Transferable Force Fields and Transport Properties

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Classical transferable force fields allow predicting physical properties and microscopic processes of pure substances and mixtures. The development is demanding because force-field parameters are highly correlated and simulations are computationally expensive. We use the PC-SAFT equation of state [1] as surrogate model to drastically accelerate the optimization procedure leading to the TAMie force-field with very good descriptions of static properties including phase equilibria of pure substances and of mixtures. Transport properties such as viscosity, thermal conductivity, and self-diffusion coefficients however, are described with considerable errors. We propose new reduced order models for transport properties based on entropy scaling [2] which can be combined with force fields in various ways.
First, Multi Fidelity Modeling [3] provides a way to combine data from experiment and simulations with a suitable transferable force-fields like TAMie in a meaningful way and thus take advantage of both worlds. Precision of experimental measurements can be combined with exploration and extrapolation capabilities of simulations.
Second, new transferable force fields that describe both static and transport properties are developed by using PC-SAFT and entropy scaling together in the optimization procedure. Transport properties can then be considered as part of the objective function, whereby the surrogate models significantly accelerate the convergence of the optimization problem.

References

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