Possibility of *Ab Initio* Effective Fragment Potential Molecular Dynamics Simulations for Predicting Thermodynamic Properties of the Functional Liquid Materials

([1]*Department of Applied Chemistry, Faculty of Science and Engineering, Chuo University*, [2]*JST ACT-X*, [3]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science*) ○Nahoko Kuroki,[1,2] Hirotoshi Mori[1,3]

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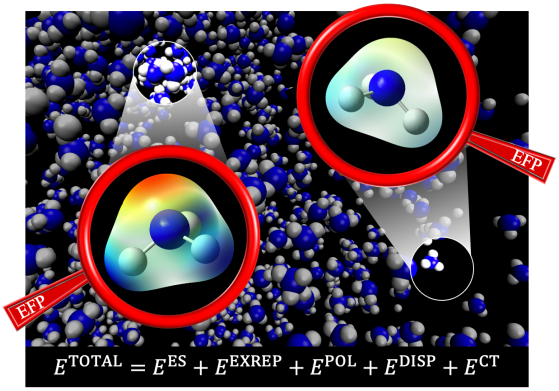
For designing optimal solvents for chemical engineering processes such as fluid transportation, separation extraction, and gas absorption, it is mandatory to predict the thermodynamic properties of the candidate solvents by *ab initio* molecular simulations. However, the computational costs of the *ab initio* molecular simulations are too high to make practical applications within enough short time. In the field of chemical engineering, it has been forced to perform non-efficient experimental tasks including try and error.

With the background, in recent years, we have developed a novel molecular simulation method based on fragment-based molecular theory (Effective Fragment Potential Molecular Dynamics; EFP-MD), which is promising for *ab initio* prediction of thermodynamic properties of functional liquid materials.[1-3] In the EFP theory, which was originally developed by Day *et al.*,[4,5] macroscopic thermodynamic properties of the functional liquids are expanded by a set of compact wave functions of the component "Fragment" molecules. We have shown that liquid structures, excess functions, and diffusion constants of functional liquid materials (ionic liquids, mixed solvents, and supercritical fluids) can be at least qualitatively well described by our EFP-MD simulations. We have also succeeded in predicting equilibrium thermodynamic properties of the functional liquids by combing the fragment-based molecular theory with machine learning techniques.



In this talk, we'll show the way to screen functional liquid materials with enough prediction speed and chemical accuracy. The corresponding experimental validations with small costs will be also presented.

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