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Atomic Cluster Expansion and application to modelling of materials

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Classical and machine learning interatomic potentials alike incorporate design choices that reflect the intuition of their authors and that are justified only a-posteriori by the performance of the model. Design choices comprise, for example, the form of the embedding function of an embedded atom potential or a specific angular dependence of a descriptor in a machine learning potential.
The atomic cluster expansion (ACE) [1-3] takes a different route. Based on the broad assumption of locality, it establishes a complete and orthonormal basis for the space of local atomic configurations. The ACE basis functions immediately comply with the basic symmetry requirements of atomic scale physics, they are invariant under translation, rotation, inversion and permutation of atoms. This enables the systematic expansion and convergence of atomic scale properties in analogy to quantum mechanics, where one is used to converging basis functions for the accurate representation of energies and forces. And the completeness enables ACE to represent common machine learning descriptors and potentials.
ACE has been implemented in the LAMMPS molecular dynamics simulation software package and its numerical efficiency is competitive or superior to other ML potentials [4]. After an introduction to ACE, I will discuss the parameterization of ACE from first principles reference data and the computation of thermodynamic and mechanical properties.
Three factors are critical for obtaining accurate and transferable ACE, (i) an extensive, diverse and high-quality reference dataset, (ii) a robust and efficient training procedure, and (iii) a thorough validation including assessment of uncertainty. I will show how our parameterization strategy incorporates the three factors and enables near automatic construction and convergence of ACE [5].
I will then discuss ACE for a number of elements, compounds and molecules and review their properties against reference data. Analysis of mechanical properties and automated free energy and phase diagram calculations [6] will be presented.

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Poster title

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