Dr. Soumen SAHA
Assistant Professor (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 anAssistant Professor in the Department of chemistry, TDB College.

**Date of appointment to the present job:**
22nd January 2021

**Other Academic/ Administrative post:**

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|---|---|
| **1) Post:** | **Program-Specific Researcher (equivalent to the Associate Professor)**<br>ESICB, Kyoto University, Kyoto, Japan |
| **Duration:** | May, 2019 to November, 2020 |
| **2) Post:** | **Designated Associate Professor**<br>Nagoya University, Nagoya, Japan |
| **Duration:** | January, 2019 to March, 2019 |
| **3) Post:** | **Post Doctoral Fellow**<br>Nagoya University, Nagoya, Japan |
| **Duration:** | November, 2016 to December, 2018 |
| **4) Post:** | **Research Associate**<br>CSIR-IICT, Hyderabad, India |
| **Duration:** | November, 2013 to September, 2016 |
| **5) Post:** | **Post Doctoral Fellow**<br>The Hebrew University, Jerusalem, Israel |
| **Duration:** | June, 2012 to September, 2013 |
| **6) Post:** | **Post Doctoral Research Associate**<br>Jackson State University, Jackson, MS 39217, USA |
| **Duration:** | May, 2011 to May, 2012 |
| **7) Post:** | **Research Associate**<br>Birla Institute of Technology and Science, Pilani, India |
| **Duration:** | November, 2010 to February, 2011 |

**Academic background:**

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|---|---|
| 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<br>[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 M Phil/Ph D etc.:**

- **PhD Topic**:Density Functional Theory Based Studies of Reactivity Descriptors to Predict the Regioselectivity of Chemical and Biological Systems

**Area of present academic/ Research interest/Research Projects& Schemes and Collaborations:**

- **Research interest:** Modeling of polymerization reaction

  Inter- and intra-group separations of lanthanides and actinides

  Studying the role of f-orbital in the reaction

- **Collaborations:**Prof. MasatakaNagaoka, Professor, Nagoya University, Nagoya, Japan

**Ph.D. Supervision:**
NIL

**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.

**Publications:**

1. **'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.

2. ***N*-dependence Problem of Local Hardness Parameter.**S. Saha and R. K. Roy; *Phys. Chem. Chem. Phys.*, **2008**, *10*, 5591.

3. **'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.

4. **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.

5. **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.

6. **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.

7. **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.

8. **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.

9. **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.

10. **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.

11. **Hardness Potential Derivatives and Their Relation to Fukui Indices.** S. Saha, R. Bhattacharjeeand R. K. Roy; *J. Comp. Chem.*, **2013**, *34*, 662.

12. **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.

13. **Modeling Chemical and Biological (Re)activity.** R. Sharma, S. Saha, P. Badrinarayan, and G. N. Sastry; *CRIPS*, **2014**, *15*, 9.

14. **Cooperative or Anticooperative: How Non-covalent Interactions Influence Each Other.** S. Saha and G. N. Sastry; *J. Phys. Chem. B*, **2015**, *119*, 11121.

15. **Quantifying Cooperativity in Water Clusters: An Attempt towards Obtaining a Generalized Equation.**S. Saha and G. N. Sastry; *Mol. Phys.*, **2015**, *113*, 3031.

16. **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.

17. **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.

18. **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.

19. **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.

20. **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.

21. **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.

22.**Theoretical Elucidation of the Effect of Counteranions on the Olefin Polymerization Activity of (Pyridylamido)Hf(IV) Catalyst by QM and REMD Studies: $MeB(C_6F_5)^{3-}$ versus $B(C_6F_5)^{4-}$.** N. Misawa, Y. Suzuki, S. Saha, N. Koga and M. Nagaoka; *Organometallics*, **2021**, *40*, 48.

23. **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.

24. **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.

25. **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.

26. **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.

**Books and Chapters:**NIL

**Seminars, Webinars and Conferencesattended:**

- **National Symposium on Challenges on Drug Discovery Research: Networking Opportunities between Academia and Industries (*2006*), Birla Institute of Technology and Science, Pilani, India** (Poster presentation).
- **Theoretical Chemistry Symposium 2006 (*TCS-2006*), Bharathidasan University, Tiruchirappali, India** (Poster presentation).
- **XIII$^{th}$ National Conference on Surfactants, Emulsion and Biocolloids with Special Focus on Biomimetic Systems (*NATCOSEB XII-2007*), Birla Institute of Technology and Science, Pilani, India** (Poster presentation).

- **International Conference on the Interface of Chemistry-Biology in Biomedical Research (*2008*), Birla Institute of Technology and Science, Pilani, India** (Poster presentation).
- **Discussion Meeting on Theoretical Chemistry (*TCS-2009*), Indian Institute of Science and Jawaharlal Nehru Centre for Advance Scientific Research, Bangalore, India** (Poster presentation).
- **National Conference on Emerging Trends in Life Sciences Research (*2009*), Birla Institute of Technology and Science, Pilani, India** (Poster presentation).
- **International Symposium Of Molecules and Materials (*2009*), Indian Institute of Science Education and Research, Kolkata, India** (Poster presentation).
- **National Symposium on recent development & Trends in Computational Chemistry (*RDTCC-2010*), North-Eastern Hill University, Shillong, India** (Poster presentation).
- **20th Conference on Current Trends in Computational Chemistry (*CCTCC-2011*), Jackson State University, Jackson, MS, USA**(Poster presentation).
- **The Fourteenth Theoretical Chemistry Symposium 2014 (TCS-2014), CSIR-NCL, Pune, India** (Poster presentation).
- **International conference on 'Frontiers in Electronic Structure Theory – 2015' (FEST-2015), CSIR-NCL, Pune (*organiser*)** (Poster presentation).
- **Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 8) 2017, IIT Bombay, Bombay** (Poster presentation).
- **Symposium for Reaction Path Search (SRPS 2019) 2019, Nagoya University, Nagoya, Japan** (Poster presentation)

**Life Membership:** NIL

**Awards:**

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

**Special Interest:**NIL.

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