Transferable neural network potential for C-H systems: versatile applications from molecules to 3D materials

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Interatomic potentials (IP) based on neural network (NN) have obtained significant attention in materials science due to their ability to capture complex atomic interactions. In this study, we present a transferable NN-based IP specifically tailored for C-H systems. The potential has been meticulously trained on cluster data, enabling its versatile applications across a wide range of materials, including molecules, 2D materials, and bulk systems. Here, we highlight the key features of this potential, focusing on its accuracy and its capacity to faithfully reproduce intricate C-H interactions. We demonstrate the potential's performance in predicting essential properties such as structural characteristics, energetics, and dynamics of C-H systems. Its applicability in diverse settings makes it an invaluable tool for researchers interested in investigating the properties of systems containing C-H bonds.