

Sr. No.	Thesis Title	Name of the Student	Year	Type
1.	Psychrophilic and Mesophilic Class C Beta-Lactamase Studied by Classical Molecular Dynamics Simulation	Chandan Das	2011	M.Sc.
2.	Ab initio Molecular Dynamics Simulation of Water Gas Shift Reaction on Rh/Al <sub>2</sub> O <sub>3</sub> surface	Parichay Chakraborty	2012	M.Sc.
3.	Mechanism of "On-Water" Reactions	Akshaya Kumar Das	2013	M.Sc.
4.	Origin of Isotope effect in the "On-Water" reactions	Projesh Kumar Roy	2014	M.Sc.
5.	Insights into the Cross-Linking in Class C Beta-Lactamases: An Effective Strategy to Inhibit Antibiotic Resistance	Soumyadyuti Samai	2014	M.Sc.
6.	Polygon as a Coordinate for Sampling Configurational Landscape of Molecular Clusters	Sreyoshi Sur	2014	M.Sc.
7.	CO Oxidation over Rh(DCO)/ $\gamma$ -Al <sub>2</sub> O <sub>3</sub>	Ujjwal Kr. Maity	2015	M.Sc.
8.	Modelling the Structure of Nitrocefin New Delhi Metallo $\beta$ -Lactamase Michaelis Complex	Debmalya Ray	2015	M.Sc.
9.	Computational Study of Formation of Rh Dimer from Mononuclear Rh <sub>1</sub> (C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> Complex Supported on Zeolite-Y	R. Barenya Krushna Sahoo	2015	M.Sc.
10.	Development of Well Sliced Metadynamics for Sampling Free Energy Surfaces as Slices	Venkat Kapil	2016	M.Sc. (5yr)
11.	Deacylation Mechanism of Aztreonam Catalysed by Class-C Beta-Lactamases: A QM/MM study	Shalini Gupta	2016	B.S.
12.	Study of Oxidative Degradation of High-Performance Polymers and Efficient Implementation of Born-Oppenheimer Molecular Dynamics	Jayashrita Debnath	2017	B.S. & M.S.
13.	Blue Moon TASS Approach: A New And Efficient Method for Rare Event Sampling	Subhendu Pal	2018	M.Sc. (2yr)
14.	Convergence and Error Estimation in Free Energy Calculations using the Weighted Histogram Analysis Method	Subarna Sasmal	2018	M.Sc. (2yr)
15.	Simulation of Urea Crystal using Molecular Mechanics Force Field to Study Polymorphism	Subrata Mandal	2018	M.Sc. (2yr)
16.	A Novel Generalised Approach for Calculating Error in Free Energy Estimation in Umbrella Sampling, Metadynamics and TASS method	Asit Pal	2019	M.Sc. (2yr)
17.	Development of Lambda-TASS for Alchemical Free Energy Calculations	Meenal Jain	2019	M.Sc. (2yr)
18.	Speeding up Electrostatic Interactions in QM/MM Calculations using Multiple Time Stepping Algorithm	Kuntal Ghosh	2020	M.Sc. (2yr)