

Dr Mukesh Kumar Singh

Mukesh Kumar Singh (MRSC)

Email address: mklsingh36@gmail.com

msingh2@ed.ac.uk

Webpage: Dr Mukesh Kumar Singh MRSC

ORCID: (0000-0003-4865-0283)

Dr Mukesh Kumar Singh - Google Scholar

RESEARCH INTERESTS

Over the last eleven years, my combined computational and experimental research has focused on

- Understanding and predicting new magnetic materials which have potential applications in miniaturised information storage, quantum encryption, magnetic refrigeration, magnetic resonance imaging, qubits in quantum computation, and molecular spintronics.
 - Recycling of metals from electronic and industrial waste.
 - Synthesising mono and polymetallic actinide complexes for small molecule activation.
 - Understanding structural, bonding, energetic and reactivity for silylene molecules.
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KEY RESEARCH SKILLS

- **Experimental:** Expert level of training in Schlenk techniques, glove box (dry and wet), single crystal and powder X-ray diffraction (XRD), ICP-OES/MS, NMR, FTIR, multistep-organic ligand synthesis, and SQUID magnetometry (VSM and MPMS).
 - **Computational:** Expert level of training in Gaussian 09/16, ORCA, MOLCAS and CP2K software.
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EDUCATION

2013 – 2019: PhD in Chemistry from the *Department of Chemistry, Indian Institute of Technology Bombay, India*, Supervisor Prof. G. Rajaraman.

2010 – 2012: Master of Science (M.Sc.) from the University of Hyderabad, Gachibowli, Hyderabad, India Chemistry, First division (75%).

2007 – 2010: Bachelor of Science (B.Sc.) from Banaras Hindu University, Varanasi, Uttar Pradesh, India Chemistry (Hons.), Botany and Zoology, First division (75%).

RESEARCH EXPERIENCE

Dec 2022 – To date

School of Chemistry, University of Edinburgh, UK

Postdoctoral Fellow with Prof. Jason Love, working on ligand design, lanthanide/actinide chemistry, recycling of metals from electronic waste.

- I have published one paper on the efficient recycling of gold and copper from electronic waste using recyclable precipitants and am involved in two projects with industrial collaborators, targeting the selective separation of pure gold from gold alloys and gold-containing minerals.
- I have been designing and creating new polydentate ligand-based mono and polymetallic transition metals, lanthanide metals and actinide metals complexes using Schlenk and glove box techniques to explore the magnetic and catalytic activities.
- I am designing a series of ligands to recover rare-earth metals from electronic waste.
- I am employing a diversity of characterisation techniques, including NMR spectroscopy, mass spectrometry, X-ray diffraction (both powder and single crystal), SQUID magnetometry, ICP-OES/MS and associated analyses.
- I have been conducting DFT and *ab initio* studies on fascinating molecules synthesised by my colleagues and national and international collaborators to investigate their structures, reactivity and magnetic properties.

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April 2020 – April 2022

School of Chemistry, University of Edinburgh, UK

Marie Skłodowska-Curie Actions (MSCA) Individual Postdoctoral Fellow with Prof. Euan Brechin, conducted combined experimental and computational studies on molecular magnets: coordination cages, frameworks, and multifunctional materials.

- I created new organic ligands through a multistep process and used them to produce coordination cages and frameworks suitable for hosting guests. These were made in both atmospheric and inert environments using Schlenk techniques.
- I used various techniques, including NMR, Mass Spectrometry, X-ray diffraction (powder and single crystal), SQUID magnetometry, and other associated analyses to characterise the molecules. I was also responsible for running single crystals of the group members on single-crystal X-ray diffractometers (XCalibur and Supernova).
- I conducted DFT and *ab initio* studies on various molecules synthesised by colleagues and collaborators from different countries, estimating spin-Hamiltonian parameters and magnetic phenomena.
- This two-year position resulted in eleven peer-reviewed papers, with me being the corresponding author of three of these papers.

March 2019 – April 2020

Department of Chemistry, Texas A&M University, USA

Postdoctoral Research Associate with Prof. Kim Dunbar, conducted computational studies on 3d/4f/3d-4f metal and metal-radical complexes.

- I conducted extensive DFT and *ab initio* studies on 3d/4f molecular magnets, synthesised by a combination of colleagues and collaborators from national and international arenas. These studies aimed to estimate spin-Hamiltonian parameters and related magnetic phenomena.
- I authored three peer-reviewed papers. I utilised various characterisation techniques such as NMR, Mass Spectrometry, and single-crystal X-ray diffraction.

Nov 2018 – March 2019

Department of Chemistry, Indian Institute of Technology Bombay, India

Research Associate with Prof. G. Rajaraman, conducted theoretical studies on molecular nanomagnets, particularly emphasising the magnetic properties of paramagnetic lanthanide, transition metals complexes and endohedral fullerenes (EMFs).

May 2012 – Dec 2012

Department of Chemistry, Indian Institute of Technology Bombay, India

Research Associate with Prof. G. Rajaraman, carried out theoretical studies on 3rd-row transition metal nanomagnets.

Aug 2012 – April 2012

School of Chemistry, University of Hyderabad, India

M.Sc. Project with Prof. Samudranil Pal, University of Hyderabad, titled "Pd(II) Complexes with Aroyl hydrazones of Aromatic Aldehydes and Ketones: Synthesis, Characterisation and Reactivity".

May 2011 – July 2011

Department of Chemistry, Indian Institute of Technology Bombay, India

Indian Academy of Science (IAS) fellow with Prof. G. Rajaraman, carried out theoretical studies on the magnetic properties of Fe^{III}-Ni^{II} dimetallic complexes.

PUBLICATIONS AND INDUSTRIAL COLLABORATIONS

I have published thirty-four international peer-reviewed papers (Dalton Trans. (9), Chem. Comm. (8), Inorg. Chem. (6), Chem. Eur. J. (4), Chem. Sci. (2), Angew. Chem. Int. Ed. (2), Sci. Adv. (1), Chem. Inorg. Front. (1), RSc Adv. (1)) together **with one review** in Coord. Chem. Rev. and a book chapter. These are cited ca. 900 times leading to an h-index of 17 and i10-index of 22. **I have been one of the corresponding authors in five published articles, with one single-author paper.** In most of my published papers, I have been the sole computational chemist who has undertaken all the calculations. I am also involved in two projects with industrial collaborators, targeting the selective separation of pure gold from gold alloys and gold-containing minerals.

Note: * represents the corresponding authorship for the applicant.

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1. "Synthesis, Reactivity, and Complexation with Fe(0) of a Tight-bite Bis(N-heterocyclic silylene)"
Z. Hendi, M. K. Pandey, K. Rachuy, **M. K. Singh**, R. Herbst-Irmer, D. Stalke and H. W. Roesky, *Chem. Eur. J.*, 2024, just accepted. (doi.org/10.1002/chem.202400389)
2. "Stabilisation of NH- Group Adjacent to Naked Silicon(II) Atom in Base Stabilized Aminosilylenes"
M. K. Pandey, Z. Hendi, X. Wang, A. Bhandari, **M. K. Singh***, K. Rachuy, S. K. Kushvaha, R. Herbst-Irmer, D. Stalke and H. W. Roesky, *Angew. Chem, Int. Ed.*, 2024, e202317416. (doi.org/10.1002/ange.202317416)
3. "Magnetic Exchange, Anisotropy and Excitonic Fluctuations in a [Ni^{II}₁₇] Anderson Wheel"
D. J. Cutler, A. J. Canaj, **M. K. Singh**, G. S. Nichol, S. Piligkos, M. Evangelisti, J. Schnack and E. K. Brechin, *Inorg. Chem. Front.*, 2024, **11**, 515-525. (doi.org/10.1039/D3QI02307A)
4. "Efficient Recycling of Gold and Copper from Electronic Waste by Selective Precipitation"
A. Nag, **M. K. Singh**, C. A. Morrison and J. B. Love, *Angew. Chem. Int. Ed.*, 2023, **62**, e202308356. (doi.org/10.1002/anie.202308356)
5. "Odd and Even Numbered Ferric Wheels"
D. J. Cutler, A. B. Canaj, **M. K. Singh**, G. S. Nichol, D. Gracia, H. Nojiri, M. Evangelisti, J. Schnack and E. K. Brechin, *Sci. Adv.*, 2023, **10**, 2304553. (doi.org/10.1002/adv.202304553)
6. "A Bis-calix[4]arene Supported [Cu^{II}₁₆] Cage"
L. R. B. Wilson, M. Coletta, **M. K. Singh**, S. J. Teat, A. Brookfield, M. Shanmugam, E. J. McInnes, S. Piligkos, S. J. Dalgarno and E. K. Brechin, *Dalton Trans.*, 2023, **52**, 8956-8963. (doi.org/10.1039/D3DT01448G)
7. "A Ferromagnetically Coupled Pseudo-calixarene [Co₁₆] Wheel That Self-assembles as a Tubular Network of Capsules"
P. A. Tsami, T. G. Tziotzi, A. B. Canaj, **M. K. Singh**, S. J. Dalgarno, E. K. Brechin and C. J. Milios, *Dalton Trans.*, 2022, **51**, 15128-15132. (doi.org/10.1039/D2DT02554J)
8. "A Graceful Break-up: Serendipitous Self-assembly of a Ferromagnetically Coupled [Ni^{II}₁₄] Wheel"
E. Agapaki, **M. K. Singh**, A. B. Canaj, G. S. Nichol, J. Schnack and E. K. Brechin, *Chem. Commun.* 2022, **58**, 9088-9091. (doi.org/10.1039/D2CC03445J)
9. "An [Fe^{III}₈] Molecular Oxyhydroxide"
D. J. Cutler, M. Coletta, **M. K. Singh**, A. B. Canaj, L. J. McCormick, S. J. Coles, J. Schnack and E. K. Brechin, *Dalton Trans.* 2022, **51**, 8945-8948. (doi.org/10.1039/D2DT01477G)
10. "Guest-induced Magnetic Exchange in Paramagnetic [M₂L₄]⁴⁺ Coordination Cages"
M. K. Singh*, A. E. Berrios, J. Vallejo, S. Sanz, J. M. Lilio, G. S. Nichol, P. S. Lusby and E. K. Brechin, *Dalton Trans.* 2022, **51**, 8377-8381. (doi.org/10.1039/D2DT01385A)
11. "In Silico Design to Enhance the Barrier Height for Magnetization Reversal in Dy(III) Sandwich Complexes by Stitching Them Under the Umbrella of Corannulene"
M. K. Singh,[‡] T. Sharma,[‡] R. Gupta, M. Khatua and G. Rajaraman, *Chem. Sci.*, 2021, **12**, 11506-11514. (doi.org/10.1039/D1SC03160K)
12. "A Dicobalt(II) Single-Molecule Magnet Via a Well-Designed Dual-Capping Tetrazine Radical Ligand"
B. Yao, **M. K. Singh**, Y. F. Deng and Y. Z. Zhang, *Inorg. Chem.*, 2021, **60**, 18698-18705. (doi.org/10.1021/acs.inorgchem.1c02094)
13. "[Fe₁₅]: A Frustrated, Centred Tetrakis Hexahedron"
D. J. Cutler, **M. K. Singh**, G. S. Nichol, M. Evangelisti, J. Schnack, L. Cronin and E. K. Brechin, *Chem. Commun.*, 2021, **57**, 8925-8928. (doi.org/10.1039/D1CC03919A)
14. "The Structural Manipulation of a Series of Ni₄ Defective Dicubanes: Synthesis, X-ray Structures, Magnetic and Computational Analyses"

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S. S. Woodhouse, T. N. Dais, E. H. Payne, **M. K. Singh**, E. K. Brechin and P. G. Pliege, *Dalton Trans.*, 2021, **50**, 5318-5326. (doi.org/10.1039/D0DT04286B)

15. "A [Mn¹⁸] Wheel-of-Wheels"

M. Coletta, T. G. Tziotzi, M. Gray, G. S. Nichol, **M. K. Singh**,* C. J. Milios* and E. K. Brechin*, *Chem. Commun.*, 2021, **57**, 4122-4125. (doi.org/10.1039/D1CC00185J)

16. "Trigonal Prismatic Cobalt(II) Single-Ion Magnets: Manipulating the Magnetic Relaxation Through Symmetry Control"

B. Yao, **M. K. Singh**, Y. F. Deng, Y. N. Wang, K. R. Dunbar and Y. Z. Zhang, *Inorg. Chem.*, 2020, **59**, 8505-8513. (doi.org/10.1021/acs.inorgchem.0c00950)

17. "Probing the Axial Distortion Effect on the Magnetic Anisotropy of Octahedral Co(II) Complexes"

Y. F. Deng, **M. K. Singh**, D. Gan, T. Xiao, Y. N. Wang, S. Liu, Z. Wang, Z. Ouyang, Y. Z. Zhang and K. R. Dunbar, *Inorg. Chem.*, 2020, **59**, 7622-7630. (doi.org/10.1021/acs.inorgchem.0c00531)

18. "Geometrical Control of the Magnetic Anisotropy in Six Coordinating Cobalt Complexes "

M. R. Saber, **M. K. Singh** and K. R. Dunbar, *Chem. Commun.*, 2020, **56**, 8492-8495. (doi.org/10.1039/D0CC03238G)

19. "Magneto-Structural Studies of an Unusual [Mn(III)Mn(II)Gd(III)(OR)₄]₄- Partial Cubane from 2, 2'-bis-p-tBu-calix [4] arene"

M. Coletta, S. Sanz, D. J. Cutler, S. J. Teat, K. J. Gagnon, **M. K. Singh***, E. K. Brechin* and S. J. Dalgarno*, *Dalton. Trans.*, 2020, **49**, 14790-14797. (doi.org/10.1039/D0DT02731F)

20. "Probing the Strong Magnetic Exchange Behaviour of Transition Metal-Radical Complexes: A DFT Case Study"

M. K. Singh*, *Dalton. Trans.*, 2020, **49**, 4539-4548. (doi.org/10.1039/D0DT00262C)

21. "A Design Criteria to Achieve a Giant Ising-Type Anisotropy in Co^{II}-Encapsulated Metallo-Fullerenes"

M. K. Singh, P. Shukla, M. Khatua and G. Rajaraman, *Chem. Eur. J.*, 2020, **26**, 464-477. (doi.org/10.1002/chem.201903618)

22. "Boosting axiality in stable high-coordinate Dy(III) single-molecule magnets"

A. B. Canaj, **M. K. Singh**, E. R. Marti, M. Damjanovic, C. Wilson, O. Cespedes, W. Wolfgang, G. Rajaraman and M. Murrie, *Chem. Commun.*, 2019, **55**, 5950. (doi.org/10.1039/C9CC00965E)

23. "Mechanism of magnetisation relaxation in {M^{III}₂Dy^{III}₂} (M = Cr, Mn, Fe, Al) "Butterfly" Complexes: How Important are the Transition Metal Ions here?"

Y. Peng, **M. K. Singh**, V. Mereacre, C. E. Anson, G. Rajaraman, A. K. Powell, *Chem. Sci.*, 2019, **10**, 5528. (doi.org/10.1039/C8SC05362F)

24. "Theoretical Studies on Hexametallc [M₃(μ₃-O/OH)]₂ (M = Fe(III), Mn(III) And Ni(II)) Clusters: Magnetic Exchange, Magnetic Anisotropy, and Magneto-Structural Correlations"

M. K. Singh and G. Rajaraman, *Inorg. Chem.*, 2019, **58**, 3175. (doi.org/10.1021/acs.inorgchem.8b03257)

25. "Experimental and theoretical exploration of magnetic exchange interactions and single molecule magnetic behaviour of bis(η¹:η²-μ₂-carboxylate) Gd^{III}₂/Dy^{III}₂ systems"

S. Ghosh, S. Mandal, **M. K. Singh**, C.-M. Liu, G. Rajaraman and S. Mohanta, *Dalton Trans.*, 2018, **47**, 11455. (doi.org/10.1039/C8DT02008F)

26. "Chemical and in silico tuning of the magnetisation reversal barrier in pentagonal bipyramidal Dy(III) single-ion magnets"

A. B. Canaj, **M. K. Singh**, C. Wilson, G. Rajaraman and M. Murrie, *Chem. Commun.*, 2018, **54**, 8273. (doi.org/10.1039/C8CC03929A)

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27. "Role of (1,3) {Cu-Cu} Interaction on the Magneto-Caloric Effect of Trimetallic {Cu^{II}-Gd^{III}-Cu^{II}} Complexes: Combined DFT and Experimental Studies"
M. K. Singh, T. Rajeshkumar, R. Kumar, S. K. Singh and G. Rajaraman, *Inorg. Chem.*, 2018, **57**, 1846. (doi.org/10.1021/acs.inorgchem.7b02775)
28. "Low-Coordinate Monometallic Lanthanide Complexes as Molecule-Based Magnets"
A. K. Bar, P. Kalita, **M. K. Singh**, G. Rajaraman and V. Chandrasekhar, *Coord. Chem. Rev.*, 2018, **367**, 163. (doi.org/10.1016/j.ccr.2018.03.022)
29. "Role of *Ab initio* Calculations in the Design and Development of Lanthanide Based Single Molecule Magnets" Book Chapter in "Organometallic Magnets" Springer Publishing Company.
T. Gupta, **M. K. Singh** and G. Rajaraman, 2018. ([Weblink](#))
30. "Acquiring a Record Barrier Height for Magnetization Reversal in Lanthanide Encapsulated Fullerene Molecules Using DFT and *Ab Initio* Calculations"
M. K. Singh and G. Rajaraman, *Chem. Commun.*, 2016, **52**, 14047. (doi.org/10.1039/C6CC08232G)
31. "Record High Magnetic Exchange and Magnetization Blockade in Ln₂@C₇₉N (Ln= Gd^{III} and Dy^{III}) Molecules: A Theoretical Perspective"
M. K. Singh, N. Yadav and G. Rajaraman, *Chem. Commun.*, 2015, **51**, 17732. (doi.org/10.1039/C5CC06642E)
32. "Can CH... π Interactions be Used to Design Single-Chain Magnets?"
M. K. Singh and G. Rajaraman, *Chem. Eur. J.*, 2015, **21**, 980. (doi.org/10.1002/chem.201404853)
33. "Inducing Magnetic Communication in Caged Dimetallic Co^{II} Systems"
J. Caballero-Jiménez, F. Habib, D. Ramírez-Rosales, R. Grande-Aztatzi, G. Merino, I. Korobkov, **M. K. Singh**, G. Rajaraman, Y. Reyes-Ortega and M. Murugesu, *Dalton Trans.*, 2015, **44**, 8649. (doi.org/10.1039/C5DT00497G)
34. "Hydroxo-Bridged Dimers of Oxo-Centered Ru^{III} Triangle: Synthesis and Spectroscopic and Theoretical Investigations"
A. Upadhyay, J. Rajpurohit, **M. K. Singh**, R. Dubey, A. Kumar Srivastava, A. Kumar, G. Rajaraman and M. Shanmugam, *Chem. Eur. J.*, 2014, **20**, 6061. (doi.org/10.1002/chem.201304826)
35. "High Metallicity Ni^{II} Cages from Hydroxamate Ligands"
C. McDonald, S. Sanz, E. K. Brechin, **M. K. Singh**, G. Rajaraman, D. Gaynor and L. F. Jones, *RSC Adv.*, 2014, **4**, 38182. (doi.org/10.1039/C4RA06064D)
36. "Syntheses, Structures, Magnetic Properties, and Density Functional Theory Magneto-Structural Correlations of Bis(μ-phenoxo) and Bis(μ-phenoxo)-μ-acetate/Bis(μ-phenoxo)-bis(μ-acetate) Dimetallic Fe^{III}Ni^{II} Compounds"
S. Hazra, S. Bhattacharya, **M. K. Singh**, L. Carrella, E. Rentschler, T. Weyhermueller, G. Rajaraman and S. Mohanta, *Inorg. Chem.*, 2013, **52**, 12881. (doi.org/10.1021/ic400345w)

Preprint and Submitted

37. "Synthesis and Characterization of Triazole-fused Rare Mixed Valent Si(I)-Si(III) and Ge(I)-Ge(III) Compound Stabilized by Amidinates"
M. K. Pandey, Z. Hendi, **M. K. Singh***, S. K. Kushvaha, X. Wang, A. Kumar, R. H. Irmer, D. Stalke and H. W. Roesky, (preprint ready).
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AWARDS, GRANTS, MEMBERSHIPS AND SCHOLARSHIPS

- Member of Royal Society of Chemistry (MRSC) **2021**.
 - Award of a Marie Skłodowska-Curie Actions Individual Fellowship (MSCA-IF) **2018**.
 - Best poster award in "The eighth edition of Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 8)-**2017**, Mumbai, India."
 - Best poster award in "The 15th International Conference on Molecule-Based Magnets (ICMM)-**2016**, Sendai, Japan."
 - Travel grant award from IIT Bombay to attend "The 15th International Conference on Molecule-Based Magnets (ICMM)-**2016**, Sendai, Japan".
 - Junior Research Fellowship (JRF) awarded by the University Grant Commission (UGC), New Delhi, India. Jan **2013**.
 - Senior Research Fellowship (SRF) awarded by the University Grant Commission (UGC), New Delhi, India. Jan **2015**.
 - Qualified for UGC-JRF twice (87 and 84, All India Rank) in JOINT CSIR-UGC NET Exam in Chemical Sciences, held on **Dec. 2011** and **June 2012**, respectively. The total number of applicants was ~200,000.
 - Qualified twice in all India-level GATE exams for Chemical Sciences (**2011 and 2012**). The total number of applicants was ~2,00,000.
 - Received Indian Academy of Sciences (IAS)-**2011** Fellowship. The total number of applicants were ~10,000.
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OUTREACH ACTIVITIES

- March 2023 – till date: As a **member of the Postdoc Committee** at the School of Chemistry, University of Edinburgh, I have taken the initiative to improve the overall experience of early-career researchers within the school. My efforts have been focused on organising a range of activities, including research seminars, social events, and career-focused talks, to support my peers' future career prospects. One notable event that I have organised is the "**IUPAC Global Women Breakfast 2024**" webinar. This event was designed to bring together women researchers from our school to discuss the latest advancements and trends in chemistry. By creating a platform for these researchers to connect and learn from one another, I hope to have contributed to increasing the visibility and representation of women in chemistry.
 - Feb 2023 – till date: During my current PDRA tenure at the School of Chemistry, University of Edinburgh, I offered my services by providing technical support to Mr. Stewart Franklin, the lab technical officer. I volunteered to cover the lab for 2-3 hours every week on Friday for nine weeks each semester. This coverage was primarily during lunch breaks and one hour before the lab's closure, providing Stewart with sufficient time to accomplish other tasks before the weekend closure. My assistance was unpaid, as my primary objective was to support the school and its employees.
 - October 2019: I participated in the "Chemistry Open House and Science Exploration" at Texas A&M University. The event attracted thousands of visitors, including school children and their parents.
 - During my PhD, I served as a member of the core organising committee for three conferences –
 - (i) APCTCC8-2018
 - (ii) MTMM-2016
 - (iii) STCC-FC-2013My responsibilities included searching for various industrial sponsors and ensuring the smooth day-to-day functioning of the conferences. This involved taking care of logistics for attendees' travel and food and scheduling talks. These conferences had a participation range between 300 to 1200 attendees.
 - Additionally, I volunteered to provide hands-on training on *ab initio* CASSCF + RASSI-SO + SINGLE_ANISO + POLY_ANISO calculations using MOLCAS at one workshop called WESCC-2016.
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WRITING PROPOSALS AND FELLOWSHIPS

I was involved in several successful proposals and fellowship write-up/submission processes throughout my research tenure. This suggests my ability to attract my research funding. Some of those are:

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- I have applied as a principal investigator for the EPSRC Quantum Technologies Career Acceleration Fellowship at King's College London and await the results. This fellowship is for five years and has a total support value of £1,859,263.52.
 - I have applied as a principal investigator for the Royal Society University Research Fellowship at University of Sussex and await the results. This fellowship is for five years and has a total support value of £1,372,633.00.
 - Marie Skłodowska-Curie Actions (MSCA) Individual Postdoctoral Fellowship (April 2020 till April 2022) as a lead applicant for two years and total support value £212,933.76.
 - During my Masters, I secured an Indian Academic of Science (IAS) Fellowship (2011), which supported me for two months of research activity at the Indian Institute of Technology Bombay, India.
 - I have also been involved in several successful proposal write-up/submission processes for the groups I have worked with. These include UKIERI-DST (with Prof Gopalan Rajaraman and Prof Euan Brechin; Molecular Magnetic Materials for Qubit Applications: Experiment and Theory) and NSF Project (with Prof Mario Wriedt and Prof Kim Dunbar; Investigation of Metal-Organic Frameworks as Platforms for the Controlled Nanostructuring of Molecular Magnets).
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INVITED TALKS, CONFERENCES, MEETINGS AND POSTER PRESENTATIONS

I have disseminated my research results in ten conferences and two workshops where I have given oral presentations, invited talks, and poster presentations. In these conferences, attendees were from academic and industrial backgrounds.

- **Invited Talk:** Department of Chemistry, University of Sussex, 17th Aug 2024.
 - **Invited Talk:** Postdoc seminar, School of Chemistry, University of Edinburgh, 27th May 2024.
 - **Invited Talk:** Physical Chemistry seminar, School of Chemistry, University of Edinburgh, 22nd October 2021.
 - Workshop on "**Problems, Errors and Pitfalls in Single Crystal Structure Analysis**" 5th -8th August 2019, Clarkson University, Potsdam, New York, USA.
 - "**New Frontiers in Chemical Science (NFCS)**" 13th -14th December 2018, Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra, India.
 - "**Asia Pacific Conference on Theoretical and Computational Chemistry (APCTCC8)**" 15th -17th December 2017, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra, India.
 - "**In-house symposium**" 4th March 2017, VMCC Auditorium, Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra, India.
 - "**The 15th International Conference on Molecule-Based Magnets (ICMM)**" Sept. 4th -8th 2016, Sendai, Japan"
 - "**19th CRSI National Symposium in Chemistry (CRSI NSC-19)**", 14th -16th July 2016, Department of Chemistry, University of North Bengal, Darjeeling, West Bengal.
 - "**Modern Trends in Molecular Magnets (MTMM)**" 19th -21st May 2016, Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra, India.
 - "**Workshop on Electronic Structure of Coordination Complexes**" 16th -18th May 2016, Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra, India.
 - "**Theoretical Chemistry Symposium 2014 (TCS-2014)**", NCL Pune, India, 18th-21st December 2014.
 - "**8th RSC-CRSI, 16th CRSI Symposium in Chemistry**", Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, India, 6th -9th February 2014.
 - "**Symposium on Theoretical and Computational Chemistry – Frontiers and Challenges (STCC-FC)**", School of Chemistry, Bharathidasan University, Tiruchirappali, India, 14th-15th June 2013.
 - "**The 3rd Indo-German Conference on Modelling Biological and Chemical (Re)activity**", NIPER & IISER Mohali, India, 26th February-1st March 2013.
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PROFESSIONAL MEMBERSHIP

- Guest Editor for *Frontiers in Chemistry* (IF 5.221)
- Reviewed publications for *Inorganic Chemistry* and *RSC advances*.
- Member of the Postdoc Committee, School of Chemistry, University of Edinburgh (from 2022)
- Member of the Royal Society of Chemistry (from 2021)

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- Fellow of the Indian Academy of Science (from 2011)
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COLLABORATORS

- **Industrial collaborations for efficient recycling of gold from electronic and industrial waste.** In the past year, I have expanded my research into different, more industrially applied areas and have learned additional techniques such as ICP-OES/MS. I successfully used new organic precipitants to precipitate gold complexes from solutions derived from red gold or gold-containing ores, achieving a purity level of 99.99%.

Academic Collaborators

- **India:** Prof. Gopalan Rajaraman, Prof. Maheswaran Shanmugam, Prof. Ashutosh Kumar (*IIT Bombay*), Prof. Vadapalli Chandrasekhar (*IIT Kanpur and TIFR Hyderabad*), Prof. Sasankasekhar Mohanta (*University of Calcutta*), Dr. Saurabh Kumar Singh (*IIT Hyderabad*), Dr. Tulika Gupta (*BHU*), Dr. Neeladri Das (*IIT Patna*).
 - **United Kingdom:** Prof. Euan Brechin, Prof. Paul Lusby, Prof. Jason Love, Dr Jennifer Garden (*University of Edinburgh*), Prof. Mark Murrie, Prof. Leroy Cronin (*University of Glasgow*), Prof. Scott Dalgarno (*Heriot-Watt University*)
 - **Germany:** Prof. Annie Powell, Prof. Wolfgang Wernsdorfer (*Karlsruhe Institute of Technology*), Prof. Thomas Weyhermüller (*Max Planck Institute for Chemical Energy Conversion*), Prof. Eva Rentschler (*Institute of Inorganic Chemistry and Analytical Chemistry*), Dr. Sergio Sanz Calvo (*Peter Grünberg Institute*), Prof. Jürgen Schnack (*Universität Bielefeld, Postfach*), Prof. Herbert Roesky (*Georg-August-Universität Göttingen*)
 - **United States:** Prof. Kim Dunbar (*Texas A&M University*)
 - **Canada:** Prof. Muralee Murugesu (*University of Ottawa*)
 - **China:** Prof. Cai-Ming Liu (*Chinese Academy of Sciences*), Dr Yi-Fei Deng and Prof Yuan-Zhu Zhang (*Southern University of Science and Technology, Shenzhen*), Prof. Zhongwen Ouyang (*Huazhong University of Science and Technology, Wuhan*)
 - **Mexico:** Prof. Yasmi Reyes-Ortega (*Benemérita Universidad Autónoma de Puebla*), Prof. Gabriel Merino (*Centro de Investigación y de Estudios Avanzados*)
 - **New Zealand:** Prof. Paul Plieger (*Massey University*)
 - **Greece:** Prof. Constantinos Milios (*The University of Crete, Voutes*),
 - **Spain:** Prof. Marco Evangelisti (*Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC – Universidad de Zaragoza*)
 - **Ireland:** Prof. Leigh Jones (*NUI Galway*), Prof. Declan Gaynor (*Medical University of Bahrain*).
 - **Japan:** Prof. Hiroyuki Nojiri (*Tohoku University*).
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