TCI SEMINAR

Computer Simulations of Chemical Reactions in Solution and Chromosome Structure Formation

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1:30 p.m. Room 1315

Professor Yi Qin Gao

Institute of Theoretical and Computational Chemistry
Peking University
Beijing, China

A sampling strategy for rare events, enhanced sampling of reactive trajectories (ESoRT), was developed, in which an ensemble of chemical reaction trajectories were efficiently generated and collected with known thermal weights, thus allowing a statistical investigation of thermodynamics, kinetics, dynamics and mechanisms of the reaction event of interest. Free of predefined CVs or RCs, the post-analysis of reaction mechanisms is performed. As an example, the reaction coordinate(s) of a (retro-)Claisen rearrangement in bulk water was variationally optimized based on a Bayesian learning algorithm. The hydrogen-bonding of water molecule to the charge-enriched site of the reactant state changes the dynamics of reaction. A characteristic shrinkage of the solvent shell during the chemical transition was identified, suggesting a necessary energy transferring process during the thermal activated chemical reaction, reminiscent of the "cage-effect". The transition path time of the reaction and the rate constants for the forward and backward reaction were calculated independent of RCs, and we were able to self-consistently connect the kinetics to the thermodynamics. The diffusion coefficient over the energy barrier was also determined according to Kramers' theory, showing the limitation of canonical transition state theory in dealing with the condensed phase reactions. In the second part of the talk, I will discuss the modelling of the chromatin structure utilizing experimental Hi-C data, which provides the spatial details of chromatin. By mapping a plethora of genome features onto the chromatin model, we quantitatively and systematically reinforce the importance of chromatin architecture for genome function. We find that the colocalization of genome features on a linear map coincides their 3D segregation, and thus the latter provides a mechanism for the regulation of various genome properties. Especially, we will discuss the effects of DNA methylation on the structure of DNA and that the overall DNA methylation patter reflects the 3-D organization fo the human chromatin.

Theoretical Chemistry Institute Seminar Series