Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Seminar

Exploring High Dimensional Free Energy Landscapes of Chemical Reactions: New Approaches and Applications

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Molecular Dynamics (MD) is widely used to study molecular level mechanism and free energetics of chemical reactions and structural transformations in soft matter systems. Although tremendous progress has been made in developing MD based methods for free energy calculations, severe limitations prevail owning to the practically realizable time-scales of dynamics. In this respect, biased sampling MD techniques are used to accelerate transitions between two metastable states on a high dimensional free energy landscape, with the aim to predict reaction mechanism, and to compute free energy barriers separating the basins. However, the computational efficiency of biased sampling methods decreases with increasing dimensionality, which in turn severely limits the predictive power of enhanced sampling approaches. Here we propose a new method called the "Temperature Accelerated Sliced Sampling" (TASS) to overcome these problems. TASS integrates temperature accelerated sampling and biased sampling of the orthogonal coordinates with the conventional Umbrella Sampling. This method enables us to choose large number of orthogonal collective coordinates for enhanced-sampling. Most importantly, we can change the dimensionality and the description of the orthogonal coordinates for different umbrella windows. This approach allows us to perform controlled exploration of a complex free energy landscape even when it is broad and unbound, like in the case of A+B type reactions, drug binding etc. After demonstrating the accuracy of our method, I will discuss its applications in modelling enzymatic and other catalytic reactions using DFT based QM/MM molecular dynamics.

Wednesday, Nov 27th 2019

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H