



Aktuelle Probleme der Werkstoffwissenschaften

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Prediction of structural stability: From structure maps to machine learning

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The computational design of materials relies on the ability to predict the crystal structure as well as the structural and functional properties for a given chemical composition and processing route. This requires adequate approaches to treat the chemical diversity (e.g. ~10 components in superalloys), the geometric complexity of the microstructure (e.g. dislocations and precipitates in steels) and the underlying physical phenomena (e.g. magnetic phase transitions in iron, finite-T properties of battery materials). I will present coarse-grained electronic-structure methods for atomistic simulations as well as data-driven structure maps for the prediction of the structural stability of transition metals and their compounds. The coarse-grained electronic-structure methods preserve the quantum-mechanical nature of the chemical bond but at the same time allow us to perform large-scale atomistic simulations that capture the complexity of microstructure and physical phenomena. They also provide descriptors that are used to construct the highly predictive structure maps by data analysis. This physical motivation of our descriptors rules the application of the structure maps highly intuitive even for chemically complex systems. As a combination of both concepts, we recently derived an electronic-structure based descriptor that provides a direct link between the local atomic environment and the binding energy which rules the descriptors highly suitable for practical machine-learning applications. Examples of applying these electronic-structure based modelling approaches for materials design will be outlined.