Curriculum Vitae
Madhurima Jana

1. NAME AND FULL CORRESPONDANCE ADDRESS :

Dr. Madhurima Jana
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2. PUBLICATIONS

S. No.	Author(s)	Title	Name of Journal	Volume	Page	Year
1.	S. Santra and **M. Jana***	Insights into the Sensitivity of Arginine Concentration to Preserve the Folded Form of Insulin Monomer Under Thermal Stress.	*J. Chem. Inf. Model*	60	3105	2020
2.	S. Sarmah, S. Pahari, V. Belwal, **M. Jana*,** A. S. Roy	Elucidation of molecular interaction of bioactive flavonoid luteolin with human serum albumin and its glycated analogue using multi-spectroscopic and computational studies	*J. Mol. Liq*	318	114147	2020
3.	G. N.Reddy; R. Parida; A. Muñoz-Castro; **M. Jana**, S. Giri	Doped Deltahedral Organo-Zintl Superalkali Cations	*Chem. Phys. Letters*	759	137952	2020
4.	S. Sarmah, S. Pahari, S. Das, V. K. Belwal, **M. Jana***, A. S. Roy	Non-enzymatic glycation of human serum albumin modulates its binding efficacy towards bioactive flavonoid chrysin: A detailed study using multi-spectroscopic and computational methods.	*J. Biomol. Struct. Dynam*	DOI: 10.1080/07391102.2019.1711196	--	2020
5.	S. Das, S. Santra, M. A. Rohman, M. Ray, **M.**	An Insight into the Binding of 6-Hydroxyflavone with Hen Egg White Lysozyme: A Combined	*J. Biomol. Struct. Dynam*	37	4019	2019

	Jana*, A. S. Roy	Approach of Multi-Spectroscopic and Computational Studies.				
6.	D. Paul, S. Santra**,** **M. Jana***	Interactions Between CD44 and HA_{16}: An Investigation on Multiple Binding Modes of the Complex by Using Molecular Dynamics Simulation Studies	*J. Ind. Chem. Soc. (Special Issue on " Theoretical and Computational Chemistry ")*	96	851	2019
7.	S. Das, S. Pahari, S. Sarmah, M. Rohman, D. Paul, **M. Jana*,** A. Roy	Lysozyme-luteolin binding: Molecular insights into the complexation process and the inhibitory effects of luteolin towards protein modification.	*Phys. Chem. Chem. Phys.*	21	12649-12666	2019
8.	R. Parida, G. N. Reddy, A. Chakraborty, S. Giri, **M. Jana***	A New Class of Superhalogen Based Anion Receptor in Li-ion Battery Electrolytes.	*J. Chem. Inf. Model (Spl issue: Women in Computational Chemistry)*	59	2159	2019
9.	G. N. Reddy, R. Parida, P. Jena, **M. Jana**, S. Giri	Superhalogens as building blocks of super lewis acids.	*Chem. Phys. Chem.*	20	1607	2019
10.	A. Chakraborty, G.N Reddy, **M. Jana*,** S. Giri	[8] Cyclo-1, 4-Naphthylene: A Possible New Member in Hole Transport Family	*Chem. Phys. Lett.*	715	153	2019
11.	S. Santra, T. Kundu, **M. Jana***	Microscopic investigation on empirical force-field model dependent structure and dynamical properties of amino acids in aqueous medium.	*J. Ind. Chem. Soc. (Invited Lecture Article),*	95	1617	2018
12.	D. Mohanta, **M. Jana***	Effects of ethanol on the secondary structure specific hydration properties of Chymotrypsin Inhibitor 2 in its folded and unfolded forms.	*Mol. Simul.*	44	1278	2018
13.	D. Mohanta, **M. Jana***	Can 2,2,2-trifluoroethanol be an efficient protein denaturant than methanol and ethanol under thermal stress?	*Phys. Chem. Chem. Phys.*	20	9886.	2018
14.	S. Biswas, S. Santra, S. Yesylevskyy, J. Maiti, **M. Jana***, R. Das	Picosecond Solvation Dynamics in Nanoconfinement: Role of Water and Host-Guest Complexation.	*J. Phys. Chem. B.*	122	3996	2018

15.	D. Mohanta, S. Santra**, M. Jana***	Conformational disorder and solvation properties of the key-residues of a protein in water-ethanol mixed solutions.	*Phys. Chem. Chem. Phys.*	19	32636	2017
16.	S. Giri, R. Parida, **M. Jana**, S. Gutiérrez-Oliva, A. Toro Labbe	Insights into the Mechanism of Ground and Excited State Double Proton Transfer Reaction in Formic Acid Dimer.	*J. Phys. Chem. A.*	121	9531	2017
17.	D. Mohanta, S. Santra, G. N. Reddy, S. Giri, **M. Jana***	Residue Specific Interaction of an Unfolded Protein with Solvents in Mixed Water-Ethanol Solutions: A Combined Molecular Dynamics and ONIOM Study.	*J. Phys. Chem. A*	121	6172	2017
18.	S. Giri, R. Inostroza-Rivera, **M. Jana***	The Beckmann rearrangement in the framework of reaction electronic flux.	*Theor. Chem. Acc.*	136	9	2017
19.	M. Yang, T. A. d'Ortoli, E. Säwén, **M. Jana,** G. Widmalm, A.D. MacKerell Jr.	Delineating the conformational flexibility of trisaccharides from NMR spectroscopy experiments and computer simulations.	*Phys. Chem. Chem. Phys.*	18	18776	2016
20.	D. Mohanta, **M. Jana***	Effect of ethanol concentrations on temperature driven structural changes of Chymotrypsin Inhibitor 2.	*J. Chem. Phys.*	144	165101	2016
21.	**M. Jana,** A. D. Mackerell Jr.	CHARMM Drude polarizable force field for aldopentofuranoses and methyl-aldopentofuranosides	*J. Phys. Chem. B*	119	7846	2015
22.	S. K. Sinha, **M. Jana,** K. Chakraborty, S. Bandyopadhyay	In silico studies of properties of water hydrating a small protein.	*J. Chem. Phys.*	14	22D502	2014
23.	**M. Jana*,** S. Bandyopadhyay	Molecular dynamics study of β-cyclodextrin-phenylalanine (1:1) inclusion complex in aqueous medium.	*J. Phys. Chem. B*	117	9280	2013
24.	**M. Jana,** S. Bandyopadhyay	Restricted dynamics of water around a protein-carbohydrate complex: Computer simulation studies.	*J. Chem. Phys.*	137	055102	2012
25.	**M. Jana,** S. Bandyopadhyay	Conformational flexibility of a protein–carbohydrate complex and the structure and ordering of surrounding water.	*Phys. Chem. Chem. Phys.*	14	6621	2012,

26.	**M. Jana**, S. Bandyopadhyay	Vibrational spectrum of water confined in and around cyclodextrins.	*Chem. Phys. Lett.*	509	181	2011
27.	**M. Jana,** S. Bandyopadhyay	Hydration properties of α-, β-, and γ-cyclodextrin from molecular dynamics simulation	*J. Phys. Chem. B*	115	6347	2011
28.	**M. Jana,** S. Bandyopadhyay	Kinetics of hydrogen bonds in aqueous solutions of cyclodextrin and its methyl-substituted forms.	*J. Chem. Phys.*	134	025103	2011
29.	**M. Jana,** S. Bandyopadhyay	Low-frequency vibrational spectrum of water around cyclodextrin and its methyl-substituted derivatives.	*Langmuir*	26	14097	2010
30.	**M. Jana,** S. Bandyopadhyay	Microscopic investigation of the hydration properties of cyclodextrin and its substituted forms	*Langmuir*	25	13084	2009

3. OTHER RELEVANT ACADEMIC/RESEARCH INFORMATION

3.1 RESEARCH INTEREST

We use state of art molecular dynamics simulations techniques and quantum mechanical tools to address several issues related to the structure and dynamics of biological molecules and materials.

- Effects of additives/cosolvent on protein structure and dynamics
- Protein folding-unfolding
- Structural aspects of Glycans and their interactions with Proteins
- Membrane-sugar interactions
- Membrane modulation in presence of small organic molecules
- Force Field development for carbohydrate and small organic molecules
- Host-guest interaction in confined media
- Reaction mechanism
- Transport properties of Li-ion battery electrolytes in presence of newly designed potential additives

3.2 SPONSORED PROJECTS

Sl. No	Name of the Project	Sponsoring Agency	Name of the PI	Name of the Co-PI	Total Value (Rs. in Lakhs)	Start Date	Close Date
1.	Effects of Alcohols on Protein Dynamics: A Molecular Dynamics Simulation Approach	SERB, DST	Dr. M. Jana	Nil	24.8	2013	2017
2.	In-silico Studies of Structural Diversity of Glycosaminoglycans and their Interactions with Protein	BRNS	Dr. M. Jana	Nil	24.94	2018	2021
3.	Microscopic Investigation of the Stability of Proteins in Amino Acid Solutions	DST-EMR	Dr. M. Jana	Nil	41.09	2018	2021

3.3 PG STUDENTS GUIDANCE

Sl. No	Name of the Student	Title of the Thesis	Year of Passing
1.	Mr. Dayananda Sharma Mr. Pratik Biswal Ms. Nivedita Rai	*Molecular Dynamics Study of TIP3P, SPC/E and TIP4P Water Models at Room Temperature*	2013
2.	Ms. Vijayalaxmi sahoo	*Temperature Dependent Molecular Dynamics Simulation Study of [BMIM][Cl]*	2014
3.	Mr. Motilal Chattaria	*Molecular Dynamics Simulation of Large Ring Cyclodextrins in Aqueous Medium*	2016
4.	Mr. Siddharth Kamal	*Molecular Dynamics Studies of Glycosaminoglycans in Aqueous Medium*	2016
5.	Mr. Tathagata Kundu	*Systematic Comparison of Empirical Force-Fields for Molecular Dynamics Simulations of Amino Acid Solutions*	2017
6.	Ms. Rituparna Mishra	*Molecular Dynamics Studies of a-, ß- and γ-cyclodextrins in water-methanol binary mixtures*	2018
7.	Mr. Malay Roul	*Interaction Between CD44 and hyaluronan: A molecular dynamics simulation approach*	2018

8.	Mr. Abhijeet Mohanty	*Molecular Dynamics Studies of Cyclodextrin-Amino Acid Inclusion Complexes*	2019
9.	Mr. Anuj Kumar Ray	*Molecular Dynamics Studies of DMPC Bilayer*	2019
10.	Mr. Prabir Sarkar	*Molecular Dynamics Studies of DMPC Bilayer With Pyrazine Derivatives*	2020
11.	Mr. Gautam Jha	*Computational Study of Magnetic Clusters of Heavy Actinides and Their Properties*	2020
12.	Mr. Samrat Sarkar	*On-going*	2021
13.	Mr. Suzatra Chatterjee	*On-going*	2021

3.4 Ph.D GUIDANCE

Sl. No	Name of the Student	Title of the Thesis/Area of Ph.D work	Co-Supervisor (if any)	Status
1.	Dr. Dayanidhi Mohanta	*Molecular Dynamics Studies of the Effects of Alcohols on Chymotrypsin Inhibitor 2*	Nil	2013-2018 Degree Awarded on 24th April, 2018
2.	Dr. G. Naaresh Reddy	*In Silico Studies of Functionalized Aromatic Heterocyclic and Zintl Ion Based Super-Atom/Alkali/Halogen*	Dr. S. Giri	2015-2020 Degree Awarded on 08th July, 2020
3.	Mr. Santanu Santra	*Proteins in cosolvent and cyclodextrin-drug interactions*	Nil	Ongoing
4.	Mr. Rakesh Parida	*Proton transfer reactions and design of additives for Li-ion battery electrolytes*	Dr. S. Giri	Ongoing
5.	Mr. Somdev Pahari	*Local bilayer properties in presence of small organic molecules*	Nil	Ongoing
6.	Ms. Shakuntala Dhurua	*Proteins in amino-acid solutions and Protein-Glycan interactions*	Nil	Ongoing
7.	Mr. Rabiul Gazi	*Pressure effects on proteins in presence of cosolvent*	Nil	Ongoing

3.5 CONFERENCES, WORKSHOPS AND LECTURE(S) ARRANGED / COORDINATED

- Coordinator, TEQIP-III sponsored webinar workshop on "*Molecular modeling of materials and biological macromolecules*" during 22-Sep-2020 to 26-Sep-2020.

- Co-Convener of the National conference on "*Biomolecular Dynamics: Experimental and Theoretical Perspectives (BDETP-2017)"* during 18th- 20th December, 2017.

3.6 CONFERENCES AND WORKSHOPS ATTENDED/INVITED LECTURES

- Invited Speaker in *10th Triennial Congress of the International Society for Theoretical Chemical Physics* **2019** (ISTCP 2019), Tromsø, Norway.

- Invited Talk in *Theoretical Chemistry Symposium 2019 (TCS* 2019), Organized by BITS Pilani.

- Delivered talk in *Recent Advances in Molecular Simulations (RAMOLS),* 2018. Organized by Thematic Unit of Excellence in Computational Materials Science at IISc Bangalore.

- Delivered an invited lecture on "*Molecular Modeling: Principles and Application*" in a Faculty development programme to the faculties and 2-year M. Sc. students in the College of Engineering and Technology (CET), Bhubaneswar. October 24-28, 2016.

- Invited Speaker in *Recent Advances on Multi-Functional Materials (RA2M-2017),* 2017 Organized by Haldia Institute of Technology and Indian Photobiology Society, Jadavpur University, West Bengal.

- Attended *Theoretical Chemistry Symposium TCS* 2016, Organized by University of Hyderabad, IIIT Hyderabad and IICT Hyderabad.

- *Computer Aided Drug Design Symposium 2014*, University of Maryland, Baltimore, USA

- Poster Presentation at *Research Day 2014*, University of Maryland, Baltimore, USA

- Oral Presentation at Quantum Theoretical Computation 2012, Pontificia Universidad Catolica de Chile (PUC), Santiago, Chile

Madhurima Jana
(04-Sep-2020)