Atsushi Yamada

CRPP, Centre de Recherche Paul Pascal, Bordeaux

Molecular Simulation Studies of Condensed Phase : Quantum and Classical Approaches for Reaction Systems and miscellaneous

In this seminar, I will talk about some molecular simulation studies of condensed phase systems. In particular, I present a study of proton transfer reaction in solution based on mixed quantum-classical approximation and show reaction quantum dynamics picture as well as quantum and solvent effects. I also briefly present some miscellaneous simulation studies of exciton dynamics on polymer and very large scale all-atom simulation of virus in solution,