Computational materials science on an atomistic basis: A multi-scale problem

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Although modern computer codes based on density functional theory (DFT) allow the reliable prediction of many material properties, they cannot be applied, when the problem of interest demands a consideration of huge configuration spaces or model systems containing many thousand atoms. Moreover, DFT based methods do not allow for exchange processes between atoms and therefore, do not consider configurational enthalpies being a prerequisite for modeling the temperature-dependence of substitutional ordering phenomena in multi-component systems.

In principle, the combination of methods allowing for studying dynamic processes on the atomistic scale as molecular dynamics (MD) (introduced in this summerschool) with DFT would be a powerful tool to overcome these limitations, if we find a key to couple these individual approaches. It will be demonstrated that one very successful concept to "open the door" is the use of so-called Cluster Expansions (CE) and Monte-Carlo Simulations (MC). It will be shown, how these "multi-methods approach" of DFT, MD, CE, and MC permits us to treat material properties up to the mesoscale without any empirical parameters as input, but with an accuracy that allows the quantitative comparison with experimental results. The focus will be on processes which possess a delicate time- and temperature-dependence like short-range order or precipitate evolution.