Molecular Solvation Theory for Material Design

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Solutions play an important role as a place to produce materials and exhibit their functions. Our group has focused on the role of solutions in the formation and function of materials and has developed a multiscale method based on the statistical mechanics theory of liquids for material design.

In-solution chemical reactions are among the most interesting in-solution chemical processes in material design. We proposed the QM/MM/3D-RISM method as a multi-scale method to handle chemical reactions in solution. In the QM/MM/3D-RISM method, the chemical reaction center is treated by QM, the surrounding reaction-inactive moieties by MM, and the solution by 3D-RISM. Recently, this method was used to elucidate the mechanism of pKa change of ligand molecules by inclusion compounds.

Another important process is the change in molecular structure in solution. It is known that macromolecules, such as a polymer or protein, aggregate or phase separate under the influence of solution molecules. Recently, we have developed an efficient method for sampling molecular structures in solution. This method is designed in the framework of the hybrid Monte Carlo method: conformations are extracted at constant time intervals of MD trajectories and solvation free energies of the conformations are determined by 3D-RISM theory, and thus a metropolis criterion for conformational transitions is used. This method enables structure sampling that satisfies the 3D-RISM ensemble.

In this presentation, In this presentation, the theories described above will be reviewed.