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Bayesian Uncertainty Quantification in Alloy Modelling and Design

Abstract

We present a fully Bayesian framework for quantifying uncertainties in alloy modeling using surrogate models in place of expensive electronic structure based computer codes. We start with the development of an exchange-correlation functional capable of uncertainty quantification capabilities for density functional theory. We discuss predictions on atomization energies and bulk properties. We then provide a Bayesian outlook of a popular alloy surrogate model: the cluster expansion. We propagate uncertainties from not knowing the best surrogate model and its parameters to alloy phase transition temperatures, phase diagrams, band gaps, and bulk properties. We provide a Bayesian justification of the validity of using surrogate models in expensive electronic structure calculations and alloy design. The structure selection problem is fundamental for training surrogate models with a limited computational budget for the prediction of a particular quantity of interest and in closing we will provide some insights on information theoretic approaches for this active learning task.