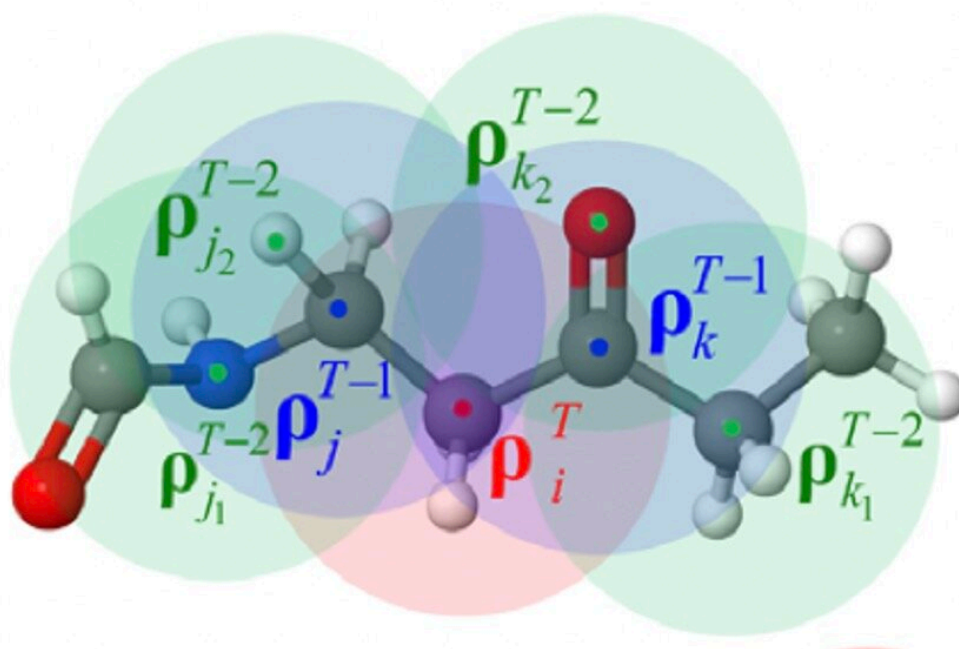


Researchers develop recursively embedded atom neural network model

October 26 2021, by Liu Jia



Schematic diagram of the REANN model showing how the density descriptor is recursively embedded. Credit: ZHANG Yaolong et al.

In a recent study published in *Physical Review Letters*, a research team led by Prof. Jiang Bin from University of Science and Technology of China (USTC) of the Chinese Academy of Sciences proposed a

recursively embedded atom neural network (REANN) model based on their previous work on creating high-precision machine-learning (ML) potential surface methods.

With the advancement of machine learning technologies, a common method to build potential functions is atom neural networks (ANNs) under which the [total energy](#) is the sum of each atomic energy dependent on the local environment. Three-body descriptors have long been considered complete to describe the local environment.

Recent work, however, has found that three-body (or even four-body) descriptors could lead to the local structural degeneracy and thus fail to fully describe the local environment. This problem has posed difficulties to improve the precision of ANNs' potential surface training.

The REANN [model](#), using a recursively embedded density descriptor, shares the same nature with the less physically intuitive message-passing [neural networks](#) (MPNNs). The researchers proved that iteratively passing messages (namely updating orbital coefficients) to introduce many-body correlations can achieve a complete description of the [local environment](#) without explicitly computing high-order features.

By testing the dataset of CH₄ and bulk water, the researchers revealed the local completeness and nonlocality of this new model and showed that compared with current ML models, it has better accuracy.

The study provides a general way to easily improve existing ML potential surface frameworks to include more complicated many-body descriptors without changing their basic structures.

More information: Yaolong Zhang et al, Physically Motivated Recursively Embedded Atom Neural Networks: Incorporating Local Completeness and Nonlocality, *Physical Review Letters* (2021). [DOI:](#)

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