



- **Dr. SANDIP KUMAR RAJAK (M.Sc,Ph.D)**
- *Assistant Professor of Chemistry & HOD*
- *Specialization in Physical Chemistry*  
sandip1ku@gmail.com

### **Research Interest**

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

### ➤ **Present Research Activities**

Sl. No.	Title	Agency	Period	Grant / Amount Mobilized (Rs. Lakh)	Category of the Project
1	A Quantum Chemical Study on Quantitative Structure Property Relationship (QSPR) and Quantitative Structure Activity Relationship (QSAR) of Molecules	UGC	2014-2016	4350000/-	<b>UGC Minor Research Project</b>

## Book Edited

1. *Quantum Mechanics: Theoretical concepts and Applications* acb publications, Kolkata, 2014, ISBN: 81-87500-77-8
2. *Environmental Hazards*, acb publications, Kolkata, 2013, ISBN:81-87500-67-0

## List of Publication in Journals

1. 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.**
2. 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**
3. 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**
4. Dulal C. Ghosh and Sandip Kr. Rajak, A quantum mechanical calculation of the variation of the reactivity parameters of Ammonia (NH<sub>3</sub>) molecule during the physical process of its umbrella (C<sub>3v</sub> –D<sub>3h</sub>) inversion and the identification of preferred conformation of reaction in the gas phase, **International Journal of Chemical Modeling, 2009,2 , 221-232**
5. 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.**
6. 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 .**
7. 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.**

## **List of Publication in Book Chapters**

1. Sandip K.Rajak, Dulal C. Ghosh, The evaluation of protonation energy of molecules in terms of quantum theoretical descriptors, **Theoretical and Computational Research in twenty first century**, Apple Academic Press, Canada, 2015, ISBN:978-1-77-188-033-6
2. Dulal C. Ghosh and Sandip K. Rajak , Dipole Moment is a Possible Diagnostic Descriptor of the Conformational Isomerism of the Ammonia Molecule. "Nanoscience and Advancing Computational Methods in Chemistry: Research Progress, Apple Academic Press, Canada, 2012, <http://www.appleacademicpress.com/news-events.html>, ISBN 978-1-4666-1607-3
3. 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, 2012, <http://www.appleacademicpress.com/news-events.html>, ISBN 978-1-4666-1607-3
4. 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. ISBN: 978-94-007-1733-6

## **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 21<sup>st</sup> Century', U.C.T.College,Berhampore,2015, ISBN:978-81-925536-0-3

**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	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
2	Risk of Intake in Fluoride Contaminated Water	Ground Water : Issues & Challenges of The 21 <sup>st</sup> Century	Sripat Singh college, Murshidabad, 29-30/12/2014	International
3	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
4	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
5	Green Chemistry for Sustainable Development.	GREEN CHEMISTRY : A WAY TO SUSTAINABLE DEVELOPMENT	Sripat Singh college, Murshidabad, 27-28/12/2012	NATIONAL
6	Nanotechnology A New Environmental Hazard,	EDUCATION FOR SUSTAINABLE DEVELOPMENT IN 21 <sup>ST</sup> CENTURE	Union Christian Training College, Murshidabad, 4-5/10/2012	NATIONAL

7	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
8	Correlating the site selectivity of protonation in some Ambidentate molecules in terms of the dual descriptor.	Recent Advances In Chemical Sciences and Related Areas	SriGopal Banerjee College, Magra, Hoogly, 18-19/11/2011	National
9	A quantum mechanical calculation of the variation of the reactivity parameters of Ammonia (NH <sub>3</sub> ) molecule during the physical process of its umbrella (C <sub>3v</sub> -D <sub>3h</sub> ) 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
10	A quantum Mechanical Computation of the dipole moment of ammonia molecule as a function of the physical process of its Umbrella (C <sub>3v</sub> -D <sub>3h</sub> ) 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 Course attended during the year:**

<b>Name of the Course/ Summer School</b>	<b>Place</b>	<b>Duration</b>	<b>Sponsoring Agency</b>
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