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Water Models: adventures in parametrization (G)

Sunday 10 June 2018 17:00 (2 minutes)

Water is the most important solvent in biological systems. Yet majority of its properties are poorly reproduced by the most commonly used models. An ideal water model needs to accurately capture both structure and dynamics over a wide range of thermodynamic conditions.
To create such a model we attempted both coarse grained¹ and atomistic parametrizations. Our experience shows the need for fitting to multiple target properities at different state points for the model to be both accurate and transferable.

1. Rodríguez-López, T., Khalak, Y., & Karttunen, M. (2017). Non-conformal coarse-grained potentials for water. *The Journal of chemical physics*, 147(13), 134108.

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