectral features (FT-IR, ¹H-NMR), chemical reactivity, NBO analyses of 2-(4-fluorophenyl)-2-(4-fluorophenylamino)acetonitrile and its docking into IDO enzyme, G. Brahmachari, A. Kumar, A. K. Srivastava, S. Gangwar, N. Misra, V. K. Gupta, Rajnikant, *RSC Advances* 5 (2015) 80967-80977.
14. An investigation of superhalogen properties of YF_n nano clusters- A quantum chemical study, A. Dwivedi, A. K. Srivastava, A. K. Pandey, *Main Group Chemistry* 14 (2015) 291-299.
15. Vibrational, HOMO-LUMO, MESP, partial charge analyses and reactivity descriptors of Amylamine, Iso-amylamine and Tert-amylamine: A comparative quantum chemical study, A. Dwivedi, A. K. Srivastava, A. Bajpai, *Spectrochimica Acta Part A* 149 (2015) 343-351.
16. Combined experimental (FT-IR, UV-visible spectra, NMR) and theoretical studies on the molecular structure, vibrational spectra, HOMO, LUMO, MESP surfaces, reactivity descriptor and molecular docking of Phomarin, A. Kumar, A. K. Srivastava, S. Gangwar, N. Misra, A. Mondal, G. Brahmachari, *Journal of Molecular Structure* 1096 (2015) 94-101.

List of Publications in Conference Proceedings:

1. DFT Studies on AlSe Nano Clusters, D. V. Shukla, A. Kumar, A. K. Srivastava, N. Misra, *Materials Today: Proceedings* 5 (2018) 9187-9190
2. 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.
3. 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.

Invited Talks/Special Lectures/Recognitions:

1. Evaluator of science projects in 27th State-Level National Children's Science Congress organized by Council of Science & Technology, Uttar Pradesh, India during 04-06 December, 2019.
2. Invited Talk at National Conference on Advances in Materials Science (NCAMS-2019), Department of Physics, Marwar Business School, Gorakhpur on 21-22 February, 2019.
3. Invited Talk at National Conference on Soft Matter (NCSM-2018) organized by Department of Physics, DDU Gorakhpur University, Gorakhpur on 27-28 March, 2018.
4. Organizer, 1st Virtual Conference on Scientific Research and Advances (VCSRA-2018) during 20-25 February, 2018.

Administrative Responsibilities:

1. Member of Website Committee in DDU Gorakhpur University, Gorakhpur from January 2020 to date.
2. Member of Steering Committee for NAAC in DDU Gorakhpur University, Gorakhpur from December 2019 to date.
3. Member of Departmental Research Committee (DRC) of Physics Department at DDU Gorakhpur University, Gorakhpur from July 2018 to date.
4. Member of Departmental Committee of Physics Department at DDU Gorakhpur University, Gorakhpur from July 2018 to date.
5. Internal Quality Assurance Cell (IQAC) Representative of Physics Department in DDU Gorakhpur University, Gorakhpur, India from September 2019 to November 2019
6. Assistant Proctor in DDU Gorakhpur University, Gorakhpur, India from July 2018 to September 2019

Personal Information:

Father, Mother: Mr. D. P. Srivastava, Mrs. S. Srivastava

Date of birth: 04/09/1988

Nationality, Marital Status: Indian, Married

Language known: English, Hindi

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