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Ultimately large-scale *ab initio* molecular dynamics with effective fragment potential opens an era for predicting physicochemical properties of mixed liquids and supercritical fluids

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Abstract (less than 300 words)

Predicting the fundamental properties of solutions is one of the essential aspects of chemical engineering. Although the design of liquid mixtures and supercritical fluids is an indispensable technology in chemical engineering, it has been impossible to simulate their kinetic behavior in detail. Of course, in the spirit of "quick and dirty" chemical engineering, it would be great if faster molecular simulations were possible, which would directly accelerate research and development. However, now that we have access to powerful computers, shouldn't we take full advantage of their capabilities and tackle chemical engineering simulations previously impossible in principle? The future of chemical engineering should be revolutionized to be "Quick and Clear" with the help of high-speed computers and first-principles molecular simulations that maximize their capabilities.

In this context, recently, we have established an accurate and efficient first-principles MD protocol (EFP-MD; Effective Fragment Potential-Molecular Dynamics [1-3]), which focuses on the apparent fact that the interacting molecules determine the nonlinear molecular interactions that govern condensed matter properties. In this talk, we will start from the basics of the EFP-MD method and introduce the application of the EFP-MD method to ionic liquids, mixed liquids, and supercritical fluids.

References

[1] N. Kuroki, H. Mori, *J. Phys. Chem. B* **123**, 194-200 (2019).

[2] N. Kuroki, H. Mori, *Chem. Phys. Lett.* **694,** 82-85 (2018).

[3] N. Kuroki, H. Mori, *Chem. Lett.* **45**, 1009-1011 (2016).