O.22 Multibinit lattice part: From ab-initio data to predictive lattice potentials

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Despite the increase of computational power, first-principles DFT simulations remain still nowadays practically limited to relatively small length scale (few hundreds of atoms per cell) and short time scale (few picoseconds). The bottleneck is the computationally demanding quantum mechanical treatment of the electrons.

Here we present from A to Z how to build practically a lattice effective potential based on a polynomial expansion including all lattice degrees of freedom [1] for any material with MULTIBINIT [2], which allow to by-pass the first-principles limitations: starting from the determination of the required DFT data to the validation of the effective potential, going through the model generation and the fitting procedure. We will for each step, remind the underlying concepts, illustrate with a concrete example and present the tools we developed to ease the process and make it accessible to anyone. In line with that, various functionalities implemented in AGATE [3] will be presented that help create the necessary first-principles data, post-processing second-principles data and extracting key informations to validate the model, simulate materials at finite temperature and even predict new behaviours. The power of our scheme will be illustrated by the treatment of perovstkite titanates $ATiO_3$ with A=Ca,Sr,Ba,Pb.

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