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Handling uncertainties in the development of tight-binding potentials : application to zirconium hydride

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In the field of material science for energy applications, zirconium hydrides are studied both for their useful application for hydrogen storage and for their negative effect on mechanical properties of the nuclear fuel cladding material (zirconium) in water cooled reactors. At the atomic scale, the tight-binding (TB) approximation has proven to be a satisfying method to develop potentials that are both accurate and computationally tractable to model zirconium hydrides. Such potentials are defined by a fixed number of parameters that need to be accurately identified for the model to be reliable. The reliability is indeed closely related to the uncertainties associated with parameters [1]. Even if the use of parametric potentials, TB or semi-empirical ones, is widely established in the literature [2], very few studies discuss the quantification of such uncertainties [3–5].

This work aims at quantifying the uncertainty associated with the calibration of TB potentials. A previously developed TB potential [6]is used, focusing on its ability to reproduce elastic constants and lattice parameters of δ (cubic) and ϵ (tetragonal) zirconium hydrides. Uncertainty Quantification (UQ) methods, based on polynomial chaos expansion and Bayesian inference, are used to estimate the parameters uncertainties, through their *a posteriori* probability distributions and starting from a limited number of experimental and DFT data. The accuracy of the TB potential - with respect to the available data - is thus improved. In addition, having characterized the uncertainty on the model parameters, we can estimate the uncertainty propagation on any computed property.

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