

Proforma for information to be provided by the Teaching Staff



1. Name : Dr. Tulika Gupta
2. Designation: Assistant Professor
3. Academic Qualifications:

Sr.	Degree	Institution	Year
1.	Secondary	Barrackpore Ramakrishna Vivekananda Mission Vidyabhawan, Kolkata	2004
2.	Higher Secondary	Barrackpore Girls' High School, Kolkata	2006
3.	B.Sc	Jadavpur University, Kolkata	2009
4.	M.Sc	IIT Guwahati, Assam	2011
5.	Ph.D	IIT Bombay, Maharashtra	2017, Feb
6.	Post-doc	Heidelberg University, Germany	2016, Nov-2017, Nov

4. Area of Specialization: Inorganic Chemistry : Modelling of Molecular Nanomagnets , accentuation on magnetic anisotropy deduction in lanthanide/actinide/transition metal systems, estimating zero-field splitting parameters of transition metal complexes employing DFT and state-of-the-art *ab initio* approach. Reaction modelling for open shell transition metal mediated catalytic reactions.
5. Contact Information: +91-8585890318 (M) ; Email id : tulikag.chem@bhu.ac.in
6. Projects Undertaken as PI/ Co PI: NA
7. Awards/ Recognitions if any:

- CSIR Foreign Travel Grant for participation in *ACCC5, Hong Kong* 2015, April
- Interviewed for BASF Summer School participation 2015, May
- SERB(DST) Travel Grant for participation in *WATOC-2014, Chile* 2014, September
- UGC Senior Research Fellowship for Doctoral Dissertation Studies 2014, January
- “Small Grants for Scientific Activities” by RSC for conducting research in *The University of Manchester, UK* 2013, August
- IIT-B Financial Support for participation in *DFT-2013, Durham, UK* 2013, September
- Associate Membership from RSC 2013, June
- UGC Junior Research Fellowship for Doctoral Dissertation Studies 2012, January
- GATE Teaching Assistantship 2011, July
- Indira Gandhi Scholarship for Masters Studies 2010, October
- Merit-Cum-Means Masters Studies Scholarship 2009, December

8. List of 10 major Publications: (in order of importance)

- *“A classification of spin frustration in molecular magnets from a physical study of large odd-numbered-metal, odd electron rings”*
Michael L. Baker, Grigore A. Timco, Stergios Piligkos, Jennifer S. Mathieson, Hannu Mutka, Floriana Tuna, Piotr Kozłowski, Michał Antkowiak, Tatiana Guidi, **Tulika Gupta**, Harapriya Rath, Robert J. Woolfson, Grzegorz Kamieniarz, Robin G. Pritchard, Høgni Weihe, Leroy Cronin, Gopalan Rajaraman, David Collison, Eric J. L. McInnes, and Richard E. P. Winpenny, *Proc. Nat. Acad. Sci. USA*, 2012, **109**, 19113-19118. (*No. of citations = 69*)
- *“Magnetic exchange in {Gd(III)–radical} complexes: method assessment, mechanism of coupling and magneto-structural correlations”*
Tulika Gupta, Thayalan Rajeshkumar and Gopalan Rajaraman, *Phys. Chem. Chem. Phys.* 2014, **16**, 14568-14577. (*No. of citations = 28*)
- *“Magnetic Anisotropy and Mechanism of Magnetic Relaxation in Er(III) Single-Ion Magnets”*
Saurabh Kumar Singh, **Tulika Gupta** and Gopalan Rajaraman, *Inorg. Chem.* 2014, **53**, 10835-10845. (*No. of citations = 46*)
- *“Unprecedented Magnetic Relaxation Via the Fourth Excited State in Low-Coordinate Lanthanide Single-Ion Magnets: A Theoretical Perspective”*
Saurabh Kumar Singh, **Tulika Gupta**, M. Shanmugam and Gopalan Rajaraman, *Chem. Commun.* 2015, **50**, 15513-15516. (*No. of citations = 38*)
- *“Analysis of the Role of Peripheral Ligands coordinated to Zn(II) in Enhancing the Energy Barrier in Luminescent Linear Trinuclear Zn-Dy-Zn Single-Molecule Magnets”*
Jean Pierre Costes, Silvia Titos-Padilla, Itziar Oyarzabal, **Tulika Gupta**, Carine Duhayon, Gopalan Rajaraman and Enrique Colacio, *Chem. Eur. J.* 2015, **21**, 15785-15796. (*No. of citations = 29*)
- *“Single-Molecule Magnetism, Enhanced Magnetocaloric Effect, and Toroidal Magnetic Moments in a Family of Ln₄ squares”*
Chinmoy Das, Shefali Vaidya, **Tulika Gupta**, Jamie M. Frost, Mattia Righi, Euan K Brechin, Marco Affronte, Gopalan Rajaraman and Maheswaran Shanmugam, *Chem. Eur. J.* 2015, **21**, 15639-15650. (*No. of citations = 29*)
- *“Role of Single-Ion Anisotropy and Magnetic Exchange Interactions in Suppressing Zero-Field Tunnelling in {3d-4f} Single Molecule Magnets”*
Tulika Gupta, Mohd. Faizan Beg and Gopalan Rajaraman, *Inorg. Chem.* 2016, **55**, 11201-11215. (*No. of citations = 10*)
- *“How Strongly the Magnetic Anisotropy and the Coordination Numbers are Correlated in Lanthanide Based Molecular Magnets?”*
Tulika Gupta and Gopalan Rajaraman, *J. Chem. Sci.*, 2014, **126**, 1569-1579. (*No. of citations = 17*)
- *“Modelling Spin Hamiltonian Parameters of Molecular Nano Magnets”*
Tulika Gupta and Gopalan Rajaraman, *Chem. Commun.* 2016, **52**, 8972-9008. (*No. of citations = 12*)
- *“Role of Ab Initio Calculations in the Design and Development of Lanthanide Based Single Molecule Magnets”*
Tulika Gupta, Mukesh Kumar Singh and Gopalan Rajaraman in Topics in Organometallic Chemistry, Springer International Publishing AG, Berlin, Heidelberg, 2018, pp. 1-74.

9. Additional Information/ Achievements:

■ **TEACHING EXPERIENCE AND MENTORSHIP**

- Supervised Masters' internship to Mr. Kishan Kumar Yadav 2018, Jan to May
- ◆ **Project Title :** "Exploring Magnetism : A Computational Perspective"
- Co-supervised Masters' internship to Mr. Marcel Eck 2017, May to June
- ◆ **Project Title :** "Mechanistic DFT studies on the catalytical reactions of CO₂ fixation using patellamide model ligands and CO₂ hydration using ruthenium-Triphos complexes"
- Delivered lecture and workshop on PHI usage to 2016, May
conference (WESCC-2016) participants in IIT-B
- Outlined workshops and lectures on computational 2012-2016
chemistry in Dr. G. Rajaraman's lab during doctoral studies
- Co-supervised Masters' project to Miss Mehakpriya 2015, May to 2016, May
- ◆ **Project Title :** "Probing Toroidal Behaviour in Polynuclear Dy^{III} SMMs"
- Co-guided Masters' project to Mr. Faizan Mohd. 2014, May to 2015, May
- ◆ **Project Title :** "Exploring Exchange Interactions in {3d-4f} SMMs"
- Guided first to tenth grade students of nearby slum area in 2012-2014
cognitive understanding of scientific concepts
- Contributed as volunteer through demonstration of scientific 2014, January
experiments to school students in "TechConnect-2014" at IIT-B
- Involved in preparation and execution of 2012, August to 2013, December
undergraduate laboratory section
- Formulated assignments for Masters level course 2013, January to April
on Magnetism

■ **INVITED TALKS**

- In 5th Asian Conference on Coordination Chemistry (ACCC5) in Hong Kong, 12th-16th July, 2015. "Regulating Magnetic Anisotropy in Lanthanide SMMs Using Theoretical Tools".
- In 10th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC-2014) in Santiago, Chile, 5th-10th October, 2014. "Quenching Quantum Tunneling of Magnetization in Lanthanide SMMs: A Theoretical Perspective".
- In the National conference on National Conference on Advances and Innovations in Chemical Sciences, Mumbai University, 12th -13th February, 2015. "Magnetic Anisotropy in Lanthanide SMMs: Decisive Factors".
- In 27th Research Scholars' Meet organized by Sathaye College, Mumbai, 20th-21st February, 2015. "Magnetic Anisotropy in Lanthanide based SMMs: Theoretical Exploration".
- In IWR School Mathematical Methods For Quantum Chemistry organized by Heidelberg University, Germany, 2nd-6th October, 2017. "Modelling (Quantum Chemical) of Magnetic Materials and Chemical Reaction Mechanisms".

■ **CONFERENCES, MEETINGS AND POSTER PRESENTATIONS**

- **“National Conference on Life and Works of Sir J C Bose in the Perspective of Modern Science and Technology”**, Jadavpur University, 20th-21st March, Kolkata, 2009, India.
- **“National conference on Frontiers In Chemical Sciences (FICS) 2010 in IIT Guwahati”**, IIT Guwahati, India, 3rd-4th Dec, 2010.
- **“3rd Indo-German Conference”**, Indian Institute of Technology Bombay, Mumbai, India, 27th-29th September 2011.
- **“New Horizons in Chemistry”**, Indian Institute of Technology Bombay, Mumbai, India, 3rd-4th October 2011.
- **“3rd Asian Conference on Coordination Chemistry”**, New Delhi, India, 17th -20th October 2011.
- **“International Conference on Chemistry & Complexity”** at IACS, Kolkata, IACS, Kolkata, 6th-8th December, 2011.
- **“Introduction to Gaussian: Theory and Practice- Workshop”** at IIT Chennai, 2nd-6th January, 2012.
- **“In House Symposium (IHS2012)”**, Indian Institute of Technology Bombay, Mumbai, India, 10th March 2012.
- **“National conference on Recent Advances in Inorganic Chemistry”**, at Bharathidasan University, Tiruchirappalli, Tamilnadu, 22nd-24th March, 2012.
- **“High Performance Computing Conference”**, Mumbai, 8th August 2012.
- **“Indian Institute of Technology Bombay-American Chemical Society Symposium”**, Indian Institute of Technology, Bombay, Mumbai, India, 1st-2nd October 2012.
- **“Technical Workshop on the Application Performance Optimization on HPC Clusters”**, Mumbai, 26th October 2012 organized by CDAC Pune and IIT-Bombay.
- **“Theoretical Chemistry Symposium 2012 (TCS12)”**, Indian Institute of Technology, Guwahati, India, 19th-22nd December 2012.
- **“International Conference on Functional Metalorganics and Hybrids”**, Kolkata, India, 8th -10th February, 2013.
- **“In House Symposium (IHS13)”**, Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India, 2nd March 2013.
- **“Symposium on Theoretical and Computational Chemistry-Frontiers and Challenges”**, School of Chemistry, Bharathidasan University, Tiruchirappalli, India, 14th-15th June 2013.
- **“15th International Conference on Density Functional Theory And Its Applications (DFT-2013)”**, Durham, United Kingdom, 9th-13th September, 2013.
- **“8th RSC-CRSI, 16th CRSI Symposium in Chemistry”**, Department of Chemistry, IIT Bombay, Mumbai, 6th-9th February, 2014.
- **“Workshop on Electronic Structure, Atomistic and Statistical Modelling in Chemistry Materials and Life Sciences”**, ICT Mumbai, 5th-7th Aug, 2014, organized by Schrödinger Material Science Suite.
- **“Golden Jubilee In-House Symposium”**, IIT Bombay, 16th-17th October, 2014.
- **“In-House Symposium”**, IIT Bombay, 2nd April, 2016.
- **“Workshop on Electronic Structure and Coordination Complexes”**, IIT Bombay, 16th -19th May, 2016.
- **“Modern Trends in Molecular Magnets”**, IIT Bombay, 19th-21st may, 2016.
- **“ChemCareers-2016, RSC”**, ICT Bombay, 27th August, 2016.
- **“5th Symposium on Advanced Biological Inorganic Chemistry (SABIC)”**, IACS Kolkata, 7th-11th January, 2017.
- **“CaRLa Winter School”**, Heidelberg, 12th-17th February, 2017.
- **11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC-2017)**, LMU Munich, Germany, 27th August-1st September, 2017.

- “NASI Conference in Technological Empowerment of Women”, New Delhi, 8th-9th March, 2018

10. Full List of Publications:

◆ (Overall Citations = 440)

■ PEER-REVIEWED PUBLICATIONS

- “A classification of spin frustration in molecular magnets from a physical study of large odd-numbered-metal, odd electron rings”

Michael L. Baker, Grigore A. Timco, Stergios Piligkos, Jennifer S. Mathieson, Hannu Mutka, Floriana Tuna, Piotr Kozłowski, Michał Antkowiak, Tatiana Guidi, **Tulika Gupta**, Harapriya Rath, Robert J. Woolfson, Grzegorz Kamieniarz, Robin G. Pritchard, Høgni Weihe, Leroy Cronin, Gopalan Rajaraman, David Collison, Eric J. L. McInnes, and Richard E. P. Winpenny, *Proc. Nat. Acad. Sci. USA*, 2012, **109**, 19113-19118. (No. of citations = 66)

- “Magnetic exchange in {Gd(III)-radical} complexes: method assessment, mechanism of coupling and magneto-structural correlations”

Tulika Gupta, Thayalan Rajeshkumar and Gopalan Rajaraman, *Phys. Chem. Chem. Phys.* 2014, **16**, 14568-14577. (No. of citations = 28)

- “Magnetic Anisotropy of Mononuclear Ni(II) complexes : On the Importance of Structural Diversity and The Structural Distortions”

Saurabh Kumar Singh, **Tulika Gupta**, Prashi Badkur and Gopalan Rajaraman, *Chem. Eur. J.* 2014, **20**, 10305-10313. (No. of citations = 23)

- “How Strongly the Magnetic Anisotropy and the Coordination Numbers are Correlated in Lanthanide Based Molecular Magnets?”

Tulika Gupta and Gopalan Rajaraman, *J. Chem. Sci.*, 2014, **126**, 1569-1579. (No. of citations = 18)

- “Magnetic Anisotropy and Mechanism of Magnetic Relaxation in Er(III) Single-Ion Magnets”

Saurabh Kumar Singh, **Tulika Gupta** and Gopalan Rajaraman, *Inorg. Chem.* 2014, **53**, 10835-10845. (No. of citations = 51)

- “Unprecedented Magnetic Relaxation Via the Fourth Excited State in Low-Coordinate Lanthanide Single-Ion Magnets: A Theoretical Perspective”

Saurabh Kumar Singh, **Tulika Gupta**, M. Shanmugam and Gopalan Rajaraman, *Chem. Commun.* 2015, **50**, 15513-15516. (No. of citations = 41)

- “A synthetic Strategy for Switching the Single-Ion Anisotropy in Tetrahedral Co^{II} Complexes

Shefali Vaidya, Apoorva Upadhyay, Saurabh Kumar Singh, **Tulika Gupta**, Subrata Tewary, Stuart K. Langley, James P. S. Walsh, Keith S. Murray, Gopalan Rajaraman and Maheswaran Shanmugam, *Chem. Commun.* 2015, **51**, 3739-3742. (No. of citations = 47)

- “Magnetic Relaxation in Single-Electron Single-Ion Cerium(III) Magnets : Insights from Ab Initio Calculations”

Saurabh Kumar Singh, **Tulika Gupta**, Liviu Ungur, Liviu F. Chibotaru, Gopalan Rajaraman, *Chem. Eur. J.* 2015, **21**, 13812-13819. (No. of citations = 26)

- “Analysis of the Role of Peripheral Ligands coordinated to Zn(II) in Enhancing the Energy Barrier in Luminescent Linear Trinuclear Zn-Dy-Zn Single-Molecule Magnets”

Jean Pierre Costes, Silvia Titos-Padilla, Itziar Oyarzabal, **Tulika Gupta**, Carine Duhayon,

Gopalan Rajaraman and Enrique Colacio, *Chem. Eur. J.* 2015, **21**, 15785-15796. (*No. of citations = 32*)

- “*Single-Molecule Magnetism, Enhanced Magnetocaloric Effect, and Toroidal Magnetic Moments in a Family of Ln₄ squares*”
Chinmoy Das, Shefali Vaidya, **Tulika Gupta**, Jamie M. Frost, Mattia Righi, Euan K Brechin, Marco Affronte, Gopalan Rajaraman and Maheswaran Shanumgam, *Chem. Eur. J.* 2015, **21**, 15639-15650. (*No. of citations = 31*)
- “*Effect of ligand substitution around the Dy(III) on the SMM properties of dual-luminescent Zn-Dy and Zn-Dy-Zn complexes with large anisotropy energy barriers. A combined theoretical and experimental magneto-structural study*”
Jean Pierre Costes, Silvia Titos-Padilla, Itziar Oyarzabal, **Tulika Gupta**, Carine Duhayon, Gopalan Rajaraman and Enrique Colacio, *Inorg. Chem.* 2016, **55**, 4428-4440. (*No. of citations = 31*)
- “*Role of Lanthanide-Ligand Bonding in the Magnetization Relaxation of Mononuclear Single-ion Magnets: A Case Study on Pyrazole and Carbene ligated Ln^{III} (Ln= Tb, Dy, Ho, Er) Complexes*”
Tulika Gupta, G. Velmurugan, Thayalan Rajeshkumar, and Gopalan Rajaraman, *J. Chem. Sci.* 2016, **128**, 1615-1630 (Accepted as Front Cover Page). (*No. of citations = 10*)
- “*Observation of Slow Relaxation and Single Molecule Toroidal Behavior in a Family of Butterfly-shaped Ln₄ Complexes*”
Sourav Biswas, Sourav Das, **Tulika Gupta**, Saurabh Kumar Singh, Michael Pissas, Gopalan Rajaraman and Vadapalli Chandrasekhar, *Chem. Eur. J.* 2016, **22**, 18532-18550. (*No. of citations = 7*)
- “*Role of Single-Ion Anisotropy and Magnetic Exchange Interactions in Suppressing Zero-Field Tunnelling in {3d-4f} Single Molecule Magnets*”
Tulika Gupta, Mohd. Faizan Beg and Gopalan Rajaraman, *Inorg. Chem.* 2016, **55**, 11201-11215. (*No. of citations = 14*)
- “*Role of the diamagnetic zinc (II) ion in determining the electronic structure of lanthanide single-ion magnets*”
Maheswaran Shanmugam, Apoorva Upadhyay, Chinmoy Das, Shefali Vaidya, Sourabh Kumar Singh, **Tulika Gupta**, Ranajit Mondal, Stuart Langley, Keith Murray, Gopalan Rajaraman, *Chem. Eur. J.* 2017, **23**, 4903-4916. (*No. of citations = 9*)
- “*Design of a family of Ln₃ triangles with the HAT ligand (1,4,5,8,9,12-hexaazatriphenylene): Single-Molecule Magnetism*”
Ismael F. Díaz-Ortega, Juan Manuel Herrera, **Tulika Gupta**, Gopalan Rajaraman, Hiroyuki Nojiri, and Enrique Colacio, *Inorg. Chem.* 2017, **56**, 5594-5610. (*No. of citations = 3*)
- “*Designing a Dy₂ SMM with two well differentiated relaxation processes by using a non symmetric bis-bidentate bipyrimidine-N-oxide ligand: Comparison with mononuclear counterparts*”
Ismael F. Díaz-Ortega, Juan Manuel Herrera, Daniel Aravena, Eliseo Ruiz, **Tulika Gupta**, Gopalan Rajaraman, H. Nojiri and Enrique Colacio, *Inorg. Chem.* 2018, **57**, 6362-6375.
- “*Magnetic Anisotropy, Magneto-Structural Correlations and Mechanism of Magnetic Relaxation in {Dy^{III}N₈} complexes: A Theoretical Perspective*”
Tulika Gupta and Gopalan Rajaraman, *Eur. J. Inorg. Chem.* 2018, DOI : [10.1002/ejic.201800350](https://doi.org/10.1002/ejic.201800350)

■ PEER-REVIEWED MONOGRAPHS

- *“Introduction to Magneto-Chemistry of Mono,Di and Trinuclear Complexes”*
Tulika Gupta, Scientia Acta Xaveriana, ISSN. 0976-1152, Volume 6, No. 1, pp. 1-94, March 2015.
- *“Introduction to Molecule Based Nano Magnetic Materials”*
Tulika Gupta, Scientia Acta Xaveriana, ISSN. 0976-1152, Volume 6, No. 2, pp. 1-48, September 2015.

■ PEER-REVIEWED REVIEW ARTICLE

- *“Modelling Spin Hamiltonian Parameters of Molecular Nano Magnets”*
Tulika Gupta and Gopalan Rajaraman, *Chem. Commun.* 2016, **52**, 8972-9008. (*No. of citations = 13*)

■ PEER-REVIEWED BOOK CHAPTER

- *“Role of Ab Initio Calculations in the Design and Development of Lanthanide Based Single Molecule Magnets”*
Tulika Gupta, Mukesh Kumar Singh and Gopalan Rajaraman in Topics in Organometallic Chemistry , Springer International Publishing AG, 2018, pp. 1-74.

Date: 07.06.2018
Place: Varanasi, BHU

Tulika Gupta

Signature