Development of QM/MM Methodology and Its Applications

SPEAKER: Yan Zhang, Shandong University
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HOST: Tong Zhu, East China Normal University

ABSTRACT OF THE TALK
QM/MM method is widely used in the simulations of large systems. We ever developed the polarized boundary models based on the equilibrium of chemical potential to treat mutual polarization between QM and MM regions. Recently, we suggested a double-optimizations-of-buffer-region (DOBR) microiterative scheme to optimize the geometries of flexible systems in QM/MM calculations. The averaged number of QM calculations for the DOBR scheme is only ~1% of that of the standard scheme and ~6% of the two-region microiterative approach. Using the DOBR method, we studied the ionizations of and excess attachment to aqueous nucleobases, nucleosides, and nucleotides in DNA damage by radiation. The results indicate that QM-region polarization by bulk water evidently affects the ionization and electron attachment. It induces a drastic decrease of the cationic and anionic energies in structural relaxations. The potential energy surfaces of the cation and anion would become very steep near the equilibrium structure. In vertical electron attachment, ~50% of excess electrons would be delocalized over the water molecules around the deoxyribonucleosides. However, the main hole (excess electrons) would be localized on DNA nucleobases after relaxations in the ionizations (excess electron attachment). Moreover, we employed the QM/MM calculations to investigate the biomolecules. The absorption spectra of bovine rhodopsin mutant E113Q in solutions suggested that the polarizations of the counterions in the vicinity of Schiff base E113Q would be a crucial factor to change the energy gap of the retinal to tune the absorption spectra. 2D-free energy profiles of the UDP-glycosyltransferase catalytic reaction reveal that the hydrogen on hydroxyl group of the substrate is first transferred to His19. Subsequently, the deprotonated substrate would react with the glucose ring. The other possible pathway is that the glycosyl group of UDP-Glc undergoes a dissociation-like mechanism to form C-O bond with the deprotonated substrate.

BIOGRAPHY
Dr. Yan Zhang is a Professor in the Institute of Molecular Sciences and Engineering at Shandong University. He obtained his Ph.D. degree from Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences in 2005. Dr. Zhang did postdoctoral research at University of Colorado Denver (with Prof. Hai Lin) and Max-Planck-Institut für Kohlenforschung (with Prof. Thiel). He joined State Key Laboratory of Molecular Reaction Dynamics of DICP (Han’s group) in 2010 and moved to Shandong University in 2018. His research interests include the development of QM/MM methods and mechanism investigations of import living process. He is a developer of ChemShell code for QM/MM simulations.