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Description of interatomic interactions with neural networks[1]
SAMAD HAJINAZAR, JUNPING SHAO, ALEKSEY N. KOLMOGOROV, Physics Department, Binghamton University — Neural networks are a promising alternative to traditional classical potentials for describing interatomic interactions. Recent research in the field has demonstrated how arbitrary atomic environments can be represented with sets of general functions which serve as an input for the machine learning tool. We have implemented a neural network formalism in the MAISE package [1] and developed a protocol for automated generation of accurate models for multi-component systems. Our tests illustrate the performance of neural networks and known classical potentials for a range of chemical compositions and atomic configurations. [1] Module for Ab Initio Structure Evolution, http://maise-guide.org

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