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Neural evolution structure generation: High Entropy Alloy

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High-entropy alloys (HEAs) are particularly interesting because of their energy-related applications. Computational modeling is necessary for targeted and rapid HEAs discovery and application, and constructing an appropriate atomic structure is the first step towards reliable predictions of materials properties. We propose a method of neural evolution structures (NESs) combining artificial neural networks (ANNs) and evolutionary algorithms (EAs) to generate High Entropy Alloys (HEAs) structures. Our inverse design approach is based on pair distribution functions and atomic properties and allows one to train a model on smaller unit cells and then generate a larger cell. With a speed-up factor of approximately 1000 with respect to the Special quasi-random structures (SQSs), the NESs dramatically reduces computational costs and time, making possible the generation of very large structures (over 40,000 atoms) in few hours. Additionally, unlike the SQSs, the same model can be used to generate multiple structures with same fractional composition.A number of NE structures have been used to compute selected properties such as the elastic constants, the bulk modulus, and the Poisson ratio, and the results are similar to those of structures generated with SQS.