Curriculum Vitae

- Dr. Sandip Kumar Rajak, ***Assistant Professor of Chemistry*** in Dumkal College, Basantapur,Murshidabad, W.B. (Affiliated to University of Kalyani) from 17.7.2008 to 29.4.2021.
- ***Associate Professor of Chemistry*** ***(30.4.2021- till date)***
- Specialization in Physical Chemistry.
- Ph.D. in Chemistry (Thesis Title: ***A Quantum Chemical Study On Protonation of Some Selected Molecules***) under University of Kalyani.
- Contact: sandip1ku@gmail.com

Research Interest

- **Interested in the field of computational and theoretical chemistry & DFT study**

List of Publication in Journals and in Book Chapters

1. Sandip Kumar Rajak, QSAR study in terms of conceptual density functional theory based descriptors in predicting toxicity of nitrobenzenes towards *Tetrahymena pyriformis*, **Indian Journal of Chemical Technology**, Vol. 28, July 2021, pp. 467-472
2. Prabhat Ranjan, Shayeri Das, Poonam Yadav, Hiteshi Tandon, Shalini Chaudhary, Babita Malik, Sandip Kumar Rajak, Vandana Suhag, Tanmoy Chakraborty, Structure and electronic properties of [AunV]λ (n = 1–9; λ = 0, ± 1)nanoalloy clusters within density functional theory framework, **Theoretical Chemistry Accounts** (2021), 140:59, https://doi.org/10.1007/s00214-021-02772-7
3. Shalini Chaudhary, Abhay Chaudhary, Sandip Kumar Rajak, Savaş Kaya, Mustafa Elik, Tanmoy Chakraborty, Theoretical computation of normalised radii, density and global hardness as a function of orbital exponent, **Journal of Mathematical Chemistry**, (2021) 59:1014–1028, https://doi.org/10.1007/s10910-021-01224-8
4. Hiteshi Tandon, Sandip Kumar Rajak, Tanmoy Chakraborty, Vandana Suhag , A relationship between magnetizability and chemical potential, **Chemical Papers**(75)6:2331-2337,2021, DOI 10.1007/s11696-020-01458-x

5. Sandip Kumar Rajak ,Probing the reactive center for site selective protonation in carbonyl sulphide in terms of conceptual density functional based site selectivity descriptors, **J. Indian Chem. Soc**, Vol. 97, No. 11b, November 2020, pp. 2391-2396

6. Sandip Kumar Rajak, Nazmul Islam and Dulal C. Ghosh , Evaluation of The Protonation Energy of Molecules using Conceptual Density Functional Theoretical Reactivity Descriptors, **Current Physical Chemistry**, 2017,7,126-132

7. Sandip Kumar Rajak and Dulal C. Ghosh ,The Evaluation of Protonation Energy of Molecules in Terms of Quantum Theoretical Descriptors, Theoretical and Computational Research in the 21st century , **Apple Academic Press, Canada,** 2014

8. Sandip K.Rajak, Nazmul Islam and Dulal C. Ghosh, A Quest For An Ansatz For The Evaluation Of Protonation Energy Of Molecules Involving Akin Quantum Mechanical Descriptors, **The SciTech, Journal of Science & *Technology*, Vol-2, Issue 1, 2013, p.1-12.**

9. Sandip K Rajak, Dulal C. Ghosh, Correlating the site selectivity of protonation in some ambidentate molecules in terms of the dual descriptor, **European Physical Journal D , 2012 :66,66**

10. Dulal C. Ghosh and Sandip K. Rajak , Dipole Moment is a Possible Diagnostic Descriptor of the Conformational Isomarism of the Ammonia Molecule. **"Nanoscience and Advancing Computational Methods in Chemistry: Research Progress, Apple Academic Press, Canada, http://www.appleacademicpress.com/news-events.html , 2012**

11. Sandip K.Rajak, Nazmul Islam and Dulal C. Ghosh, ,Probing the Reactive Center for Site Selective Protonation in a Molecule by the Local Density Functional Descriptors., **Nanoscience and Advancing Computational Methods in Chemistry:Research Progress, Apple Academic Press, Canada, http://www.appleacademicpress.com/news-events.html , 2012**

12. Sandip K.Rajak, Nazmul Islam and Dulal C. Ghosh, Modeling of the Chemico-Physical Process of Protonation of Molecules Entailing Some Quantum Chemical Descriptors , **Journal of Quantum Information Science, 2011, 1, 87-95**

13. Sandip K.Rajak, Nazmul Islam and Dulal C. Ghosh, Modeling of the Chemico-Physical Process of Protonation of Carbon Compounds ,**Carbon Bonding and Structures: Advances in Physics and Chemistry,Springer,2010.**

14. Dulal. C. Ghosh, Nazmul Islam and Sandip Kr. Rajak, Application of the New Scale of Electronegativity Based on the Absolute Radii of Atoms in the Computation of some Descriptors of the Real World: 1. Computation of the Dipole Moments of Some Heteronuclear Diatomic Molecules., **International Journal of Chemical Modeling, 2009, 2, 361-374.**

15. Dulal. C. Ghosh, Nazmul Islam and Sandip Kr. Rajak, Application of the New Scale of Electronegativity Based on the Absolute Radii of Atoms in the Computation of some Descriptors of the Real World. 2. Evaluation of equilibrium Internuclear Bond Distances of Some Heteronuclear Diatomics, **International Journal of Chemical Modeling, 2009,2, 375-382 .**

16. Dulal C. Ghosh and Sandip Kr. Rajak, A quantum mechanical calculation of the variation of the reactivity parameters of Ammonia (NH_3) molecule during the physical process of its umbrella (C_{3v} –D_{3h}) inversion and the identification of preferred conformation of reaction in the gas phase, **International Journal of Chemical Modeling, 2009, 2 , 221-232**

17. .Dulal C. Ghosh, Raka Biswas, Tanmoy Chakraborty, Nazmul Islam and Sandip Kr. Rajak, The wave mechanical evaluation of the absolute radii of atoms, **Journal of Molecular Structure: THEOCHEM, 2008, 865, 60–67.**

Book Edited

1. ***Environmental Hazards*, acb publications, Kolkata, 2013, ISBN:81-87500-67-0**

List of Publication in the seminar proceedings

1. **Environmental Health Hazards, proceedings for UGC sponsored national seminar 'Environmental Hazards', Dumkal College,murshidabad,2013, ISBN:81-87500-67-0**

2. **Nanotechnology A new Environmental Hazards, proceedings for UGC sponsored national seminar 'Education For Sustainable Development(ESD) in 21st Century', U.C.T.College,Berhampore,2015, ISBN:978-81-925536-0-3**

Minor Research Project :

Sl. No.	Title	Agency	Period	Grant / Amount Mobilized (Rs.)
1	A Quantum Chemical Study on Quantitative Structure Property Relationship (QSPR) and Quantitative Structure Activity Relationship (QSAR) of Molecules	UGC	2014-2016	435000/-

Presented paper in State Level/National Level Seminar/ Conference/International Symposium

Sl. No.	Title of the Paper	Title of the conference/ Seminar	Organized by	Whether International/ National/ State/ Regional/ College or University Level
1	Evaluation of The Protonation Energy of Molecules using Density Functional Theoretical Reactivity Descriptors	Advancements in Chemical Science: Issues and Challenges	Dept of chemistry ,Bidhan Chandra College 4.2.2020-5.2.2020	International
2	A correlation of Drug Activities (Anti-Bacterial and Anti-fungal) in the Structure of some hetero cyclic compound containing benzimidazole and beta-lactam moiety in terms of the Density Functional Descriptors-A QSAR and QSPR study	Recent Advances in Chemistry	Sripat Singh college, Murshidabad 21/12/2015	NATIONAL
3	Risk of Intake in Fluoride Contaminated Water	Ground Water : Issues & Challenges of The 21st Century	Sripat Singh college, Murshidabad, 29-30/12/2014	International
4	A Quantum Chemical Study on Quantitative Structure Activity Relationship (QSAR) on corrosion inhibition.	Current Trends in Chemistry	Sripat Singh college, Murshidabad, 23/12/2013& 24/12/2013	State Level
5	A Quantum Chemical Study on Quantitative Structure Property Relationship (QSPR) And Quantitative Structure Activity Relationship (QSAR) Of Molecules.	RELATING UG LEVEL CHEMISTRY TO CURRENT ADVANCES	Krishnanagar Women's Colege, Krishnanagar, Nadia, 28-29/9/2013	NATIONAL
6	Green Chemistry for Sustainable Development.	GREEN CHEMISTRY : A WAY TO SUSTAINABLE DEVELOPMENT	Sripat Singh college, Murshidabad, 27-28/12/2012	NATIONAL
7	Nanotechnology A New Environmental Hazard	EDUCATION FOR SUSTAINABLE DEVELOPMENT IN 21ST CENTURE	Union Christian Training College, Murshidabad, 4-5/10/2012	NATIONAL

8	A quest for an ansatz for the evolution of protonation energy of molecules involving akin quantum mechanical descriptors	CHEMISTRY : OUR LIFE, OUR FUTURE	Sripat Singh college, Murshidabad, 31-01-2012	State Level
9	Correlating the site selectivity of protonation in some Ambidentate molecules in terms of the dual descriptor.	Recent Advances In Chemical Sciences and Related Areas	Sri Gopal Banerjee College, Magra, Hoogly, 18-19/11/2011	National
10	A quantum mechanical calculation of the variation of the reactivity parameters of Ammonia (NH_3) molecule during the physical process of its umbrella (C_{3v} –D_{3h}) inversion and the identification of preferred conformation of reaction in the gas phase.	OF MOLECULES AND MATERIALS (A Survey of Recent Concepts)	Indian Institute of Science Education & Research(IISER), Kolkata, 28-29/12/2009	International
11	A quantum Mechanical Computation of the dipole moment of ammonia molecule as a function of the physical process of its Umbrella (C_{3v} –D_{3h}) inversion and correlation of its vanishing dipole.	Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structure Evaluation	University of Burdwan, 20-22/02/2009	NATIONAL

Academic Staff College Orientation/Refresher/ Short Term Course attended during the year:

Name of the Course/ Summer School	Place	Duration	Sponsoring Agency
Orientation course	ASC-North Bengal University	4wks (02.03.2012-29.03.2012)	UGC
Refresher Course in Chemistry	ASC-Rajasthan University	3 wks (27.1.2014-15.02.2014)	UGC
Short Term Courses on Data Analysis/ SPSS and Minitab	HRDC-Aligarh Muslim University, Aligarh (Murshidabad Campus)	25.12.2015-31.12.2015	UGC
Refresher Course in Chemistry	UGC-HRDC-Jawaharlal Nehru University	2.1.2017-27.1.2017	UGC
Short Term Training Courses on Nanotechnology & Related IPR Issues	University of Kalyani	01.8.2018-10.08.2018	University of Kalyani & DST-Purse Programme
Short Term Program on Disaster Management	UGC-HRDC-University of Hudrabad	25.7.2022-30.7.2022	UGC