

Assistant Professor in Chemistry
Department of Education
A. M. School of Educational Sciences
Assam University (A Central University)
Silchar 788011, Assam, India

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Experience

Assistant Professor in Chemistry Oct. 2017 – till date
Department of Education Assam, India
A. M. School of Educational Sciences
Assam University (A Central University), Silchar

National Postdoctoral Fellow Feb. 2017 – Oct. 2017
Postdoctoral Research with Prof. Swapan K Pati Bengaluru, Karnataka
Theoretical Sciences Unit
Jawaharlal Nehru Centre for Advanced Scientific Research

CTS Research Visitor Nov. 2016
Department of Chemistry & Center for Theoretical Studies Kharagpur, India
Indian Institute of Technology Kharagpur

Postdoctoral Research with Prof. Gabriel Merino Sept. 2015 – Aug. 2016
Departamento de Fisica Aplicada, CINVESTAV Merida Merida, Mexico

Research Assistant Jun. – Jul. 2015
Department of Chemistry & Center for Theoretical Studies Kharagpur, India
Indian Institute of Technology Kharagpur

Education

Ph.D., Indian Institute of Technology Kharagpur 2009 – 2015
Department of Chemistry Kharagpur, India
Supervisor: Prof. P. K. Chattaraj
Thesis: All-metal and nonmetal clusters and their gas storage potential

M.Sc., University of Pune 2009
Centre for Advanced Studies in Chemistry Pune, India
Department of Chemistry
Supervisor: Prof. A. S. Kumbhar
Project: Synthesis and characterization of different Cu(I) and Cu(II) Polypyridyl complexes

B.Sc., University of Burdwan 2006
Department of Chemistry, Raghunathpur College, Purulia WB, India

Journal Publications

During Assistant Professorship:

1. G. G. Nnabuike, Sukanta Mondal, S. Salunke-Gawali, A. S. Patil, R. J. Butcher, J. A. Obaleye, "Structural features of nickel (II) mixed ligand complexes with mefenamic acid and nitrogen donor ligands" **J. Mol. Struct.**, 2020. [**Impact factor: 2.011**]
DOI: <https://doi.org/10.1016/j.molstruc.2020.129632>
2. R. Parida, G. N. Reddy, E. Osorio, A. Muñoz-Castro, Sukanta Mondal*, S. Giri*, "Unique magnetic shielding and bonding in Pnicogen nortricyclane Zintl clusters", **Chem. Phys. Lett.** (2020) 749, 137414. [**Impact factor: 2.029**]
3. J. C. Gonzalez, Sukanta Mondal, F. Ocayo, R. Guajardo-Maturana, A. Muñoz-Castro*, "Nature of C₆₀ and C₇₀ fullerene encapsulation in a porphyrin- and metalloporphyrin-based cage: Insights from dispersion-corrected density functional theory calculations", **Int. J. Quantum Chem.** (2020) 120, 3, e26080. [**Impact factor: 2.263**]
4. G. Jana, R. Pal, Sukanta Mondal*, P. K. Chattaraj*, "Do the Ni binding modes on C₁₂N₁₂ cluster influence its H₂ trapping capability?", **Adv. Mater. Lett.** (2020) 11, 4, 20041500. [**Impact factor: 1.150**]
5. M. Homray, Sukanta Mondal, A. Misra*, P. K. Chattaraj*, "Bond Stretch Isomerism in Be₃²⁻ driven by Renner-Teller Effect", **Phys. Chem. Chem. Phys.** (2019) 21, 7996. [**Impact factor: 3.567**]
6. Sukanta Mondal*, P. Sarkar, A Muñoz-Castro*, "Planar ten-membered 10- π -electron aromatic (CH)₅(XH)₅ {X = Ge, Sn} systems" **J. Mol. Model.** (2018) 24, 264. [**Impact factor: 1.346**]

During Postdoctoral Research:

7. S. Das, Sukanta Mondal, S. K. Pati*, "Mechanistic Insights into Hydrogen Activation by Frustrated N/Sn Lewis Pairs" **Chem. Eur. J.** (2018) 24, 2575. [**Impact factor: 4.857**]
8. Sukanta 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. [**Impact factor: 2.029**]
9. J. Barroso, Sukanta Mondal, J. L. Cabellos, E. Osorio, S. Pan, and G. Merino*, "Structure and Bonding of Alkali-Metal Pentalenides" **Organometallics** (2017) 36, 310. [**Impact factor: 4.060**]
10. Sukanta Mondal, J. L. Cabellos, S. Pan, E. Osorio, J. J. Torres-Vega, W. Tiznado, A. Restrepo and G. Merino*, "10- π -Electron Arenes a la Carte: Structure and Bonding of the [E-(C_nH_n)-E]ⁿ⁻⁶ (E = Ca, Sr, Ba; n = 6–8) Complexes" **Phys. Chem. Chem. Phys.** (2016) 18, 11909. [**Impact factor: 3.567**]

11. S. Pan, R. Saha, S. Mandal, Sukanta Mondal, A. Gupta, M. A. Fernández-Herrera, G. Merino*, P. K. Chattaraj*, "Selectivity in Gas Adsorption by Molecular Cucurbit[6]uril" **J. Phys. Chem. C** 120, 13911, 2016. [Impact factor: 4.270]
12. Sukanta Mondal, E. Osorio, S. Pan, J. L. Cabellos, S. Martinez, E. Florez, and G. Merino*, "Why CpAl–Cr(CO)₅ is Linear while CpIn–Cr(CO)₅ is Not? Understanding the Structure and Bonding of the CpE–Cr(CO)₅ (E = Group 13 element) Complexes" **Theor. Chem. Acc.** (2016) 135, 240. [Impact factor: 2.233]
13. S. Jalife, Sukanta Mondal, J. L. Cabellos, G. Martínez-Guajardo, S. Pan, M. A. Mendez-Rojas, I. Fernandez, G. Frenking*, and G. Merino*, "Breaking the Isolated Pentagon Rule by Encapsulating Xe₂ in C₆₀: The Guest Defines the Shape of the Host" **Chem. Select** (Communications) (2016) 1, 2405. [Impact factor: 1.811]
14. S. Jalife, Sukanta Mondal, E. Osorio, J. L. Cabellos, G. Martínez-Guajardo, M. A. Fernandez-Herrera, and G. Merino*, "Nonclassical 21-Homododecahedryl Cation Rearrangement Revisited" **Org. Lett.** (2016) 18, 1140. [Impact factor: 6.555]
15. S. Jalife, Sukanta Mondal, J. L. Cabellos, G. Martinez-Guajardo, M. A. Fernandez-Herrera, and G. Merino*, "The Cubyl Cation Rearrangements" **Chem. Commun.** (2016) 52, 3403. [Impact factor: 5.996]
16. E. Florez, N. Acelas, C. Ibarguen, Sukanta Mondal, J. L. Cabellos, G. Merino, and A. Restrepo*, "Microsolvation of NO₃⁻: structural exploration and bonding analysis" **RSC Adv.** (2016) 6, 71913. [Impact factor: 3.070]
17. Y. Jin, Y. Tian, X. Kuang, C. Lu, J. L. Cabellos, Sukanta Mondal, and G. Merino*, "Structural and Electronic Properties of Ruthenium-Doped Germanium Clusters" **J. Phys. Chem. C** (2016) 120, 8399. [Impact factor: 4.270]

During PhD:

18. Sukanta Mondal, M. Ghara, and P. K. Chattaraj*, "Hydrogen Trapping Potential of (HF)_m (m = 1–8) and (H₂O)_n (n = 1–10) Clusters" **Comp. Theo. Chem.** (2015) 1071, 18. [Impact factor: 1.403]
19. S. Chattaraj, K. Srinivasu, Sukanta Mondal, and S. K. Ghosh*, "Hydrogen Trapping Ability of the Pyridine–Lithium⁺ (1:1) Complex" **J. Phys. Chem. A** (2015) 119, 3056. [Impact factor: 2.600]
20. Sukanta Mondal, and P. K. Chattaraj*, "Stability and Structural Dynamics of Be₃²⁻ Clusters" **Chem. Phys. Lett.** (2014) 593, 128. [Impact factor: 2.029]
21. Sukanta Mondal, and P. K. Chattaraj*, "Noble Gas Encapsulation: Clathrate Hydrates and their HF Doped Analogues" **Phys. Chem. Chem. Phys.** (2014) 16, 17943. [Impact factor: 3.567]
22. Sukanta Mondal, S. Giri, and P. K. Chattaraj*, "Possibility of Having HF Doped Hydrogen Hydrates" **J. Phys. Chem. C** (2013) 117, 11625. [Impact factor: 4.270]

23. Sukanta Mondal, S. Giri, and P. K. Chattaraj*, "Methane Hydrates and their HF Doped Analogues" **Chem. Phys. Lett.** (2013) 578, 110. [**Impact factor: 2.029**]
24. Sukanta Mondal, S. Ghosh, and P. K. Chattaraj*, "A Molecular Dynamics Study on SI Hydrogen Hydrate" **J. Mol. Model.** (2013) 19, 2785. [**Impact factor: 1.346**]
25. Sukanta Mondal, K. Srinivasu, S. Ghosh*, and P. K. Chattaraj*, "Isomers of C₁₂N₁₂ as Potential Hydrogen Storage Materials and the Effect of the Electric Field Therein" **RSC Advances** (2013) 3, 6991. [**Impact factor: 3.070**]
26. S. Pan, Sukanta Mondal, and P. K. Chattaraj*, "Cucurbiturils as Promising Hydrogen Storage Materials: A Case Study of Cucurbit[7]uril" **New J. Chem.** (2013) 37, 2492. [**Impact factor: 3.288**]
27. S. Kumar, G. Mani*, Sukanta Mondal, and P. K. Chattaraj*, "Pyrrole-Based New Diphosphines: Pd and Ni Complexes Bearing the PNP Pincer Ligand" **Inorg. Chem.**, (2012), 51, 12527. [**Impact factor: 4.850**]
28. A. Chakraborty, S. Bandaru, R. Das, S. Duley, S. Giri, K. Goswami, Sukanta Mondal, S. Pan, S. Sen and P. K. Chattaraj*, "Some Novel Molecular Frameworks Involving Representative Elements" **Phys. Chem. Chem. Phys.** (2012) 14, 14784. (Published as a cover article). [**Impact factor: 3.567**]
29. P. K. Chattaraj, S. Bandaru and Sukanta Mondal, "Hydrogen Storage in Clathrate Hydrates", **J. Phys. Chem. A** (2011) 115, 187. [**Impact factor: 2.600**]

Book Chapters

1. Sukanta Mondal, A. Chakraborty, S. Pan, and P. K. Chattaraj*, "Designing of Some Novel Molecular Templates Suitable for Hydrogen Storage Application: A Theoretical Approach", **Nanoscience and Computational Chemistry: Research Progress** (2013), by A. G. Mercader, E. A. Castro, and A. K. Hagi, Apple Academic Press: CRC Press, a Taylor & Francis Group.
2. A. Chakraborty, Sukanta Mondal, and P. K. Chattaraj*, "Conceptual DFT and Chemical Reactivity" in "**Theoretical and Computational Advances: From Atoms to Molecules to Materials**" ed. D. Kumar, (2017), ISBN: 978-93-5196-507-7, Self Publishing, Lucknow (U. P.) India.

Reviewer

1. Journal of Molecular Modeling, Springer Link.
2. International Journal of Hydrogen Energy, Elsevier.

Selected Grants, Awards, & Achievements

1. Fellow of the Indian Chemical Society, Fellowship Number is F/8188 (Life Member), 2019.

2. Recipient of UGC BSR Research Start-Up Grant from University Grants Commission, MHRD, Govt. of India, 2019.
3. Selected in CTS Visitor's Programme (Second time), IIT Kharagpur, India, for a short research stay, 2018.
4. Recipient of SERB National Postdoctoral Fellowship (2017), Department of Science and Technology, Government of India.
5. Selected in CTS Visitor's Programme, IIT Kharagpur, India, for a short research stay, 2016.
6. Recipient of SNI (Sistema Nacional de Investigadores) Level – 1, 2016, CONACYT, Mexico.
7. Senior Research Fellow, 2011, Indian Institute of Technology Kharagpur, India.
8. Junior Research Fellow, 2009, Indian Institute of Technology Kharagpur, India.
9. Qualified the joint CSIR-UGC Junior Research Fellowship (JRF) and eligibility for Lectureship- National Eligibility Test (NET), December, 2008.
10. Qualified the Graduate Aptitude Test in Engineering, GATE-2008, India.
11. Recipient of merit based scholarship, NCL Scholarship during the master's study (2007-2009) from National Chemical Laboratory, Pune, India.
12. Cleared all India based postgraduate entrance test conducted by Department of Chemistry, University of Pune and National Chemical Laboratory in 2007.

Selected Conferences, Posters, and Talks

1. **Invited talk** (Title: Selective host-guest organization in the initial stage of sI methane hydrate nucleation) in the international conference '16th Theoretical Chemistry Symposium (TCS 2019)' organized by the Birla Institute of Technology & Science, Pilani, Pilani Campus, Pilani, Rajasthan 333031, India.
2. **Special lecture** (Title: Hydrogen and methane gas encapsulation in clathrate hydrates) in the "Chemistry Colloquium" of Department of Chemistry, University of North Bengal, Siliguri, West Bengal 734013, India (January 2019).
3. **Oral presentation** (Title: Clathrate Hydrates) in the National Conference on Emerging Materials, March 2018, organized by the Department of Chemistry, Assam University (A Central University), Silchar 788 011, India.
4. Presented a poster in the International Conference on Systems and Processes in Physics, Chemistry and Biology (ICSPPCB-2018) organised by the Department of Physics, Assam University (A Central University), Silchar 788 011, India.

5. **Oral Presentation** (Title: Hydrogen and methane storage in clathrate hydrates and HF doped clathrate hydrates) in 51st Annual Convention of Chemists 2014, Indian Chemical Society' December 9-12, 2014 at the Department of Chemistry, Kurukshetra University, Kurukshetra, India.
6. **Invited talk** on the topic "Hydrogen storage in clathrate hydrates and HF doped clathrate hydrates" in '2nd International Symposium on Energy Challenges and Mechanics (ECM2)' 19-21 August 2014, Aberdeen, **Scotland, United Kingdom**.
7. Presented a poster in **DAE BRNS** Symposium on Current Trends in Theoretical Chemistry (CTTC-2013), September 26-28, 2013, Bhabha Atomic Research Centre, Mumbai, India.
8. Presented a poster in Theoretical Chemistry Symposium (**TCS-2012**), December 19 – 22, 2012, IIT Guwahati, India.
9. Participated and contributed in a poster presented from the Theoretical Chemistry Lab. (Prof. P. K. Chattaraj) in the 'Diamond Jubilee Symposium on Recent Trends in Chemistry (DJSRTC-2011)' at IIT Kharagpur, October 21-23, 2011, India.
10. **Oral presentation** regarding the advancement of project **HYPOMAP** (New materials for hydrogen powered mobile applications), at National Chemical Laboratory, May 7-8, 2011, Pune, India.
11. Participated in the School on Understanding Molecular Simulations: Theory and Applications (UMS-2010), which was organized at IIT Kanpur from November 3-13, 2010, India.
12. Attended the International Conference "Of Molecules and Materials" on 28-29 December -2009 at IISER-Kolkata, India.

Service to the Assam University, Silchar

Sports Board Member	Dec. 2018 - Dec. 2021
Assam University (A Central University), Silchar	Assam, India

Miscellaneous

1. Research Visitor	Dec. 2018
Department of Chemistry, University of North Bengal	Darjeeling, India
2. CTS Research Visitor	Jun. 2018
Department of Chemistry & Center for Theoretical Studies	Kharagpur, India
Indian Institute of Technology Kharagpur, India	