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# The perfect fit? Balancing predictive power and computational complexity for an atomistic model as prerequisite for nano-scale simulations

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When aiming at quantitative predictions for materials that require huge system sizes in simulation – such as polymers – models at coarse-grained level are the natural choice. However, capturing the chemical identity of beads that are void of any individual structure resembling the original compound is a critical point for achieving meaningful predictions. As the coarse grained model inherits the features from an atomistic precursor, the latter needs to be most predictive. This may be achieved by calibrating the detailed model carefully to experimental data, thereby enhancing the atomistic model structure with most realistic behaviour [1].

Diverse strategies like e.g. simplex optimization [2][3], interactive design parameter optimization [4][5], i.e. local optimization versus global search, have been applied to study the polymer precursor ethylene-epoxide and have been intensively investigated in order to identify a viable route to a perfectly tailored atomistic model. Obviously, each strategy has its profits and limitations, the bottom-line being that a final model needs to yield results that are not only accurate, but also to be robust with respect to transfer between independent program packages. For ethylene-oxide several competing models have been published [1,6][7][8][9][10], however not all are suited for a later coarse graining step. The present field report details newly created models, as well as the tested methods, thus it documents the progress with respect to the long term objective of accurate property predictions for nano-scale simulations.

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