Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Seminar

Understanding the critical role of electrostatic and non-electrostatic interactions in important biological systems

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The investigation of the role of the electrostatics in systems of widespread interest employing computational techniques is an emerging area of research. The influence of built-in local electric fields (LEFs) present in modulating the cation selectivity of naturally occurring macrocyclic ionophore systems such as valinomycin has been explored using computational techniques. Furthermore, we have deciphered the catalytically active conformation and explained the origin behind the natural-like catalytic power of an artificial metalloenzyme using large-scale MD simulations and rigorous QM and QM/MM calculations. While the electrostatic model is widely established for enzyme catalysis, this study reports for the first-time an unprecedented catalytic role of non-electrostatic interactions into it and suggests a new principle towards designing enzymes with natural efficiency.

Tuesday, Oct 29th 2024

11:30 Hrs

Auditorium, TIFR-H