Multi-criteria Optimisation of Molecular Models of Water

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Molecular models of water are widely used; and there are many of them. In their development, parameters are fitted, in order to represent certain properties well. Due to the inevitable simplifications of the model, not all properties can be described equally well; hence, there are conflicting objectives. Multi-criteria optimisation (MCO) is the method of choice for tackling such problems. However, MCO is computationally expensive and has therefore not been used before for optimising water models. Brute force methods are infeasible, as this would require a very large number of computationally expensive molecular simulations. To overcome this problem, the *reduced units method* [1] is used here. This method exploits the fact that computer simulations internally use dimensionless properties. The input and output properties are usually provided in physical units. In the simulation, they are transformed into dimensionless properties by introducing reference values. These transformations are such that a given dimensionless simulation result contains information on an infinite number of physical situations. This can be used to drastically reduce the simulation effort required in the MCO. This approach is applied here to optimise non-polarisable water models. Three properties are considered as objectives: vapour pressure, saturated liquid density and enthalpy of vaporisation. MCO yields not only a single optimal solution but a set of optimal solutions, the so-called Pareto set. The Pareto set gives an overview of what can be achieved with a given model class. It is shown that using the new MCO approach, molecular models of water can be found which yield significantly better results for the studied properties than the best existing models, such as SPC/E and TIP4P/2005. The new MCO method for the development of molecular models is efficient, robust, and broadly applicable.

References

[1] T. Merker, J. Vrabec, H. Hasse, Soft Mater. 10 (2012) 3-25.