第409回触媒科学研究所コロキウム

Free Energy Pathways of Enzymatic Reactions Catalyzed by PLP-Transaminase

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We will present some of our recent studies on quantum-classical hybrid simulations of complex chemical reactions in aqueous solutions. The focus will be on chemical processes which do not take place so easily in normal ab initio molecular dynamics simulations. One such reaction is the process of transamination. Transaminase is a PLP (Pyridoxal 5'-Phosphate) dependent enzyme which reversibly catalyzes the transamination reaction. Aspartate Transaminase (AspTase) is a key enzyme of amino acid metabolism process. In the present talk, we will discuss our recent studies on the mechanism and free energy pathways of the transamination reaction in the active site of AspTase using hybrid quantum-classical molecular dynamics simulation with the aid of the metadynamics techniques. Results will also be presented for the transimination reaction for the Aspartate substrate which precedes the transamination reaction and also for another transamination reaction involving Serine Hydroxyl Methyl Transaminase (SHMT).

Prof. Amalendu Chandra currently holds the position of N.C. Nigam Chair Professor at the Department of Chemistry, Indian Institute of Technology Kanpur. He also held the position of Dean of Research and Development at IIT Kanpur during 2014-17. He is a Fellow of Indian Academy of Sciences, Indian National Science Academy, and also National Science Academy India. He received the Alexander von Humboldt Fellowship in 2002, Shanti Swarup Bhatnagar Prize from Council of Scientific and Industrial Research, Government of India, in 2007, and J.C. Bose Fellowship from the Department of Science and Technology in 2013. He is a Member of the Editorial Advisory Boards of the Journal of Physical Chemistry, Journal of Molecular Liquids and also a few other journals. His research interests include theoretical and computational studies of chemical dynamics in liquids, surfaces and interfaces, clusters and biomolecular systems using both classical and quantum methods. He is currently a Visiting Professor at Institute of Molecular Science, Okazaki, Japan.

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