

**Final List of Poster Presenters #TheorChem**

Poster No.	Name	Poster Title
TC1	Pooja	Structure, stability and properties of Cyclo[18]carbon-Zn-Cyclo[18]carbon super sandwich complex: DFT calculation
TC2	Gaurav Vishwakarma	Formation of cubic and hexagonal ices and their determination by infrared spectroscopy
TC3	Kalishankar Bhattacharyya	Atomistic Insights of IrOx Water Splitting Catalyst in Electrochemical Conditions
TC4	Jaibir Singh	Modifying linear free energy relationship under cooperative vibrational strong coupling
TC5	Nidhi Gupta	Study of intermixing effects in Ge/Si(001) growth using kinetic Monte Carlo simulations
TC6	Bhupesh	Thermodynamic Aspects of Solid Propellant Gas Generator for Aircraft Application
TC7	Biswajit Sahariah	Deciphering the Backbone Non-covalent Interactions that Stabilize the Polyproline II (PPII) Conformation
TC8	Susmita sarkar	The Secret of Ambivalent Mechanisms of Osmolytes to Counteract Salt-stress
TC9	Gaurav Jhaa	Structure and Bonding in Fully Oxidized Graphene Nanosheets
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
TC11	Sohail Hamid Dar	Bonding Quagmire in Transition metal - Diborane $\sigma$ -Complexes: Counterintuitive Dominance of Overlap over Energy in Frontier MOs
TC12	Tripti Ahuja	Toward Vibrational Tomography of Citrate on Dynamically Changing Individual Silver Nanoparticles
TC13	Kompella V K Srinath	Computational Investigations of Diastereoselectivity in Coordination-Driven Self-assembly
TC14	abhik ghosh moulick	Correlated dipolar and dihedral fluctuations in a protein
TC15	NEENU KRISHNA P U	Radioactive polonium chelation by Naturally occurring Gentisic acid; A theoretical study
TC16	B. S. Krishnamoorthy	Electronic and Geometrical Structure, Stability and Spectral Properties of Cobaltaboranes [(C5H5)CoB4H7X where, X = F, Cl, Br, I.] - A Theoretical Insight
TC17	Dr. MADHU GUPTA	A Comparative Approach to Study the Oxidation Of Acetaminophen In Alkaline Medium Through Quantum And Kinetic Approach