<u>CURRICULUM VITAE</u> Dr. MAHESWARAN SHANMUGAM Professor

PERSONAL PROFILE

Current address

Department of Chemistry Indian Institute of Technology Bombay Powai, Mumbai Maharashtra – 400076. Email: eswar@chem.iitb.ac.in s.maheswaran@gmail.com Permanent address

2/110 New street Kiliyanallur Trichy- 621 213. Tamil Nadu

Date of Birth: 01 June 1980, Sex: Male Nationality: Indian

EDUCATION

Ph. D., in Inorganic Chemistry, 2003-2006
The University of Manchester, Manchester, UK
Master of Sciences in Chemistry, 2000-2002
Bharathidasan University, Trichy, India
Bachelor of Sciences in Chemistry, 1997-2000
Bharathidasan University (Bishop Heber College) Trichy, India

PUBLICATIONS

I have published more than 60 papers (2003-2023) in peer-reviewed leading international journals including *Proc. Nat. Acad. Sciences, Angew. Chem. Int. Ed., J. Am. Chem. Soc., Materials Horizons, Chem.Eur. J, Chem. Commun., J. Mater. Chem., Inorg. Chem., Dalton Trans., to name a few and these articles are cited more than 4000 times. Please see the detailed list below.*

RESEARCH INTEREST

Coordination and supramolecular chemistry, Catalysis, Multiferroic materials, Molecular magnetism, Molecular coolants, Spectroscopy and Small molecule activation (reduction of CO₂ into useful Chemicals), Multiferroics.

PROFESSIONAL RESEARCH EXPERIENCE

- Professor (March 2019-Present)
- Associate Professor (March 2015- March 2019)
- Assistant Professor, (March 2011-March 2015) Indian Institute of Technology Bombay, Powai, Mumbai.

- Postdoctoral research fellow, August 2009 January 2011 University of California, Davis, USA.
- Postdoctoral research fellow, November 1, 2006 July 2009 University of California, Berkeley, and University of California, San Francisco, USA.

RESEARCH STAY

- 1. Marie-Curie young investigator exchange programme (Supervisor: Prof. Roberta Sessoli, Department of Chemistry, University of Florence, Florence, Italy (Jan-Jun 2005))
- 2. Prof. Marrie Annie Arrio and Prof. Christophe C. Moulin, Universite Pierre et Marie Curie, Paris VI, France (Nov 2005).
- **3.** M.Sc., research Project @ Bharathidasan University, Trichy, Tamil Nadu, India (July 2001-June2002; Supervisor Prof. R. Ramesh)
- 4. **M. Sc., Summer research fellow** *(a)* Indian Institute of Technology, Kanpur, UP, India (May2001-July2001; supervisor: Prof. Sabya Sachi Sarkar)

Summary of Research Highlights:

Our research group mainly focuses on developing a novel synthetic methodology to reveal a new generation of coordination complexes which will be studied in detail for their molecular magnetic property (Single-molecule magnet or single ion magnets), molecular coolants and molecular qubit application. Another major thrust area of our research is developing a cheap and earth-abundant catalyst for -CH functionalization and activation of small molecules with particular emphasis on CO₂ to Methanol. Further understanding of the mechanism of the catalytic reaction is of the utmost importance to further develop a new generation of the catalyst with improved activity, which is also an active part of our research group. Recently, we have initiated the functionalization of molecules on graphene channels to develop a new generation of nanoelectronic devices. Further on the sustainable energy harvesting aspect, we intend to work on molecular-based ferroelectric and piezoelectric materials. Besides, our group also focuses on the design of multiferroic materials.

My research group actively takes up challenging problems, to improve the blocking temperature of the molecular magnets, functionalization of molecules on surfaces, developing a cheap, abundant and reactive catalyst for various organic molecule functionalization and activation. Based on our intense investigation, we have proposed several novel methodologies and contributed to the research community to better understand underlying principles and mechanisms. Some of the research highlights from our group

➤ Developing robust, wearable, and biocompatible energy harvesting devices with bulk oxides (ceramics and perovskites) is extremely hard to achieve due to their zero mechanical flexibility, heavy metal toxicity, and tunability of properties. Alternatively, discrete inorganic complexes can be an excellent choice to overcome the above-stated issues, thanks to appropriate molecular engineering. We engineered an above-room-temperature ferroelectric discrete molecular complex [Cu(L-phe)(bpy)(H₂O)]PF₆·H₂O (1) which is suitable for piezoelectric energy harvesting due to its large values of piezoelectric coefficient (d₃₃=10 pm V⁻¹) and spontaneous polarization (Ps=1.3 µC cm⁻²). Among the devices prepared with the composite films of polyvinyl alcohol (PVA) and various weight % composition of 1, the 10 Wt % composite shows the highest output voltage of 8 V, a

power density of 0.85 μ W cm-2, and output current of 5 μ A, which is highest for any discrete inorganic complex reported to date (*Angew. Chem. Int. Ed., 2023*, Accepted <u>https://doi.org/10.1002/ange.202216680</u>).

- A robust low coordinate Cobalt(II) complex was found to show excellent catalytic efficiency and selectivity for the reduction of CO₂ into methanol. This is the first cobalt complexes found to show excellent TON and TOF besides longevity. (*Angew. Chem. Int. Ed., 2023*, Under revision).
- Graphene is an excellent 2D-atomic layer thin crystalline honeycomb lattice with superior mobility, mechanical strength, carrier concentration etc. Hence, this material has potential application in transforming nanoelectronics devices as a field effect transistor. But this hope is being majorly hampered by its intrinsic electronic band structure that there is no band gap between the valence and conductance band. Using the molecular dopant one can precisely modulate the charge carrier concentration and mobility, therefore realizing molecular nanoelectronics devices are not too far from reality. In this line of interest, a set of lanthanide complexes has been used as a dopant for the first time, stabilizing an n-doped graphene field effect transistor which is extremely rare in the literature (*Mater. Horiz.*, 2019, 6, 743). Through this research, we have shown the potential application of the inorganic dopants (which is been investigated very scarcely) compared to the organic dopants. This will open up an enormous opportunity and the molecular nanoelectronics devices should be realized sooner than anticipated.
- Isolation of more than one electron-reduced redox active metal complex is essentially an uphill process. We have shown that three electron-reduced redox-active ligand bearing Co(II) and Co(I) ion was structurally characterized and it is an excellent catalyst for promoting the stereoselective and regioselective hydrophosphination of terminal alkynes. (Dalton Trans., 2019, 2019, 48, 7378 (Themed issue: Asia's Young Talent; Invited article))
- A cheap earth abundant base metal catalyst has been unveiled for stereoselective and regioselective hydrophosphination reaction of not only terminal alkynes but also internal alkynes. Through the detailed mechanistic investigation, we have intercepted various intermediates involved in the catalytic cycle. This is the first-time spectroscopic evidence is given for the various intermediates involved in the catalytic cycle (*Organometallics* 2018, 37, 2297-2304)
- Controlling single-ion magnetic anisotropy by ligand design is extremely challenging and scarce in the literature. To the best of our knowledge, for the first time, we have proposed in two decades of molecular magnetism research how to switch and control the magnetic anisotropy of single ion magnet behavior in Co(II) tetrahedral complexes. We have reported through our systematic studies about the parameters that control not only the sign and magnitude of single-ion anisotropy of Co(II) complexes (*Inorg. Chem., 2019, under revision, Inorg. Chem., 2018, 57, 3371-3386; Chem. Eur. J. 2017, 23, 4903-4916, Inorg. Chem., 2016, 55, 9564-9578; Chem. Commun., 2015, 51, 3739, Highlighted as a Cover page).*
- Quantum tunneling is one of the major issues which hampers any effort to increase the blocking temperature, we have shown that simply by incorporating transition metal ions near the vicinity of Dy(III) ion with the right choice of bridging ligand could enhance the exchange interaction thus suppresses the QTM. The rationale for this observation is

reported which is important information to the community, particularly for Chemist (*Chem. Eur. J. 2014*, 20, 14235).

- An ideal octahedral geometry around the lanthanide ion is predicted to be unsuitable for the design of a single-molecule magnet (SMM); nevertheless, complex a Dy(III) octahedral complexes coordination sites decorated by redox active radical ion exhibits slow relaxation of magnetization with a record high anisotropy barrier for a six-coordinate Dy(III) complex. A rationale for this unusual behavior is detailed and reveals the strength of the synthetic methodology developed to enhance the exchange interaction thus suppress the QTM. (*Inorg. Chem., 2018,* 57, 9002)
- A new novel synthetic approach has been revealed to the community which is by simply incorporating the diamagnetic metal ions the energy barrier can be increased significantly which is a new approach distinctly different from the existing method (*Inorg. Chem.*, 2017, 56, 14260-14276, *Chem. Commun.*, 2014, *50*, 8838-8841, highlighted as Cover page)
- Simply by exploiting the diffused d-orbital of a transition metal ion, such as Ru(III) enhances the exchange interaction which we believe is the largest exchange interaction known in any ruthenium-based complexes. (*Inorg. Chem.*, 2018, 57, 14967, *Chem.-Eur. J.*, 2014, 20, 6061-6070).
- The importance of mass density ratio in determining MCE efficiency was highlighted and reported recently. (*Inorg. Chem.* 2018, 57, 6584, *Chem. Eur. J.*, 2015, 21, 15639 and *Dalton Trans.* 2014, 43, 259-266)"

LIST OF PROJECT GUIDED ABROAD

- 1. "Isolation of redox active iminopyridine complexes of Aluminium and its catalytic activities" Ms. Nasrin Kazem (2009), University of California, Davis.
- 2. "Gallium redox active complexes and its reactivity with the oxidizing agents" Kristin Kowalik (2010), University of California, Davis.

LIST OF PROJECT GUIDED FROM IIT BOMBAY

Master's project completed

- 1. "Investigation of the effect of Ligand field on magnetic properties of lanthanide complexes" Sujan Biswas (2011-2012)
- 2. "Synthesis and characterization of 3d-metal complexes with Schiff base ligand" Nagulmeera Shaik (2012-2013)
- 3. "Synthesis and characterization of phosphaalkene containing PNP ligands" Varun Sisiram (Jan 2013-Oct 2013, Summer intern)
- 4. "3d metal complexes for Magnetic coolant applications" Rajdip Das (2013-2014)
- 5. "Modulating the exchange interaction using redox active imino-pyridine ligands" Abhijit Hansda (2013-2014).
- 6. "Synthesis of oxo-bridged Ruthenium complexes and its mixed valence species" Subhajit Paul (May 2014-May 2015)
- 7. "Synthesis of 3d and 3d/4f metal complexes with fused ring Schiff based ligand and their characterization" Jitendra Prasad Mehta" (May 2015-May 2016)
- 8. "Synthesis of 3-d transition metal-based complexes with pyrene-based bulky ligand" Siddharth Khadipure (July2015-May 2016)

- 9. "Isolation of redox active ligand containing transition metal complexes" Srikanth Balijapelly (Jan 2015-June 2015)
- 10. "Probing the electronic and magnetic properties of 3d and 3d-4f Schiff base complexes" Athulyadas, Amrita University (Jan 2016-June 2016)
- 11. "Porous Coordination Polymers and Metal-organic polyhedral for magnetic coolant and proton conduction application" Vinod Bansal (May 2016- Apr 2017)
- 12. "Isolation of coordinatively unsaturated transition metal complexes and their applications" Rinku Yadav (May 2016- Apr 2017)
- 13. "Synthesis of transition metal complexes of thio-crown ether ligand and probing its magnetic behavior" (Jan 2017-June 2017)
- 14. "Redox-active macrocyclic ligand containing lanthanide complexes as single molecule magnets" Farsa Ram (Since May 2017- Apr 2018)
- 15. "Coordinatively unsaturated transition metal complexes for CO₂ activation" Jitendra Sharma (Since May 2017- Apr 2018)
- 16. "Hydrophophination of alkynes using Cobalt catalyst" Amit Kumar (May 2018 Apr 2019)
- 17. "Isolation of unusual cobalt catalyst and their hydrofunctionalization activity of alkynes and alkenes" Deepak Kumar Sahoo (May 2019 Apr 2020)"
- 18. "Main group metal catalyst for double hydrophosphinylation of Nitriles and alkynes" Gautam Kumar Mehta (May 2021-Apr 2022).
- 19. "Main group metal catalyst for double hydrophosphinylation of Alkenes" Anjana (May 2022-Apr 2023)
- 20. "Easy plane anisotropy in pseudo tetrahedral Cobalt (II) based complexes: A magnetic, EPR and computational study" Mr. Amit Tiwari (IRCC Intern, since Jan-2018)
- 21. "Oligonuclear transition metal complexes as catholyte/anolyte materials for Non-aqueous redox flow battery application" Ravalika Sajja (Jan 2019 June 2019).
- 22. "Designing fluorophores for the early detection of Breast cancer" Archana Rajendran (Jan 2023-June 2023)

Research assistant (completed)

1. "Sterically hindered pincer ligands for stabilizing low coordinate transition metal complexes" Jitendrasingh Rajpurohit (2012-2013)

Ph.D., students Graduated

- 1. Dr. Apoorva Upadhyay (July 2011-Jan 2016) Thesis title: "Factors Governing Single-Molecule-Magnet" behavior of 4f and 3d-4f Schiff base metal complexes".
- Dr. Shefali Vaidya (July 2011-Feb 2017) Thesis title: "Modulating the sign and Magnitude of single-ion magnetic anisotropy in Cobalt(II) pseudo tetrahedral complexes"
- 3. Dr. Chinmoy Das (July 2012-Apr 2018) Thesis title: "New generation of 3d and 4f metal complexes as single-molecule magnets, single molecule toroics, and molecular refrigerants"
- 4. Dr. Naushad Ahmed (July 2012-Jan 2019) Thesis title: "Influence of Magnetic Exchange, Electronic Structure and Geometry on the Magnetization Relaxation Dynamics of 3d, 4f and 3d-4f Metal Complexes"

- Dr. Jitendrasingh Rajpurohit (July 2013-May 2019)
 "Stabilizing coordinatively unsaturated and Unusual Oxidation State of Transition Metal Complexes and probing their Catalytic Activity"
- 6. Dr. Pragya Shukla (July 2013-Feb 2020) "Modulating the factor to improve the Single Molecule Magnet behavior of 4f and 3d-4f coordinated compounds"
- 7. Dr. Shalini Tripathi (July 2014- Sept 2020) "Developing magneto-structural correlation to switch and tune single ion magnetic anisotropy of Cobalt(II) complexes: Experimental Insights and Predictions"
- 8. Dr. Mohd Wasim (Dec 2014-June 2021) "When molecules meet the 2D-Materials: Challenges and Opportunities to realize Molecule-Based Information Storage and Electronic Devices"
- Dr. Pardeep Jangra (Dec 2015-Nov 2021)
 "A new generation of transition metal (Fe and Co) catalysts for hydro-functionalization and bio-inspired catalysis"
- 10. Dr. Kamal Uddin Ansari (July 2014-Dec 2021)
 "Investigation of Electronic and Magnetic Properties of Discrete Transition Metal Complexes and Heterometallic Lanthanide Complexes"

Ph.D., Students (Ongoing)

- 1. Ms. Rajashi Haldar (Since 2019) "Molecular Engineering to develop 3d and 3d-4f metal based molecular Ferroelectrics and Mutiferroics"
- Ms. Vasudha Sharma (Since 2020) "Activation of small molecules (CO₂) into useful chemical feedstock (methanol) using robust 3d-transition metal catalysts: Development of synthetic methods and understanding the mechanism of the catalytic reaction"
- 3. Ms. Dipanti Borah (Since 2020) *"Targeting single molecule magnets with high blocking temperature for developing molecular based information storage devices"*
- 4. Ms. Vijaya T R (Since 2021)
 "Structure-Property correlation for stabilizing axial magnetic anisotropy in six-coordinate Cobalt(II) complexes and developing electrocatalyst for efficient water oxidation"
- 5. Ms. Rukshar Bano (Since 2022) "Directing template approach for the selective C5, C6 functionalization of heteroarenes"
- 6. Mr. Bapan Jana (Since 2022) "Application of Molecular Ferroelectrics and Multiferroics"
- Mr. K. Vignesh (Since 2022) "Molecular based Piezoelectric materials for mechanical energy harvesting application"
 Mr. B. Ganeshmoorthi (Since 2023)
- 8. Mr. B. Ganeshmoorthi (Since 2023) *"Multiferroic Multifunctional Materials based on Extended Structures"*9. Mr. Ramesh Kumar (Since 2023)
- "Developing robust catalyst for N₂/CO₂ activation"
- 10. Mr. Deepanshu Chauhan (Since 2019): Co-PI

"Single molecule Magnets and Single Molecule Torics: Experimental and Theoretical Perspective"

11. Mr. Satheeshkumar (Since 2023): Co-PI

"Multiferroics based on Single molecule Toroics and Ferroelectricity: Experimental and theoretical insights"

Postdoc., project completed

- 1. Dr. Sujit Sasmal "Identifying the SMM property in monomeric transition metal complexes using Sulfur based Schiff base ligands" (May 2013-July 2013)
- 2. Dr. Dipti Lakhe Chawde "Tuning the MCE parameters of magnetic coolants" (Since Jul 2014-Jun 2015)
- 3. Dr. Shanish Kumar "Coordinatively unsaturated transition metal complexes using phosphine based ligands for CO₂ reduction" (Feb 2016-Feb 2018)
- 4. Dr. N. Praveen "Early detection of fibril formation of α-synuclein using transition metal complexes" (March 2016-March 2019)
- **5.** Dr. Suman Das "Phosphorylation of alkene, alkyne and organo-nitriles by using anionic indium metal complexes" (Jun 2021- August 2022)
- 6. Dr. Amaleswari Rasamsetty "Synthesis of low coordinated 3d and 3d-4f metal based singlemolecule magnets" (June 2018- May 2022)
- 7. Dr. Daulat Phapale "Spectroscopic Characterization of Paramagnetic Intermediates during Electrochemical Water Oxidation Catalyzed by Ru(III) Complexes" (Dec 2019-Dec 2022)
- 8. Dr. Sadananda Kumbhakar "Stabilizing low coordinate Lanthanide complexes using bulky amide ligands" (Since 2023).

TEACHING

- CH-557 Topics in Chemistry; Single crystal x-ray diffraction course has been introduced to the candidates for the first time. Students had been trained for structure refinement and structure solution methods (July 2011, July 2012, July 2013, July 2014, July 2015, July 2016)
- CH-429 Analytical methods in Chemistry; Various spectroscopy techniques have been newly introduced such as electron paramagnetic resonance, SQUID apart from routine IR, NMR, Mass-spec to the students. (Jan 2012, Jan 2013, Jan 2014, Jan 2015 and Jan 2016)
- 3. CH-802S Seminar course for the graduate students (July 2013, Jan 2014, Jan 2018)
- 4. CH-821 Topics in Chemistry (July 2014, July 2015, July 2016)
- 5. CH-105 Inorganic and Organic Chemistry (Jul 2017, Jul 2018, Jul 2019, Jul 2020, Jul 2021)
- 6. CH-578 Topics in Chemistry (Jan 2018, Jan 2019, Jan 2020, Jan 2021)
- 7. CH-105 Tutorial
- 8. CHS-801 Seminar Course (July 2014)
- 9. CH-117 lab
- 10. CH-831 lab Advanced Laboratory Techniques (Jan 2017)
- 11. CH-415 lab Inorganic Chemistry lab- II (Jul 2018)
- 12. CH-432 Inorganic Chemistry lab –III (Jan 2019)
- 13. CH-227 Introduction to Coordination Chemistry

- 14. CH-578 Topics in Chemistry (July 2017, July 2018, July 2019, July 2020, July 2021)
- 15. CH-827 Inorganic Complexes (Jan 2022, Jan 2023, Jan 2024)

COLLABORATORS

- > Prof. Satoshi Horike, Kyoto University, Japan
- Prof. G. Rajaraman, Department of Chemistry, IIT Bombay, Powai, Mumbai, Maharashtra, India
- Prof. C. Subramaniam, Department of Chemistry, IIT Bombay, Powai, Mumbai, Maharashtra, India
- Prof. Eric McInness, School of Chemistry, The University of Manchester, Manchester, UK.
- > Prof. Arzhang Adrvan, School of Chemistry, Oxford University, Oxford, UK
- Prof. Ashutosh Kumar, Department of Biological Sciences and Bioengineering, IIT Bombay, Powai, Mumbai 400076.
- Prof. Samir Maji, Department of Biological Sciences and Bioengineering, IIT Bombay, Powai, Mumbai 400076.
- > **Prof. Marco Affronte,** Department of Physics, University of Modena, Italy.
- > Prof. Keith S. Murray, University of Monash, Australia
- > Prof. Lorenzo Sorace, Department of Chemistry, University of Florence, Italy.
- > Prof. Dipankar Mandal, INST, Mohali, India.

DETAILS OF GRANTS RECEIVED

Serial number	Title of Project	Duration	Funding agency	Money Sanctioned (Rupees)
11IRCCSG006	LanthanidebasedSinglemoleculeMagnets for ImproveddataStorageapplications	2011-2014	IIT Bombay (Seed Grant)	26,24,000
12DST004	Design of Lanthanide Based Single- Molecule-Magnets and Validation through Experimental Studies	2012-2015	Department of Science and Technology	49,77,000
12BRNS007	Synthesis of uranium co-ordination complexes and probing its electronic and magnetic properties	2012-2015	Board of Nuclear Research Sciences	17,00,000
12DST075	A new generation of molecular nanomagnets (Co-PI)	2013-2016	Department of Science and	3,40,40,000

			Technology- Nanomission	
13CSIR11	Tuning the MCE parameters $(-\Delta S \text{ and } \Delta T_{ad})$ of molecular coolants	2013-2016	CSIR	~20,00,000
14DST-ID4	Activation of O ₂ molecules by porous coordination polymer and direct observation of its magnetic behavior	2014-2016	INDO-IJCSP	~12,00,000.00
SERB	Building block approach to the dense extended network $(Cr^{3+}, Cu^{2+}, Ni^{2+})$ and/or Gd^{3+} for efficient adiabatic magnetic cooling	2016-2019	DST	~40,00,000.00
15INSA003	Developing magneto- structural correlation to switch and tune the single-ion magnetic anisotropy of Co(II) complexes.	2016-2019	INSA	15,00,000.00
15IRAWAD011	Revealing new synthetic strategy for isolation of redox active radical complexes of transition and 4f ion complexes and probing its electronic and magnetic properties	2015-2018	IRCC-IIT Bombay	5,00,000.00
15PDF002	Early detection of fibril formation of α- synuclein using transition metal complexes	2016-2018	DST-SERB	~27,00,000.00
	Rational design to stabilize Ising or axial single-ion magnetic anisotropy in Co(II) complexes	2018-2021	CSIR	12,00,000.00/-

Synthesis of next generation precursors for metal ALD and electroplating	2018-2019	AMAT Consultancy	18,00,000.00/-
Targeting Single- Molecule Magnets with High-Blocking Temperature	2020-2023	SERB	39,00,000.00/-
Is molecular engineering the key for newer breakthroughs in quantum information processing	2020-2023	SERB-SUPRA	83,00,000/-
Molecular Engineering to develop Lanthanide based Multiferroics	2023-2026	CSIR	9,00,000/-
Magneto-electric Multiferroics: Design of new molecular materials based on 3d, 4f and 3d-4f ions.	2023-2026	BRNS	35,00,000/-
Designing efficient and robust catalysts for the mitigation of CO2 and its conversion as C1 or C2 products	2023-2026	IISc-STARS	40,00,000/-
Targeting Biocompatible and Discrete ferroelectric metal complexes (3d, 4f, 3d-4f) for mechanical energy harvesting	2024-2027	SERB-CRG	78,00,000/-
Quantifying Magnetic Anisotropy in 3d and 4f metal ions: A high- precision Study via Magneto-Torque Techniques	2024-2024	IoE-SCPP: IIT Bombay	10,00,000/-

CONFERENCES, MEETINGS, POSTER PRESENTATIONS

- 1. Dalton discussion 9: Functional molecular assemblies programme, Manchester, UK (Apr 2006)
- 2. Chemistry of coordination space, London, UK (Jul 2006)
- 3. The UK molecular magnet network Mag-Net 2005, Cambridge, UK (Sep 2005)
- 4. Co-ordination chemistry discussion group, Leicester, UK (Jul 2004)
- 5. Quantum effect in molecular nanomagnets (QuEMolNa), Valencia, Spain (Apr 2004)
- 6. The Fairchild prion review meeting, San Francisco, USA (Jan 2009)
- 7. The Fairchild prion review meeting, San Francisco, USA (Jan 2007)
- 8. UK network on molecular magnetism, Cambridge, UK (Sep 2005)
- 9. Molecular nanomagnetism (MOLNANOMAG), Florence, Italy (Jun 2005)
- 10. Quantum effects in molecular nanomagnets (QuEMolNa), Valencia, Spain (Apr 2004)
- 11. Chemistry of Functional materials, Goa, India, August 2011
- 12. "MTIC-XIV" Hyderabad, India, December 2011
- 13. Asian Coordination Chemistry Conference, New Delhi, October 2011
- 14. Participated in a conference held in Florida, USA 2012 entitled in "International Conference on Molecular Magnetism (ICMM)
- 15. "MTIC-XIV" IIT Roorkee, India, December 2013
- 16. Chemical Research Society India (CRSI) meeting held in IIT Bombay February 2014.

INVITED TALK

- 1. "Molecular Based Multiferroic Materials: Challenges and Opportunities" MTIC-XX IISc Bangalore (Dec 2023)
- 2. Application of Transition metal complexes for sustainable energy-harvesting and fuels, IIT Kanpur (July 2023).
- 3. "Probing the Origin of Feroo/Antiferromagnetic exchange interaction in Cu(II)-4f Complexes" Mother Therasa Women University, Kodaikanal (July 2023)
- 4. "CO₂ transformation to Sustainable energy and Fuels using low coordinate 3d metal catalysts" IITB-NTU Workshop, IIT Bombay (Oct 2023)
- 5. "Probing the Origin of Feroo/Antiferromagnetic exchange interaction in Cu(II)-4f Complexes" MTMM-IIT Kharagpur (Dec 2022)
- 6. "Application of transition metal complexes for sustainable energy-harvesting and fuels" RAIC, IIT Bombay (Oct 2022)
- 7. "Spin Admixed and Spin crossover phenomena in a Square Planar Fe(III) complex" ACMM-2, IISER Bhopal, India (Dec 2022)
- 8. "Modulation of Single-Ion Magnetic Anisotropy of Tetrahedral and Octahedral Co(II) Ion by Ligand Design" ACMM-1 Fukuoka, Japan (Mar 2021)
- 9. "Stabilizing unusual oxidation state of Nickel ion using redox active ligand upon molecular dioxygen activation" Loyola College, Chennai (Feb 2019).
- 10. "Non-heme iron complexes for sulfido atoms transfer reactions" International conference on Advanced Chemical and Structural Biology-ICACSB-2019, PRIST University, Chennai (Feb 2019).
- 11. "Molecular based electronic devices: controlling the electrical properties of GFETs by lanthanide complexes" International Conference on Molecular Magnetism, Rio, Brazil (Sep 2018).
- 12. "Molecules to Materials: Modulating the electrical properties of GFETs by lanthanide complexes" Main group Molecules to Materials, IISc, Bangalore (Oct 2018).

- 13. "Can we control the single-ion magnetic anisotropy of Tetrahedral Co(II) ion by ligand design?" Indo-French Conference at IISc, Bangalore (Nov 2018)
- 14. "Probing the Electronic and Magnetic Properties of Cobalt and Nickel Complexes: An experimental and theoretical Investigations", Goa University (Dec 2019).
- 15. "3d and 4f metal complexes for the molecular device and catalytic application" ICMRE-Anna University Vizhupuram Jan 2018"
- 16. "What controls the SIM behavior of 3d and 4f ions? Synthesis and its application" MTIC-2017, IISER Pune.
- 17. "Introduction to lanthanide based molecular magnetism" Indo-Aarhus workshop at Goa (Nov 2017)
- 18. "3d and 4f metal complexes and its magnetic, catalytic and molecular device application" Chemical Frontiers, Goa (August 2017) "Controlling zero-field splitting in tetrahedral Co(II) complexes through ligand design" Aarhus University, Denmark (June 2017).
- 19. "Influence of exchange interaction on relaxation dynamics of lanthanide ions" University of Copenhagen, Denmark (June 2017)
- 20. "Unusual Oxidation State of Nickel Ion Stabilized by Redox Active Ligand Through Dioxygen Activation" Madurai Kamaraj University, Madurai, Tamil Nadu (March 2017).
- 21. "Molecular nanomagnet and its application" Vivekanandha college of arts and Science for Women, Tiruchengodu (Feb 2016).
- 22. "Effect of Magnetic Anisotropy on Magnetic Coolant Property of Square Based Ln4 (where Ln = Dy, Tb, Gd) Complexes Kyushu University (May 2015).
- 23. "3d and 4f Single-ion magnets: Switching the Magnetic Anisotropy and Enhancing Effective Energy Barrier in an Unconventional Method" Kyoto (May 2015).
- 24. What influences Quenching of Quantum Tunnelling of Magnetization in Ni2Dy2 Single-Molecule Magnet? Tohoku (May 2015).
- 25. "Biological and technological application of coordination complexes", Bishop Heber College (Jan 2014).
- 26. "Single-Molecule-Magnets and its applications" Mother Teresa Women's University, Kodaikanal (March 2013)
- 27. "Molecular nanomagnets: Transition from transition metal complexes to inner-transition metal complexes" New Horizons in Chemistry, IIT-Bombay, March 2013.
- 28. "Manganese phosphonate clusters: Synthesis and studies of their electronic and magnetic properties" Department of Chemistry, Bharathidasan University, Trichy, India (Oct 2006).

HONORS AND AWARDS

- **CRSI Bronze medal the research contribution in Chemistry (2023-2024)**
- IIT Bombay Research Publication Award (2019)
- Indian National Science Academy Young Investigator Award (2015)
- > IIT Bombay Young Investigator Award (2015)
- **BRNS** young investigator award (2012)
- > Overseas research scholarship (ORS; 2003-2006)
- University research scholarship (URS; 2003-2006; awarded for doctoral studies at the University of Manchester, Manchester, UK)
- Marie-Curie exchange programme young scientist research fellowship (Jan 2005 Jun 2005)

- Qualified (Lecturership-NET) in national eligibility test (NET) conducted by CSIR_UGC, India in December 2002.
- Indian Academy of Sciences summer research fellow (May 2001 Jul 2001)
- ➤ Associate Member of Royal Society of Chemistry (AMRSC) (2003 2006)
- Member of American Chemical Society (Since 2010)
- Second rank in Postgraduate studies
- > Ninth rank in the university level (Undergraduate course, among several colleges)
- Second rank in college in B. Sc., (2/80)

PUBLICATIONS

Papers / book chapters published from IIT Bombay

Book chapters

- Chapter 8, "Co(II) complexes as Single-ion Magnets" Shalini Tripathi, Atanu Dey, Maheswaran Shanmugam*, Ramakirushnan Suriya Narayanan and Vadapalli Chandrasekhar, accepted in Topic in Organometallic magnets, 2018, DOI: 10.1007/3418_2018_8 Publisher: Springer.
- Chapter 9, "Co(II)/(III)-Lanthanide(III) complexes as Single-molecule Magnets" Atanu Dey, Shalini Tripathi, Maheswaran Shanmugam, Ramakirushnan Suriya Narayanan, and Vadapalli Chandrasekhar*, accepted (2018) in *Topic in Organometallic magnets*, 2018, DOI: 10.1007/3418_2018_9 Publisher: Springer.

Publications

- "Capturing the Elusive [RuV=O]+ Intermediate in Water Oxidation" Phapale, Daulat; Sharma, Vasudha; Saini, Abhishek; Sharma, Sunita; Kumar, Pardeep; Kumar, Rakesh; Shanmugam, Muralidharan; Draksharapu, Apparao; Dutta, Arnab; McInnes, Eric; Collison, David; Rajaraman, Gopalan; Shanmugam, Maheswaran, *ACS Catalysis*., 2024, Accepted.
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