DR. SOUMEN SAHA

Assistant Professor
M. Sc. (Chemistry), Ph.D.
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» Overview:

Dr. Soumen Saha did his B.Sc. in Chemistry Hons from Suri Vidyasagar College, Suri. He was a postgraduate student of Bengal Engineering College, Shibpur, currently known as IIEST, Shibpur. He has received his Ph.D. degree in the year of 2010 from Birla Institute of Technology and Science (BITS), Pilani, India. He has nearly 10 years research experience after his Ph.D. degree. He has worked as a postdoctoral fellow in Jackson State University, USA; The Hebrew University, Jerusalem, Israel; CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad, and lastly in Nagoya University and Kyoto University, Japan. Before joining here he was designated as an associate professor in Japan. He was awarded Israel's most prestigious fellowship by the 'planning and budget committee' of the Israel government. Currently, he is working as an Assistant Professor in the Department of chemistry, TDB College to teach Physical Chemistry as well as Quantum Chemistry courses for the budding undergraduate and postgraduate students.

» Date of appointment to the present job:

22/01/2021

» Other Academic/ Administrative post:

- Member of College Environment Committee
- Member of Seminar Committee
- Member of Students Welfare and Stipend Committee

» Academic background:

- 2010 Doctor of Philosophy (Theoretical and Computational Chemistry) in Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India.
- 2003 Master of Science in Chemistry from Bengal Engineering and Science University [Formerly Bengal Engineering College (D.U)], Shibpur, West Bengal, India.
- 2001 Bachelor of Science in Chemistry (Honours with Mathematics and Physics as subsidiary subjects) from Suri Vidyasagar College, The University of Burdwan, India.

» Information about Ph.D./ M.Phil.:

» Ph.D.:

- **Date of Award:** 2nd November, 2010
- **Title of Thesis:** *Density Functional Theory Based Studies of Reactivity Descriptors to Predict the Regioselectivity of Chemical and Biological Systems*.

» Professional Qualifications:

- **NET:** Joint CSIR-UGC, 2003

» Publications in Journals:

1. Sequence Analysis, Structure Prediction of Receptor Proteins and In Silico Study of Potential Inhibitors for Management of Life Threatening COVID-19. HK Basak, S Saha, J Ghosh, U Paswan, S Karmakar, A Pal, A Chatterjee; Letters in Drug Design & Discovery, 2022, 19, 108.
2. In silico Evaluation of Savirin Derivatives As Inhibitors of the agr Quorum Sensing System of Staphylococcus aureus. H. K. Basak, U. Paswan, J. Ghosh, S. Saha and A. Chatterjee; Anal. Chem. Lett., 2021, 11, 661.
3. Towards Developing a Criterion to Characterize Non-covalent Bonds: A Quantum Mechanical Study. N. Kumar, S. Saha and G. N. Sastry, Phys. Chem. Chem. Phys., 2021, 23, 8478.
4. Atomistic Simulation of the Polymerization Reaction by a (Pyridylamido) hafnium (IV) Catalyst: Counteranion Influence on the Reaction Rate and the Living Character of the Catalytic System. N. Misawa, Y. Suzuki, K Matsumoto, S. Saha, N. Koga and M. Nagaoka; J. Phys. Chem. B, 2021, 125, 1453.
5. Theoretical Elucidation of the Effect of Counteranions on the Olefin Polymerization Activity of (Pyridylamido) Hf (IV) Catalyst by QM and REMD Studies: MeB(C6F5)3– versus B(C6F5)4–. N. Misawa, Y. Suzuki, S. Saha, N. Koga and M. Nagaoka; Organometallics, 2021, 40, 48.
6. Theoretically Predicting the Feasibility of Highly-fluorinated Ethers as Promising Diluents for Non-flammable Concentrated Electrolytes. A. Bouibes, S. Saha (co-first author) and M. Nagaoka; Scientific Reports, 2020, 10, 21966.
7. Microscopic Origin of the Solid Electrolyte Interphase Formation in Fire-Extinguishing Electrolyte: Formation of Pure Inorganic Layer in High Salt Concentration. A. Bouibes, N. Takenaka, S. Saha and M. Nagaoka; J. Phys. Chem. Lett., 2019, 10, 5949.
8. Probing the Most Stable Isomer of Zirconium Bis(phenoxy-imine) Cation: A Computational Investigation. S. Saha, M. Takayanagi, K. Matsumoto, S. K. Sankaran, Y. Tanaka, N. Koga and M. Nagaoka; J. Phys. Chem. A, 2018, 122, 2198.
9. Differential Cationization of Fatty Acids with Monovalent Cations Studied by ESI-MS/MS and Computational Approach. B.S. Reddy, P.Pavankumar, L.Sridhar, S. Saha, G.N. Sastry and S.Prabhakar; Rapid Commun. Mass Spectrom., 2018, 32, 1126.
10. On the Origin of Spurious Errors in Many-body Expansion for Water Cluster. S. Saha, M. R. Vivek and G. N. Sastry; J. Chem. Sci., 2017, 129, 1053.
11. Palladium-Catalyzed Tandem-Cyclization of Functionalized Ynamides: An Approach to Benzosultams. A. S. Reddy, A. L. S. Kumari, S. Saha and K. C. K. Swamy; Adv. Synth. Catal., 2016, 358, 1625.
12. Quantifying Cooperativity in Water Clusters: An Attempt towards Obtaining a Generalized Equation. S. Saha and G. N. Sastry; Mol. Phys., 2015, 113, 3031.

13. Cooperative or Anticooperative: How Non-covalent Interactions Influence Each Other. S. Saha and G. N. Sastry; J. Phys. Chem. B, 2015, 119, 11121.
14. Modeling Chemical and Biological (Re)activity. R. Sharma, S. Saha, P. Badrinarayan, and G. N. Sastry; CRIPS, 2014, 15, 9.
15. DFT-based Reactivity Study of (5,5) Armchair Boron Nitride Nanotube (BNNT). S. Saha, T. C. Dinadayalane, D. Leszczyska and J. Leszczynski; Chem. Phys. Lett., 2013, 565, 69.
16. Hardness Potential Derivatives and Their Relation to Fukui Indices. S. Saha, R. Bhattacharjee and R. K. Roy; J. Comp. Chem., 2013, 34, 662.
17. Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. S. Saha, T. C. Dinadayalane, J. S. Murray, D. Leszczyska and J. Leszczynski; J. Phys. Chem. C, 2012, 116, 22399.
18. Open and Capped (5,5) Armchair SWCNTs: A Comparative Study of DFT based Reactivity Descriptors. S. Saha, T. C. Dinadayalane, D. Leszczyska and J. Leszczynski; Chem. Phys. Lett., 2012, 541, 85.
19. On the Complementarity of Comprehensive Decomposition Analysis of Stabilization Energy (CDASE) – Scheme and Supermolecular approach. A. Sarmah, S. Saha, P. Bagaria (Gupta) and R. K. Roy; Chem. Phys., 2012, 394, 29.
20. CDASE-A Reliable Scheme to explain the Reactivity Sequence between Diels-Alder Pair. S. Saha, R. K. Roy and S. Pal; Phys. Chem. Chem. Phys., 2010, 12, 9328.
21. Studies of Regioselectivity of Large Molecular Systems using DFT Based Reactivity Descriptors. R. K. Roy and S. Saha; Annu. Rep. Prog. Chem., Sect. C: Phys. Chem., 2010, 106, 118.
22. A Comprehensive Decomposition Analysis of Stabilization Energy (CDASE) and its Application in Locating the Rate Determining Step of Multi-step Reactions. P. Bagaria, S. Saha, S. Murru, V. Kavala, B. K. Patel and R. K. Roy; Phys. Chem. Chem. Phys., 2009, 11, 8306.
23. Are the Hirshfeld and Mulliken Population Analysis Schemes Consistent with Chemical Intuition? S. Saha, R. K. Roy and P. W. Ayers; Int. J. Quantum Chem., 2009, 109, 1790.
24. 'One-into-Many' Model: An Approach on DFT Based Reactivity Descriptor to Predict the Regioselectivity of Large System (Addition/Correction). S. Saha and R. K. Roy; J. Phys. Chem. B, 2008, 112, 1884.
25. N-dependence Problem of Local Hardness Parameter. S. Saha and R. K. Roy; Phys. Chem. Chem. Phys., 2008, 10, 5591.
26. 'One-into-Many' Model: An Approach on DFT Based Reactivity Descriptor to Predict the Regioselectivity of Large System. S. Saha and R. K. Roy; J. Phys. Chem. B, 2007, 111, 9664.

» Books and Chapters:

N. A.

» Seminars, Conferences, Webinars and workshops attended:

- Seminars: 00
- Conferences: 06
- Symposium: 07

» Life Membership:

N. A.

» Awards/ Academic Achievements:

- Awarded as Planning and Budgeting Committee (PBC), Israel Govt., Fellow in The Hebrew University, Jerusalem, Israel, on October 2012.

» Professional Courses:

- **Orientation Programme/FIP/FDP:** 01
- **Refresher Course:** 00
- **Short Term Course:** 00

» Others/ Miscellaneous:

- **Academic Visit Abroad:**

  He has worked as a postdoctoral fellow in Jackson State University, USA; The Hebrew University, Jerusalem, Israel, and lastly in Nagoya University and Kyoto University, Japan.

- **Collaborations:**

1. Prof. Masataka Nagaoka, Professor, Nagaoka Laboratory, Graduate School of Information Science, Nagoya University, Chikusa-ku, Nagoya 464-8601, Japan.
2. Prof. Abhik Chatterjee, Professor, Department of Chemistry, Raiganj University, Raiganj, UttarDinajpur, 733134, West Bengal, India.
3. Dr. Debasish Mandal, Assistant Professor, School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala - 147004, Punjab, India.