

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

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Biased sampling of collective coordinates is a widely used strategy to accelerate rare events and compute free energy changes in molecular dynamics simulations. However, computational efficiency of such methods decreases with increasing number of collective coordinates. This severely limits the predictive power of enhanced sampling approaches. Here we propose a new method called the “Temperature Accelerated Sliced Sampling” (TASS) that integrates temperature accelerated sampling and biased sampling of the orthogonal coordinates with the conventional umbrella sampling approach. This enables us to choose large number of orthogonal collective coordinates in umbrella 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 which 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.

Dr. Nisanth N. Nair currently holds the position of Associate Professor at the Department of Chemistry, Indian Institute of Technology Kanpur (IIT Kanpur) and Visiting Professor at the Institute of Catalysis, Hokkaido University. He joined IIT Kanpur in 2008 as Assistant Professor after his four years of post-doctoral work with Prof. Dominik Marx, Ruhr-University, Bochum (Germany). His research interests include development of computational methods for free energy calculations, QM/MM computations, and hybrid DFT based ab initio MD simulations. He also works in modelling enzymatic reactions, catalytic reactions in zeolites, and oxidation reactions on polymer surfaces. He was elected as the “P K Kelkar Young Faculty Research Fellow” by IIT Kanpur in 2012 and “Young Associate” by the Indian Academy of Sciences, Bangalore in the same year. He received the “Young Scientist Medal” by the Indian National Science Academy in 2013. Recently, he has been awarded the “Distinguished Lectureship Award” by the Chemical Society of Japan.

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