Gourhari Jana, PhD

School of Mechanical Engineering and Materials Science, Washington State University, 99163, USA
+91-9647225828 gourharijana75@gmail.com, gourhari.jana@wsu.edu Gourhari Jana Gourhari Jana

Education:

- **PhD** Chemistry, Indian Institute of Technology Kharagpur, India — July 2015–November 2020
- **MSc** Chemistry, Vidyasagar University, India, % marks: 84.42 — July 2013–May 2015
- **BSc** Chemistry (Hons), Midnapore College, VU, India, % marks: 67.25 — July 2010–June 2013
- **Higher Secondary Education** (**12th**) in Science, WBCHSE Board, India, % marks: 86.00 — July 2008–June 2010
- **Secondary Education** (**10th**), WBBSE Board, India, % marks: 84.90 — July 2006–June 2008

Professional Experience:

- **Postdoc** Washington State University, WA, Pullman, USA — September 2025–Present
- **Visiting Scientist** Faculty of Physics, University of Warsaw, Poland — April 2025–June 2025
- **Research Associate-I** Indian Association for the Cultivation of Science, Kolkata, India — April 2024–April 2025
- **Postdoc** Michigan State University, East Lansing, Michigan, USA — March 2022–March 2024
- **Postdoc** Indian Institute of Technology Bombay, Mumbai, India — January 2021–January 2022
- **Research Associate (Adhoc)** S. N. Bose National Centre for Basic Sciences, India — October 2020–January 2021

Teaching/Mentoring Experience:

- **Project Mentor** University of Michigan, USA, # students: 2 — March 2022–Present
- **Project Mentor** Indian Institute of Technology Kharagpur, India, # students:10 — July 2015–November 2020
- **Teaching Assistantship** Indian Institute of Technology Kharagpur, India, # Postgraduate Level Courses: 4, # Undergraduate Level Courses: 1, Summer intern students: 6, MSc Project students: 4. — July 2015–November 2020

Experience and Research Interest:

Theoretical & Computational Chemistry

- **Electronic Structure Calculations** using Density Functional Theory (DFT) and conventional *ab initio* methods
- **Quantum Mechanics & Ab Initio Molecular Dynamics**
- **Density Functional Theory (DFT)** including Conceptual-DFT, Time-Dependent DFT (TD-DFT), and Broken-Symmetry DFT
- **Quantum Theory of Atoms in Molecules (QTAIM)** for molecular structure characterization
- ***Ab Initio* Adiabatic and Diabatic Global Potential Energy Surface (PES) Generation**
- **Application of Beyond Born-Oppenheimer Theory (BBO) in Quantum Scattering Processes**
- **Bonding & Non-Bonding Interaction Analysis**
- **Implicit & Explicit Solvation Models**
- **Aromaticity Analysis** and electronic delocalization studies

Molecular Modeling & Materials Design

- **Design of Molecular, Cluster, 2D and 3D Catalytic Materials** and their Chemical Reactivity Descriptors
- **Local and Global Minima Search** for structure optimization
- **Design and Development of Novel Nanomaterials** for catalysis and sensing applications
- **Design and Development of van der Waals and Non-van der Waals Complexes**, including topological aspects
- **Renewable Energy Materials**, including energy and hydrogen storage applications
- **Mechanically Interlocked Compounds & Molecular Machines**

Catalysis & Reaction Mechanisms

- **Catalysis** (heterogeneous and homogeneous) in gas, liquid, and solid phases
- **Electrocatalysis** for energy applications
- **Reaction Mechanism Analysis** including thermodynamics and kinetics
- **Rare Gas Chemistry & Ultracold Reactions**

Polymers & Drug Discovery

- **Molecular Dynamics and Interactions on the formation of polymers**
- **Design of Polymers and their Mechanistic Approaches**
- **Polymerization Mechanisms & Material Performance Optimization**

Quantitative Structure-Activity Relationship (QSAR) & Chemical Informatics

- **QSAR, QSPR, and QSTR-Based Studies** for biological activity and toxicity prediction

Research Summary:

Postdoctoral Research

Worked on Polymer Crystallization, Reaction mechanism for polymer materials design, catalysis reaction mechanism, Electro-chemical cell reactions, Reduction of CO_2 into valuable products, Electronic structure calculations (Open and Closed Shell), DFT, BS-DFT, TDDFT and Conceptual DFT, Ground and Excited-state calculation, Spin Cross Over (SCO), ab initio technique, Quantum Molecular Dynamics like Atom-centered Density Matrix Propagation (ADMP) and Born Oppenheimer Molecular Dynamics (BOMD) methods, Nonlinear optical property, Light-induced excited-spin-state trapping (LIESST) calculation.

- Designated to work on quantum chemistry, quantum molecular dynamics, Time-dependent DFT for spectral study, the study of the chemical bonding natures, chemical reactivity using atoms in molecule, ultracold reactions channel, thermodynamics and kinetics stability check, quantum mechanics and DFT, Electrochemical cell or redox reactions, macromolecular interactions, QSAR based toxicity analysis and drug design.
- Contributed significantly on Time-dependent excited state spin coupling and natural transition orbital analysis using PySOC code during first Research Associate position at the S.N. Bose National Centre for Basic Sciences.
- Investigated the light-induced excited-spin-state trapping (LIESST) and spin cross-over (SCO) during the first postdoc at the Indian Institute of Technology Bombay.
- Played a significant role in developing reactive force fields, quantum calculations, and other theoretical developments, including method/code development, polymerization mechanisms.
- Worked on catalysis and cheap catalyst design, redox reaction study, oxygen and hydrogen evolution reaction (OER and HER) and fuel cell, water splitting employing quantum mechanics, as well as other theoretical developments, including polymerization, novel reaction mechanisms, rotaxane property study, cubane chemistry and materials design.
- *Ab initio* adiabatic potential energy surfaces and conical intersections; quasi-classical trajectory calculations on two-state PES with nonadiabatic coupling as friction; single- and multi-state chemical reaction dynamics in Jacobi and hyperspherical coordinates; and application of Beyond Born–Oppenheimer theory in spectroscopy and scattering processes.
- Non-covalent interaction studies for energetic crystals and at interfaces of polymeric composites. Relate as to how electron localization and delocalization indices change under initiation of chemical reactions.

Doctoral Research

Explored the electronic structure calculation of interesting molecular systems employing DFT, including noble gas employed insertion, non-insertion, and inclusion compounds, noble-metal catalyst design, insights of ES-click polymerization reactions, chemisorption and physisorption of hydrogen on unprecedented molecular systems and clusters, and micro hydration behavior of novel inorganic clusters. Search of novel mechanisms for thermodynamically feasible but kinetically protected reaction channels. Utilized conceptual density functional theory and its allied reactivity descriptors for the semi-quantitative study of molecular reactivity, Delved into weak non-covalent interaction indices.

- Monitored the stability and metastability of molecular systems, clusters, and bonding and non-bonding interactions (weak and strong).
- Investigated the theoretical findings and clarified experiment observations using the density functional theory-based simulations.
- Concentrated on examining the structure, stability, reactivity, and pertinent bonding situation in chemical systems involving weak interactions, including different non-reactive species consisting of noble gases (Ng), coinage metals (so-called noble metals: Cu, Ag, and Au), and molecular hydrogen.
- Examined the global minimum structure and energy search using particle swarm optimization and firefly algorithms.
- Employed Quantitative Structure-Toxicity Relationship Models based on Hydrophobicity and Electrophilicity (Ecotoxicological QSARs).

Awards/Fellowships:

Awards & Honors

1. **Young Achiever Award (YAA)**, Institute of Scholars (InSc), 2021.
2. **Young Researcher Award (YRA)**, Institute of Scholars (InSc), 2021.
3. **Research Excellence Award (REA)**, Institute of Scholars (InSc), 2019.
4. **Acharya Prafulla Chandra Ray Memorial Award**, Indian Chemical Society (ICS) in International Seminar on RA2M, 2018.
5. **International Year of Chemistry-2011 (IYC-2011)** Award, 2011.
6. **Best Poster Award** in "International Year of Chemistry (IYC)" and "Symposium on Frontiers in Polymer Chemistry (FPC)", 2011.

Scholarship & Funding

1. **Senior Research Fellowship (SRF)** awarded by Indian Institute of Technology Kharagpur, West Bengal, India, 2017-2020.
2. **Junior Research Fellowship (JRF)** awarded by Indian Institute of Technology Kharagpur, West Bengal, India, 2015-2017.
3. **Graduate Aptitude Test in Engineering (GATE)** with All India Rank: 65 (Score-734), 2016.
4. **Joint CSIR-UGC National Eligibility Test (NET) Fellowship**, (All India Rank under CSIR scheme: 50), June 2017
5. **Department of Science and Technology (DST) INSPIRE Scholarship** awarded by Ministry of Science and Technology, India, 2010-2015.
6. **Merit-cum-Means (MCM) Scholarship** awarded by Department of Higher Education, India, 2010-2013.
7. **National Merit Scholarship** awarded by Ministry of Human Resource Development, Department of Higher Education, India, 2010-2011.
8. **Certificate of Merit for Securing Highest Marks** (430) in H.S. Examination, First Rank in Chandipur Dev. Block, 2010.

Computational Skills:

- **Program Packages:**
- **(i) Molecular-level Simulation Codes:** Gaussian09/16 (ground-state calculation), D3-Mol, MOLPRO (excited-state calculation), ORCA, PySOC, Q-Chem, ADF2013/14/19(EDA-NOCV calculation), AIMALL & Multiwfn (chemical bonding), NWChem, NBO 6.0 (NPA charge calculation), UCA-FUKUI (chemical reactivity calculation).
  (ii) Period-level Computational Codes: Materials Studio, VASP, CASTEP, CP2K, MOLCAS, Crystal 17, VNL-ATK.
- **Languages:** Python
- **Plotting Interfaces:** Xmgrace, GNU Plot, Interactive-Editor, Origin 6/8
- **Modelling & Visualization GUI:** Gauss View 3.0/5.0/6.0, Vesta, Chemcraft, Avogadro, Cylview, ORTEP, Mercury, Molekel, VMD, PyMol, MolDraw, Crystal Explorer, Molden, IQMol, XcrysDen
- **Operating Systems:** Ubuntu(/WSL), Linux, CentOS, Windows XP/7/8/10

Publications:

970=Total Citations
18=h-index
26=i10index
46= Research Articles (19 *first author*, 2 *corresponding author*), 3= Book chapters.

Google Scholar: https://scholar.google.com/citations?user=f8ndQd8AAAAJ&hl=en
Research Gate: *https://www.researchgate.net/profile/Gourhari_Jana*
ORCID ID: *https://orcid.org/0000-0001-7864-8489*

Peer-Reviewed Journals (published)

2025

[46] **G. Jana**, P.K. Chattaraj, "A careful scrutiny of the aromaticity in anionic polynitrogen clusters", *Phys. Chem. Chem. Phys.*, **2025**. https://doi.org/10.1039/D5CP01974E

[45] **G. Jana**, P.K. Chattaraj, "Exploring Advanced Nanostructures and Functional Materials for Efficient Hydrogen Storage: A Theoretical Investigation on Mechanisms, Adsorption Process, and Future Directions", *Front. Chem.*, **2025**, 17, 1525140. https://doi.org/10.3389/fchem.2025.1525140

2024

[44] Po-Wei Huang, K. R. Sanchez-Lievanos, D. Maldonado, **G. Jana**, J. L. Mendoza-Cortes, K. E. Knowles, and Marta C. Hatzell, "Surface Ligands Impact Nitrogen Photofixation on Metal Oxide Nanocrystals", *ACS Energy Lett. Energy Express.* **2024** *Adv. Funct. Mater*. https://doi.org/10.1002/adfm.202413319, 2413319.

2023

[43] A N. Safaie[a], A. Rodriguez[a], **G. Jana**[a], J. Smak, J. L. Mendoza-Cortes, R. C. Ferrier, Jr., "Unveiling the Mechanisms of Epoxide Polymerization with N—Al Adduct Catalysts: A Comprehensive Experimental and Theoretical Investigation" *Poly. Chem.*, **2023**, https://doi.org/10.1039/D3PY00482A**.** (IF= 5.36)

[42] **G. Jana**, JL Mendoza-Cortes, "Thermodynamics, Kinetics, and Optical Properties of Rotaxane: A First-Principles Molecular Dynamics Study" *J. Phys. Chem. A*, **2023**, *127*, 2671–2687**.** (IF= 2.86)

[41] S. Mondal, **G. Jana**, H.K. Srivastava, G.N. Sastry, P.K. Chattaraj, "Structure and stability of the sH binary hydrate cavity and host-guest versus guest-guest interactions therein: A DFT approach", *J. Comput. Chem.* **2023**, *144*, 1446–1553**.** (IF= 3.23)
[40] R. Pal, **G. Jana**, P.K. Chattaraj, "Structure and Stability of a New Set of Noble gas Insertion Compounds, XNgOPO(OH)2 (X = F, Cl, Br; Ng = Kr, Xe, Rn): An in silico Investigation", *Theo. Chem. Acc.*, **2023**, *142 (34), 1-11*. (https://doi.org/10.1007/s00214-023-02973-2). (IF= 3.23)

2022
[39] R. Jha, **G. Jana**, P. K. Chattaraj, "Possible catalytic activity of N,N-coordinated mono-cationic copper bound Pyrazol-1-yl(1H-pyrrol-2-yl)methanone complex: a computational study", *Proc. Indian Natl. Sci. Acad*. **2022**. (https://doi.org/10.1007/s43538-022-00072-7**).**
[38] K. Misra, B. Halder, F. Banerjee, **G. Jana**, H.S. Maity, A.B. Kachave, A. Nag, "Synthesis and computational study of beta-amino alcohols starting from value-added plant polyphenol using água-de-coco do Ceará (ACC) as a green reaction medium", *Polycyclic Aromatic Compounds*, **2022**.
DOI: 10.1080/10406638.2022.2069136 (IF= 3.74)

2021
[37] **G. Jana***, R. Pal, S. Pan, P. K. Chattaraj, "XNgNSi (X = HCC, F; Ng = Kr, Xe, Rn): A New Class of Metastable Insertion Compounds Containing Ng-C/F and Ng-N Bonds and Possible Isomerization therein", *J. Phys. Chem. A* **2021,** *125*, 10514-10523. (IF= 2.86)
[36] **G. Jana**, H. Mondal, P. K. Chattaraj, "H_2 Adsorption by Noble Gas Insertion Compounds: A Computational Study", *J. Ind. Chem. Soc*. **2021,** 98, 100060 (IF= 0.15)
[35] A. Mitra, **G. Jana**, R. Pal, P. Gaikwad, S. Sural, P. K. Chattaraj, "Determination of Stable Structure of a Cluster using Convolutional Neural Network and Particle Swarm Optimization", *Theor. Chem. Acc.* **2021**, *140*, Article Number 30 (IF= 2.23).
[34] P. Mondal, **G. Jana**, T. S. Pal, P. K. Chattaraj, N. K. Singha, "Self-healable functional polymers based on Diels–Alder 'click chemistry' involving substituted furan and triazolinedione derivatives: a simple and very fast approach", *Polym. Chem.* **2021**, *12*, 6283-6290. (IF= 4.76)
[33] S. R. Nambiar, **G. Jana**, S. Pan, P. K. Chattaraj, "Do Superalkalis and Superhalogens Enhance Existing Chemical Reactions?", *Chem. Phys. Lett*. **2021**, *762*, 138131. (IF= 2.03)

2020
[32] **G. Jana**, P. K. Chattaraj, "Effect of Substitution on the Bonding in He Dimer Confined within Dodecahedrane: A Computational Study", *J. Comput. Chem*. **2020**, *41*, 2398-2405. (IF= 3.23)
[31] **G. Jana**, R. Pal, S. Mondal, P. K. Chattaraj, "Do the Ni Binding Modes on $C_{12}N_{12}$ Cluster Influence Its H_2 Trapping Capability?", *Adv. Mater. Lett.* **2020**, *11*, Article Number 20041500. (IF= 1.15)
[30] A. Mitra, **G. Jana**, P. Agrawal, S. Sural, P. K. Chattaraj, "Integrating Firefly Algorithm with Density Functional Theory for Global Optimization of Al_4^{2-} Clusters", *Theor. Chem. Acc*. **2020**, *139*, Article Number 32. (IF= 2.23)
[29] P. Mondal, **G. Jana**, P. K. Behera, P. K. Chattaraj, N. K. Singha, "Fast 'ES-Click' Reaction involving Furfuryl and Triazolinedione Functionalities towards Desinging a Healiable Polymethacrylate", *Macromolecules* **2020**, *53*, 8313-8323. (IF= 5.92)
[28] S. Pan, **G. Jana**, R. Saha, L Zhao, P. K. Chattaraj, "Intriguing Structural, Bonding and Reactivity Features in Some Beryllium Containing Complexes", *Phys. Chem. Chem. Phys*. **2020**, *22*, 27476-27495 (IF= 3. 57)
[27] R. Pal, **G. Jana**, P. K. Chattaraj, "Ligand Stabilized Transient "MNC" and Its Influence in MNC→MCN Isomerization Process: A Computational Study (M = Cu, Ag, and Au)", *Theor. Chem. Acc*. **2020**, *139*, Article Number 15. (IF= 2.23)
[26] S. Mandal, A. Mandal, **G. Jana**, S. Mallik, S. Roy, A. Ghosh, P. K. Chattaraj, D. K. Goswami, "Low Operating Voltage Organic Field-Effect Transistors with Gelatin as a Moisture-Induced Ionic Dielectric Layer: the Issues of High Carrier Mobility", *ACS Appl. Mater. Interfaces* **2020**, *12*, 19727-19736. (IF= 8.76)
[25] B. Samanta, A. De, **G. Jana**, P. K. Chattaraj, N. Ganguly, M. Gomez-Rodriguez., "NEVAE: A Deep Generative Model for Molecular Graphs", *J. Mach. Learn. Res*. **2020**, *21*, 1-33. (IF= 4.09)
[24] A. Morales-Bayuelo, J. Sánchez-Márquez, **G. Jana**, P. K. Chattaraj, "A Conceptual DFT Analysis of the Plausible Mechanism of Some Pericyclic Reactions", *Struct. Chem*. **2020**, *31*, 1745–1756. (IF= 1.55)

2019
[23] **G. Jana**, R. Jha, S. Pan, P. K. Chattaraj, "Microsolvation of Lithium-Phosphorus Double Helix: A DFT Study", *Theor. Chem. Acc*. **2019**, *138*, Article Number 75. (IF= 2.23)
[22] **G. Jana**, A. Mitra, S. Pan, S. Sural, P. K. Chattaraj, "Modified Particle Swarm Optimization Algorithms for the Generation of Stable Structures of Carbon Clusters, C_n (n = 3-6, 10)", *Front. Chem*. **2019**, *7*, 485. (IF= 3.69)
[21] **G. Jana**, R. Pal, S. Sural, P. K. Chattaraj, "Quantitative Structure - Toxicity Relationship: An "In Silico Study" using Electrophilicity and Hydrophobicity as Descriptors", *Int. J. Quantum. Chem*. **2019**, *120*, e26097. (IF= 2.26)
[20] S. Pan, **G. Jana**, G. Merino, P. K. Chattaraj, "Noble-Noble Strong Union: Gold at its Best to Make a Bond with a Noble Gas

Atom", *ChemistryOpen Rev*. **2019**, *8*, 173-187. (IF= 2.21)
[19] P. Mondal, **G. Jana**, P. K. Behera, P. K. Chattaraj, N. K. Singha, "A New Healable Polymer Material based on Ultrafast Diels-Alder 'Click' Chemistry using Triazolinedione and Fluorescent Anthracyl Derivatives; A Mechanistic Approach", *Polym. Chem*. **2019**, *10*, 5070-5079. (IF= 4.76)
[18] R. Saha, **G. Jana**, S. Pan, G. Merino, P. K. Chattaraj, "How Far Can One Push The Noble Gases Towards Bonding?: A Personal Account", *Molecules* **2019**, *24*, 2933. (Review Article) (IF= 3.27)
[17] R. Dutta, **G. Jana**, D. Mondal, A. Pyne, S. Sil, P. K. Chattaraj, N. Sarkar, "The Role of Viscosity on Various Dynamical Processes of Different Fluorophores in Ionic Liquid-Cosolvent Mixtures: A Femtosecond Fluorescence Upconversion Study", *Photochem. Photobio. Sci*. **2019**, *18*, 1359-1372. (IF= 2.83)
[16] R. Pal, G. Pal, **G. Jana**, P. K. Chattaraj, "An In Silico QSAR Model Study using Electrophilicity as a Possible Descriptor against T. brucei", *Int. J. Chemoinf. Chem. Eng*. **2019**, *8*, 57-68. (IF= 1.88)
[15] B. Samanta, A. De, **G. Jana**, P. K. Chattaraj, N. Ganguly, M. Gomez-Rodriguez, "Nevae: A deep generative model for molecular graphs", Proceedings of the AAAI Conference on Artificial Intelligence **2019**, *33*, 1110-1117. (IF= 3.40)
[14] A. Kumar, R. Ananthakrishnan, **G. Jana**, P. K. Chattaraj, S. Nayak, S. K. Ghosh, "An Intramolecular Charge Transfer Induced Fluorescent Chemosensor for Selective Detection of Mercury (II) and its Self-Turn-On Inside Live Cells at Physiological pH", *ChemistrySelect*. **2019**, *4*, 4810-4819. (IF= 1.81)

2018
[13] **G. Jana**, S. Pan, E. Osorio, L. Zhao, G. Merino, P. K. Chattaraj, "Cyanide-Isocyanide Isomerization: Stability and Bonding in Noble Gas Inserted Metal Cyanides (Metal = Cu, Ag, Au)", *Phys. Chem. Chem. Phys*. **2018**, *20*, 18491-18502. (IF= 3.57)
[12] **G. Jana**, S. Pan, P. L. Rodríguez-Kessler, G. Merino, P. K. Chattaraj, "Adsorption of Molecular Hydrogen on Lithium–Phosphorus Double-Helices", *J. Phys. Chem. C* **2018**, *122*, 27941-27946. (IF= 4.18)
[11] S. Pan, **G. Jana***, E. Ravell, X. Zarate, E. Osorio, G. Merino, P. K. Chattaraj, "Stable NCNgNSi (Ng= Kr, Xe, Rn) Compounds with Covalently Bound C-Ng-N Unit: Possible Isomerization of NCNSi through the Release of the Noble Gas Atom", *Chem. Euro. J*. **2018**, *24*, 2879-2887. (IF= 4.86)
[10] **G. Jana**, S. Pan, G. Merino, P. K. Chattaraj, "Noble Gas Inserted Metal Acetylides (Metal= Cu, Ag, Au)", *J. Phys. Chem. A* **2018**, 122, 7391-7401. (IF= 2.86)
[9] **G. Jana**, R. Pal, P. K. Chattaraj, "Hydrogen Storage in Lithium Adsorbed and Polylithiated (OLi_2) Heteroatom (B, N) Modified (2, 2) γ-Graphyne Nanotube and Its CO Sensing Potential: A Computational Study", *J. Ind. Chem. Soc*. **2018**, *95*, 1457-1464. (IF= 0.15)
[8] P. Mitikiri, **G. Jana**, S. Sural, P. K. Chattaraj, "A Machine Learning Technique towards Generating Minimum Energy Structures of Small Boron Clusters", *Int. J. Quantum Chem*., **2018**, *118*, e25672. (IF= 2.26)
[7] R. Pal, **G. Jana**, S. Sural, P. K. Chattaraj, "Hydrophobicity versus Electrophilicity: A New Protocol toward Quantitative Structure–Toxicity Relationship", *Chem. Bio. Drug. Des*. **2018**, *93*, 1083-1095. (IF= 2.40)
[6] S. Mondal, T. Goswami, **G. Jana**, A. Misra, P. K. Chattaraj, "A Possible Reason behind the Initial Formation of Pentagonal Dodecahedron Cavities in sI-Methane Hydrate Nucleation: A DFT Study", *Chem. Phys. Lett*. **2018**, *691*, 415-420. (IF= 2.03)
[5] A. Morales-Bayuelo, J. Sánchez-Márquez, **G. Jana**, P. K. Chattaraj, "Analyzing Torquoselectivity in a Series of Unusual Ring-Opening Reactions through Bond Reactivity Indices and the Adaptive Natural Density Partitioning method", *Int. J. Quantum. Chem*. **2018**, *118*, e25778. (IF= 2.26)

2017
[4] **G. Jana**, S. Pan, P. K. Chattaraj, "Binding of Small Gas Molecules by Metal–Bipyridyl Monocationic Complexes (Metal= Cu, Ag, Au) and Possible Bond Activations therein" *J. Phys. Chem. A* **2017**, *121*, 3803-3817. (IF= 2.86)
[3] **G. Jana**, S. Pan, G. Merino, P. K. Chattaraj, "MNgCCH (M= Cu, Ag, Au; Ng= Xe, Rn): the first set of compounds with M–Ng–C bonding motif", *J. Phys. Chem. A* **2017**, *121*, 6491-6499. (IF= 2.86)
[2] S. Pan, **G. Jana**, A. Gupta, G. Merino, P. K. Chattaraj, "Endohedral Gas Adsorption by Cucurbit[7]uril: A Theoretical Study", *Phys. Chem. Chem. Phys*. **2017**, *19*, 24448-24452. (IF= 3. 57)

2016
[1] **G. Jana**, R. Saha, S. Pan, A. Kumar, G. Merino, P. K. Chattaraj, "Noble Gas Binding Ability of Metal-Bipyridine Monocationic Complexes (Metal= Cu, Ag, Au): A Computational Study" *ChemistrySelect* **2016**, *1*, 5842-5849. (IF= 1.81)

Book Chapters (published)

[1] **G. Jana**, R. Pal, S. Sural, P. K. Chattaraj, "Quantitative Structure-Toxicity Relationship Models Based on Hydrophobicity and Electrophilicity" for the Book Ecotoxicological QSARs; Volume Editor: Prof. Kunal Roy, *SpringerProtocols* **2019**, *27*, 661-679.

[2] **G. Jana**, R. Pal, "Generation of Global Minimum Energy Structures using Machine Learning Technique", Edited book (Elsevier Publishers) on 'Atomic Clusters with Unusual Structure, Bonding and Reactivity', Elsevier, **2021**.
[3] **G. Jana**, R. Pal, P. K. Chattaraj, "A New Set of Thermochemically Stable Nitrile and Isonitrile Insertion Compounds with Their Possible Trapping at Ambient Temperature", Edited book (Nova Publishers) on Cyanide: Occurrence, Applications and Toxicity ', **2022**.

Complete List

Note: a = co-first author, * = corresponding author

Editorial Board Member and Review Editorship

- **Journal Reviewer and Board Member**: **Review Editor** of *Frontiers in Chemistry* (Theoretical and Computational Chemistry Section),
- **Editorial Board Member and Review Editor** of *International Journal of Computational and Theoretical Chemistry* and IEEE Transactions on Artificial Intelligence.
- **Iterative International Publishers (IIP)** Proceedings Editor for the Edited Book Series Volume 3 2023.
- **Journal Reviewer**: **Reviewer** of *Royal Society of Chemistry*.

Journal Review (Total number): 15 (peer-reviewed)

Selected Conferences/Oral Presentations:

Oral Presentations

1. **Young Scientists' Conference**, India International Science Festival, Kolkata, India. (2019)
2. **56 Annual Convention of Chemists 2019 & International Conference** on Recent Trends in Chemical Sciences, ICS & School of Chemistry Ravishankar Shukla University, Chhattisgarh, India. (2019)
3. International Seminar on "**Recent Advances in Molecules & Materials, RA2M-2018**", Haldia Institute of Technology and The Indian Chemical Society, India. (2018)
4. **Machine Learning for Medical Image Analysis (WMLMIA 2018)**, IIT Kharagpur, India, (2018).
5. **IUPAC CCCE 2021 - 48th World Chemistry Congress (WCC) & 104th Canadian Chemistry Conference and Exhibition (CCCE)** (2021).

Poster Presentations

1. International Seminar on **Recent Advances in Molecules & Materials (RA2M)**, Haldia Institute of Technology and The Indian Chemical Society, India. (2018)
2. **International Conference on Systems and Processes in Physics, Chemistry and Biology**, (ICSPPCB), Assam University, India, (2018)
3. **Machine Learning for Medical Image Analysis (WMLMIA)**, Indian Institute of Technology Kharagpur, India. (2018)
4. National Seminar on **Recent Advances in Functional Inorganic & Nanomaterials Chemistry (RAFNIC)**, Indian Institute of Technology Kharagpur, India. (2017)
5. **15th Indian Theoretical Chemistry Symposium**, University of Hyderabad, India, (2016)
6. International Year of Chemistry (IYC) Symposium on **Frontiers in Polymer Chemistry (FPC)**, Indian Institute of Technology Kharagpur and Society of Polymer Science, India. (2011; Best Poster Presenter)
7. Conference on **Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems,** held during December 11- 14, 2024, **at IISER Kolkata**
8. A Symposium on **Recent Advances in Physical Chemistry Research (SRAPCR-2025) 10th - 13th April, 2025 at IACS Kolkata**.

Workshops and Conferences

1. **Young Scientists' Conference**, India International Science Festival, Kolkata, India. (2019)
2. Workshop on **Towards Smart Functional Materials: An Interdisciplinary Approach** sponsored and organized by Indian Academy of Sciences, Bangalore and Department of Chemistry, IIT Kharagpur, India. (2019)
3. Workshop on **Machine Learning for Medical Image Analysis (WMLMIA)**, Department of Chemical Engineering, IIT Kharagpur, India. (2018)
4. Workshop on **Introduction to Python**, IEEE Student Branch, IIT Kharagpur & URJA School of Energy Science and Engineering Student Club, India. (2017)
5. Workshop on Reference Manager **Mendeley & Endnote**, Department of Chemical Engeneering, IIT Kharagpur, India. (2016)
6. **Association of Chemistry Teachers (ACT-IYC) concept test in Chemistry**, Midnapore College, Midnapore, India. (2011; Securing 58% marks)

Teaching Experience	**Teaching Assistantship**, Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur, India. 1. Course: Computational Chemistry (Int. M.Sc., M.Sc., RS), Student Strength: 43. 2. Course: Computational Chemistry Laboratory (Int. M.Sc., M.Sc., RS), Student Strength: 40 3. Course: Molecular Spectroscopy & Molecular Structure (Int. M.Sc., M.Sc., RS), Student Strength: 43 4. Course: Physical Chemistry Laboratory (M.Sc.), Student Strength: 84 5. Course: Physical Chemistry Laboratory (B.Tech.), Student Strength: 80 **Mentoring as Project Assistant** **Summer Project Students: (**Ranita Pal, Nayanthara K J., Swati Snigdha Priyadarsini, Sachin Ramesh Nambiar, Anmol Sahu, Suman Bhaumik, Sudha Swatta Roy, Swarnshikha Sinha) **M.Sc. Project Students: (**Ayan Majumder, Sk Habibullah, Nanigopal Bera, Pratiksha Gaikwad, Goutam Pal) Also guided all the junior PhD students in the laboratory.

Course work Attended (29 Credit)

1. Course: Methods in Molecular Simulations (Sub. No. TS70001), Credit 4.
2. Course: Advanced Numerical Analysis (Sub. No. MA60059), Credit 4.
3. Course: Advanced Quantum Chemistry (Sub. No. CY60105), Credit 3.
4. Course: Computational Chemistry (Sub. No. CY60101), Credit 3.
5. Course: Molecular Spectroscopy & Molecular Structure (Sub. No. CY61044), Credit 4.
6. Course: Organic Photochemistry and Pericyclic Reactions (Sub. No. CY60003), Credit 3.
7. Course: English for Technical Writing (Sub. No. HS63002), Credit 4.
8. Course: Deep Learning Foundations and Applications (Sub. No. AI61002), Credit 4.

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