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Self diffusion of water molecules simulated by model inter-atomic potentials determined by a combination of first-principles calculation and multi-canonical ensembles: exchange-correlation functional dependence
YOSHIHIDE YOSHIMOTO, Dept. of Computer Science, Graduate School of Information Science and Technology, The University of Tokyo — Water is an ubiquitous substance and is both scientifically and technologically important. In this study, the self diffusion of water molecules are simulated using Kumagai-Kawamura-Yokokawa type inter-atomic potentials [1] whose parameters are determined by a combination of first-principles calculation and multi-canonical ensembles [2,3]. Because of the property of multi-canonical ensemble, the determined potentials keep the thermodynamics of the reference first-principles simulations to a maximum extent. The author used PBE, PBE0, B3LYP, and B3LYP with DFT-D3 exchange-correlation potentials for the reference first-principles calculations to determine the model parameters. The obtained diffusion coefficients significantly depend on the choice of the exchange correlation functionals and the combination of B3LYP and DFT-D3 [4] produced the best agreement with the experimental one.

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