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Accurate temperature dependent interatomic potential for dense matter based on ab initio calculations JIAYU DAI, HUAYANG SUN, JIANMIN YUAN, National University of Defense Technology — Combining molecular dynamics, ab initio molecular dynamics is capable of simulating various dynamic behaviors relevant to temperatures, pressures and laser fields. However, because of the computational cost and limitation by parallel methods, AIMD is usually applied to systems containing a few hundreds of atoms, which condemns its application to the study of dynamic compression, phase transition, and transport behaviors. Although classical molecular dynamics can investigate large systems of more than 10^6 atoms, it requires accurate and wide range temperature-dependent interatomic potentials which are seldom available, in particular for the dense matter. Here, we construct new temperature-dependent interatomic potentials using neural network method, based on the structures and energies from AIMD using tens of atoms. The new potential is implemented in CMD and the computational efficiency is found improved by 10^3 times. Using the new potential, the calculated energies, pressures and melting points in a wide range of temperature and pressure are almost the same as that from the AIMD method. Based on this new approach, it is possible to investigate dynamic compression processes and phase transitions within the accuracy of ab initio method.

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