Special PChem seminar

3/28/19 @2pm

SCI294

Toward incorporation of quantum chemical effect of solvation into molecular dynamics simulations

For condensed systems, quantum chemical effects of solvation play important roles in various properties. Thus, the incorporation of quantum chemical effects of solvation into molecular dynamics simulations has been a major concern. Because quantum mechanical/molecular mechanical (QM/MM) models are well-balanced with respect to computational cost and accuracy, they are popular and powerful options to treat gigantic system such as solutions. However, when it comes to dynamics simulations, it is not straightforward to incorporate the quantum chemical effect of salvation via QM/MM because of solvent diffusion. Although, to address this problem many research groups have proposed corrective QM/MM techniques that are termed adaptive QM/MM method, most of them cannot achieve accurate and stable simulations because of temporal and spatial discontinuity problems. To overcome the discontinuities, we proposed a new adaptive QM/MM method, size-consistent multi-partitioning (SCMP) QM/MM, and successfully demonstrated that the SCMP method achieve stable molecular dynamics simulations by effectively taking into account quantum chemical effects of solvation. In the presentation, I would like to introduce the basic concept and the recent progress in further development of the SCMP method, and also demonstrate some successful applications.

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