

Partial List of Accepted Participants for Poster Presentation #TheorChem			
Poster Number	Name	Poster Title	Email id
TC1	Pooja	Structure, stability and properties of Cyclo[18]carbon-Zn-Cyclo[18]carbon super sandwich complex: DFT calculation	pp720111@student.nitw.ac.in
TC2	Gaurav Vishwakarma	Formation of cubic and hexagonal ices and their determination by infrared spectroscopy	g18iitm@gmail.com
TC3	Kalishankar Bhattacharya	Atomistic Insights of IrO _x Water Splitting Catalyst in Electrochemical Conditions	ksb@kofo.mpg.de
TC4	Jaibir Singh	Modifying linear free energy relationship under cooperative vibrational strong coupling	ph18068@iisermohali.ac.in
TC5	Nidhi Gupta	Study of intermixing effects in Ge/Si(001) growth using kinetic Monte Carlo simulations	nidhig@iitk.ac.in
TC6	Bhupesh	Thermodynamic Aspects of Solid Propellant Gas Generator for Aircraft Application	baparate@gmail.com
TC7	Biswajit Sahariah	Deciphering the Backbone Non-covalent Interactions that Stabilize the Polyproline II (PPII) Conformation	biswasahariah@gmail.com
TC8	Susmita sarkar	The Secret of Ambivalent Mechanisms of Osmolytes to Counteract Salt-stress	ssusmita@tifrh.res.in
TC9	Gaurav Jhaa	Structure and Bonding in Fully Oxidized Graphene Nanosheets	gauravjhaa17@gmail.com
TC10	Ranita Pal	Metastable XNgNSi (X = HCC, F; Ng = Kr, Xe, Rn) Compounds with Ng-C/F and Ng-N Bonds and Possible Isomerization therein	pal.ranita04@gmail.com
TC11	Sohail Hamid Dar	Bonding Quagmire in Transition metal - Diborane σ -Complexes: Counterintuitive Dominance of Overlap over Energy in Frontier MOs	darsohailpu94@gmail.com
TC12	Tripti Ahuja	Toward Vibrational Tomography of Citrate on Dynamically Changing Individual Silver Nanoparticles	dahuja@iitd.ac.in

TC13	B. S. Krishnamoorthy	Electronic and Geometrical Structure, Stability and Spectral Properties of Cobaltaboranes [(C ₅ H ₅)CoB ₄ H ₇ X where, X = F, Cl, Br, I.] - A Theoretical Insight	bskimo@gmail.com
TC14	Kompella V K Srinath	Computational Investigations of Diastereoselectivity in Coordination-Driven Self-assembly	srinathkompella93@gmail.com
TC15	abhik ghosh moulick	Correlated dipolar and dihedral fluctuations in a protein	abhik.ghoshmoulick@gmail.com
TC16	Dr. MADHU GUPTA	A Comparative Approach to Study the Oxidation Of Acetaminophen In Alkaline Medium Through Quantum And Kinetic Approach	GUPTAMADHU30@REDIFFMAIL.COM
TC17	NEENU KRISHNA P U	Radioactive polonium chelation by Naturally occurring Gentisic acid; A theoretical study	neenukrishnapu10@gmail.com