Development of neural network-based interatomic potentials for acceleration of structure prediction

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Interatomic models based on neural networks (NNs) have emerged as attractive alternatives to traditional potentials. Being general and flexible learning machines, NNs can be tuned to describe diverse atomic environments with near *ab initio* accuracy. In an effort to automate the construction of NN models for multielement systems, we have developed a systematic data generation protocol to sample relevant parts of configuration space and a stratified training scheme to fit models sequentially from the bottom up: first for unaries, then for binaries, and so on [1]. This approach implemented in our MAISE package [2] has allowed us to generate a library of accurate NNs across a block of chemical elements. Practical use of such NN interatomic models in structure prediction has demonstrated that they are efficient enough to accelerate *ab initio* global structure searches by orders of magnitude and reliable enough to identify overlooked stable materials [3,4].

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