



Centre/School/Special Centre: Physical Sciences

Department: Chemistry

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Dr. Suryabhan Singh

Assistant Professor

Qualifications

Ph. D. Chemistry (2011): Banaras Hindu University

Supervisor: Prof. Subrato Bhattacharya

Title of Thesis: *Synthesis, structures and properties of thiophene-2-thiocarboxylate and pyridine-2,6-bis(thiocarboxylate) derivatives of some transition and main group metals.*

M. Sc. Chemistry (2007): Banaras Hindu University

B. Sc. (Hons.) Chemistry (2005): Banaras Hindu University

Area of Interest/Specialization: Inorganic Chemistry

- Mono/bi/polynuclear (Metal Organic Framework) complexes of transition and main group metals.
- Development of crystals and investigation of their solid state structure and weak interactions in particular metal-metal and hydrogen bonding.
- To study their catalytic, gas storage (in case of MOFs), electrical and optoelectronic properties.
- Explore the structural chemistry of metal complexes by Density functional theory calculations by Natural bonding orbital calculations at DFT and *ab-initio* level.
- Applications of Time dependent density functional theory (TDDFT) calculations for metal complexes.

Experience

May 2018/Sept 2019 Post-Doctoral Fellow under supervision of **Dr. A. K. Singh**, Department of Chemistry, Indian Institute of Technology Indore, on the topic “**Synthesis characterization and reactivity of transition metal complexes with multiple**

NHC donor ligands”.

- April
2017/April
2018
- Post-Doctoral Fellow under supervision of **Prof. P. Mathur**, Department of Chemistry, Indian Institute of Technology Indore, on the topic “**Designing polynuclear 3d and 4f metal clusters bearing bridging chalcogenides for applications of as single molecule magnets**”.
- Nov.
2013/Nov.
2016
- Dr. D. S. Kothari Post-Doctoral Fellow under supervision of **Prof. S. Natarajan**, SSCU, Indian Institute of Science, Bangalore on the topic “**Development of new metal-organic frameworks (MOFs) for catalytic and gas storage (H₂, CO₂, CH₄) applications**”.
- July
2010/May
2013
- Senior Research Fellow under the supervision of **Prof. S. Bhattacharya**, Department of Chemistry, BHU on the topic “**Synthesis, structures and properties of thiophene-2-thiocarboxylate and pyridine-2,6-bis(thiocarboxylate) derivatives of transition and main group metals**”.
- July
2008/June
2010
- Junior Research Fellow under the supervision of **Prof. S. Bhattacharya**, Department of Chemistry, BHU on the topic “**Synthesis, structures and properties of thiophene-2-thiocarboxylate and pyridine-2,6-bis(thiocarboxylate) derivatives of transition and main group metals**”.
- March
2008/June
2008
- Junior Research Fellow under the supervision of **Prof. S. Bhattacharya**, Department of Chemistry, BHU on the topic “**Studies of synthesis, characterization and reactivity of organobimetallic complexes containing sulfide and disulfide ligands**” (CSIR Project).

Awards and Honors

- Post-Doctoral Fellowship by IIT Indore, India, April, 2017
- Dr. D. S. Kothari Post-Doctoral Fellowship by UGC, India, 2013
- Senior Research Fellowship by CSIR, India, 2010
- Junior Research Fellowship (NET-JRF) by CSIR, India, 2007

Research Projects

S. N.	Name of grant	Funding Agency	Year	Amount (Rs)	Duration
1.	UGC – Startup Grant	UGC, New Delhi	June 2020	10,00000/-	Two years

International Collaboration/Consultancy: No

List of Publications (All)

1. Co-operative influence of co-crystallized solvent in sustaining supramolecular architectures of Zn(II)/Cd(II) homoleptic pyridyl functionalized dithiocarbamates complexes via non-covalent interactions. V. Kumar and **Suryabhan Singh**, *J. Sulfur Chem.*, **43**, 252-263, 2022.
2. Cationic ruthenium(II)-NHC pincer complexes with hemilabile COD: Solid-state structural characterization and theoretical study of an η^2 -(E,Z)-COD ligand. D. Yadav, R. K. Singh, **Suryabhan Singh**, P. M. Shirage, A. K. Singh, *J. Organomet. Chem.* 953, 122061, 2021.
3. Synthesis, Crystal Structure, and Properties of Heteroleptic Cu(I) dithiocarbamate complex containing diphenyl phosphiniferrocene (dppf). V. Kumar and **Suryabhan Singh**, *J. Str. Chem.*, 62, 1723-1731, 2021.
4. Cationic ruthenium(II)-NHC pincer complexes: Synthesis, characterisation and catalytic activity for transfer hydrogenation of ketones. D. Yadav, S. Misra, D. Kumar, **Suryabhan Singh**, A. K. Singh, *Appl. Organomet. Chem.*, 35, e6287, 2021.
5. Ferrocene decorated unusual mercury(II) dithiocarbamate coordination polymers: crystallographic and computational studies. A. Singh, A. Singh, **Suryabhan Singh**, G. Kociok-Köhn, M. Muddassir and A. Kumar, *CrystEngComm*, **23**, 2414–2423, 2021.
6. Evolution of metal-thiocarboxylate chemistry in 21st century. **Suryabhan Singh**, *J. Mol. Str.*, **1234**, 130184, 2021.
7. New main-group ferrocenyldithiocarbamates and conversion to ferrocene oxazolidine-2-thione and -2-one. R. Yadav, **Suryabhan Singh**, M. Trivedi, G. Kociok-Köhn, N. P. Rath, R. D. Köhn, M. M Muddassir and A. Kumar, *New J. Chem.*, **44**, 3268-3277, 2020.
8. Silver-Nitrilotriacetate Coordination Polymers: Supra-molecular and Photoluminescence Properties. **Suryabhan Singh**, *Inorg. Chim. Acta*, **495**, 118939, 2019.

9. Coordination Behaviour of 2-(Methylthio)Pyrazine with Ag(I) in the presence of Different Counter Anions and Emission Properties. **Suryabhan Singh, A. Raghuvanshi, P. Mathur and A. K. Singh**, *Polyhedron*, 169, 8-13, **2019**.
10. Cu(I)/Ag(I)-3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine-p,p'-disulfonate Based Coordination Polymers: Synthesis, Structures and Photoluminescent Properties. **Suryabhan Singh**, *ChemistrySelect*, 3, 6786-6790, **2018**.
11. Supramolecular architecture of organotin(IV) N-methyl ferrocenyl N-ethanol dithiocarbamates: crystallographic and computational studies. A. Kumar, A. Singh, R. Yadav, **Suryabhan Singh**, G. Kociok-Köhn and M. Trivedi, *Inorg. Chim. Acta*, 471, 234-243 **2018**.
12. Water linked 3D Coordination Polymers: Syntheses, Structures and Applications. **Suryabhan Singh*** and Anupam Bhim, *J. Solid State Chem.*, 244, 151-159, **2016**.
13. Hydrogen Energy Future with Formic Acid: A Renewable Chemical Hydrogen Storage System. A. K. Singh, **Suryabhan Singh*** and A. Kumar, *Catal. Sci. Technol.*, 6, 12-40, **2016**.
14. Structural diversities in Cu(I) and Ag(I) sulfonate coordination polymers and their anion exchange properties. **Suryabhan Singh*** and R. Karthik, *CrystEngComm*, 17, 7363-7371, **2015**.
15. Synthesis, Crystal Structure and Spectroscopic and Electrochemical Properties of Bridged Trisbenzoato Copper-Zinc Heterobinuclear Complex of 2, 2'-Bipyridin. A. Koch, A. Kumar, **Suryabhan Singh**, R. Borthakur, D. Basumatary and R. A. Lal, *J. Mol. Structure*, 1083, 381-388, **2015**.
16. Phenylmercury(II) methylferrocenyldithiocarbamate functionalized dye-sensitized solar cells with hydroxyl as an anchoring group. R. Chauhan, G. K.-Köhn, M. Trivedi, **Suryabhan Singh**, A. Kumar and D. P. Amalanerkar, *J. Solid State Electrochem.*, 19, 739-747, **2015**.
17. Studies of structural diversity due to inter-/intra-molecular hydrogen bonding and photoluminescent properties in thiocarboxylate Cu(I) and Ag(I) complexes. **Suryabhan Singh*** and S. Bhattacharya, *RSC Advances*, 4, 49491-49500, **2014**.
18. New ternary compounds containing Zn-Cu and Zn-Ag from single molecular source precursors. **Suryabhan Singh**, J. Chaturvedi and S. Bhattacharya, *RSC Advances*, 4, 11469-11474, **2014**.

19. A Cu(II) mediated new desulfurization pathway involving elimination of ethylene sulfide. N. Sareen, **Suryabhan Singh** and S. Bhattacharya, *Dalton Trans.*, 43, 4635-4638, **2014**.
20. ROS and RNS induced apoptosis through p53 and iNOS mediated pathway by a dibasic hydroxamic acid molecule in leukemia cells. K. Banerjee, A. Ganguly, P. Chakraborty, A. Sarkar, **Suryabhan Singh**, M. Chatterjee, S. Bhattacharya and S. K. Choudhuri, *Eur. J. Phar. Sci.*, 52, 146-164, **2014**.
21. Syntheses and structural studies of heterobimetallic thiocarboxylate complexes containing zinc and silver. **Suryabhan Singh**, J. Chaturvedi, and S. Bhattacharya, *Inorg. Chim. Acta*, 407, 31-36, **2013**.
22. Syntheses and structural studies of heterobimetallic thiocarboxylate complexes containing zinc and copper. **Suryabhan Singh**, J. Chaturvedi, A. S. Aditya, N. R. Reddy and S. Bhattacharya, *Inorg. Chim. Acta*, 396, 6-9, **2013**.
23. Studies of titanocene and zirconocene pyridine-2,6-bis-thiocarboxylates exhibiting partial desulfurization. **Suryabhan Singh** and S. Bhattacharya, *Inorg. Chim. Acta*, 395, 230-236, **2013**.
24. Supramolecular organotin(IV) framework derived from pyridine-2,6-bis(thiocarboxylate) ligand. **Suryabhan Singh** and S. Bhattacharya, *Inorg. Chem. Comm.*, 24, 144-147, **2012**.
25. Solvent dependent crystallization of a few Hg(II) thiocarboxylates. **Suryabhan Singh**, J. Chaturvedi and S. Bhattacharya, *Inorg. Chim. Acta*, 385, 112-118, **2012**.
26. Studies of synthesis, structural features of Cu(I) thiophene-2-thiocarboxylates and unprecedented desulfurization of Cu(II) thiocarboxylate complexes. **Suryabhan Singh**, J. Chaturvedi and S. Bhattacharya, *Dalton Trans.*, 41, 424-431, **2012**.
27. The Chemistry of Cadmium-Thiocarboxylate Derivatives: Synthesis, Structural Features, and Application as Single Source Precursors for Ternary Sulfides. **Suryabhan Singh**, J. Chaturvedi, S. Bhattacharya and H. Nöth, *Inorg. Chem.*, 50, 10056-10069, **2011**.
28. Synthesis of triphenyltin(IV) hydrosulfide. **Suryabhan Singh** and S. Bhattacharya, *Inorg. Chim. Acta*, 367, 230-232, **2011**.
29. Silver(I) catalyzed oxidation of thiocarboxylic acids into the corresponding disulfides and synthesis of some new Ag(I) complexes of thiophene-2- thiocarboxylate. **Suryabhan Singh**, J. Chaturvedi, S. Bhattacharya and H. Nöth, *Polyhedron*, 30, 93-97, **2011**.

30. N-(Prop-2-yn-1-yl)-1,3-benzothiazol-2-amine. A. Agarwal, M. K. Singh, **Suryabhan Singh**, S. Bhattacharya and S. K. Awasthi, *Acta Cryst.*, E67, 2637-2638, **2011**.
31. Synthesis and Structural Studies of Organotin(IV) and Organolead(IV) Thiophene-2-thiocarboxylate. **Suryabhan Singh**, S. Bhattacharya and Heinrich Nöth, *Eur. J. Inorg. Chem.*, 5691-5699, **2010**.

Recent Books/Book Chapters/Monographs etc

1. Nanomaterials via Single-Source Precursors, Synthesis, Processing and Applications: Single Source Precursors for Main Group Metal Sulfides and Solar Cell Applications. **Suryabhan Singh**, A. K. Singh and A. Kumar, Elsevier, **2022**.

Research Supervision: Nil

Administrative Responsibilities

- Polling Officer, the Students' Council Election – 2019.
- Member of University Wall Calendar, Table Calendar and Diary Committee 2019-2020.
- Coordinator of Badminton Male in University Interschool Sports Meet-2019-2020.
- Mentor of B.Sc. I Sem.- 2021-22
- Member of UG and PG Admission Committee of the department.
- Member, Various Departmental Committees.
- Member, Organizing conferences/seminars/workshops, GGV.

Additional Information

Total number of Publications: **31** (international), H index: **10**, Conference/Symposium/Workshop: **25**, Reviewer for many international journals such as Dalton Trans., Polyhedron, J. Mol. Str., ChemSelect, ACS Omega *etc.*