

Organization of neural network for predicting the potentials of interatomic interaction

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The report presents a program that implements an object-oriented model of an artificial neural network for predicting the potentials of interatomic interaction. The complete functional form of a neural NNP network, supported activation functions, radial and angular symmetry functions (ACSF), and the atomic environment detection function are considered. (circumcision). The description of the user interface, online and batch modes of operation, validation and approbation of the neural network is presented. A converter of atomic systems data from the Fortnet open software package has been developed. Examples of data obtained in the process of batch training of a neural network are shown. To parallelize the learning process, an updated NNP network architecture consisting of atomic subnets is proposed.