Is it possible to predict supercritical properties by *ab initio* molecular dynamics simulation?: Effective Fragment Potential version 2 - Molecular Dynamics (EFP2-MD) simulation study

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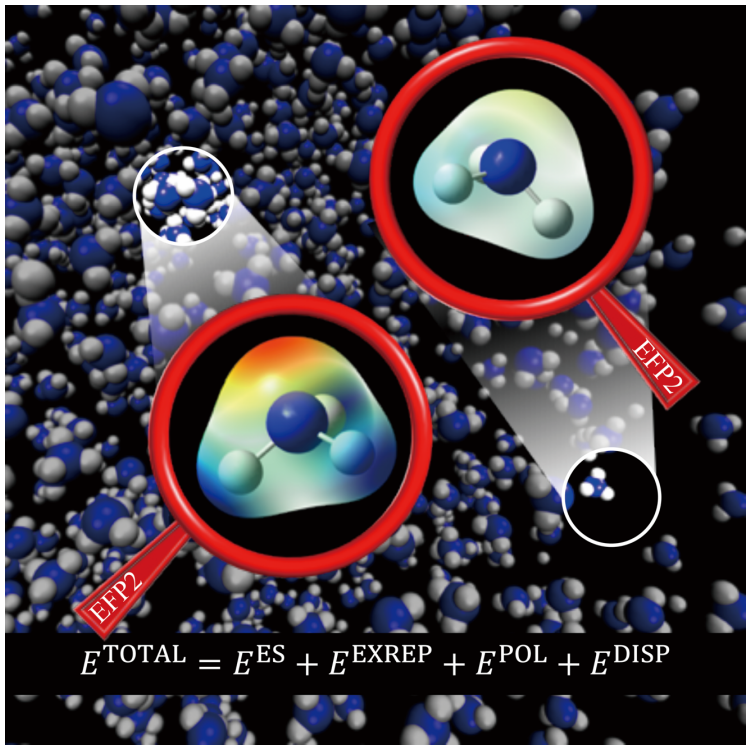
Effective fragment potential version 2-molecular dynamics (EFP2-MD) simulations, where the EFP2 is a polarizable force field based on ab initio electronic structure calculations, were applied to predict the static and dynamic liquid properties of compressed liquid NH_3. By analyzing the temperature dependence of the radial distribution function, the autocorrelation functions of velocity ($C_v(t)$) and reorientation ($C_r(t)$), and the self-diffusion constant, we clarified that the ab initio EFP2 force field can effectively describe the properties of compressed liquids. These descriptions can be performed with at least semiquantitative accuracy and at a sufficiently low computational cost. In the EFP2-MD protocol, no force field training is required. This training is mandatory when simulating liquid properties with classical MD techniques (especially in extreme conditions with high pressures and temperatures). EFP2-MD is a promising technique for predicting the physicochemical properties of novel functional compressed liquids, including supercritical fluid phase properties.



References

1. N. Kuroki and H. Mori, *J. Phys. Chem. B* **123** (2019), 194-200. (Selected as inside cover)