

Modelling beyond manual intervention -- Approach routes to a most useful molecular description

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Nowadays simulations are widely used to support the development process for new materials. Typically, through simulations researchers are capable of predicting the general trends quite well, but the informative value of quantitative statements is very often limited due the lack of specifically designed force fields.

We address this problem by setting up robust workflow routines that execute standard procedures autonomously (like e.g. equilibration). Moreover, we integrate these routines into superordinate procedures that allow for unaffected model refinement by automated parameter optimization. To this end, parameters describing a model compound are fitted to reproduce experimental reference values as closely as possible.

However, the quality of the initial model (in terms of concordance with key reference properties) decides whether this route can be taken straightaway or not. In case of poor model quality we may need to narrow down the search space before applying the above standard optimization routines. To do so we learn from randomly chosen parameter sets via advanced interpolation techniques. This allows us a global view over the parameter space after a period of recording data points and to enter the above optimization routine with a promising initial model.

The benefit of fast, automated, and reliable routines (also in combination with a global parameter search) to optimize model parameters will be illustrated by some atomistic force field models for small solvent molecules/polymer precursors and ionic liquids.