

Atomistic simulation of materials and processes using neural network potentials

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The importance of atomistic simulation is ever increasing in materials science. However, the heavy computational cost of ab initio methods has been an obstacle against wide application of atomic simulation. Recently, machine-learned potential is attracting wide attention as it combines the efficiency of classical force field and accuracy of ab initio methods. In this presentation, I will introduce on the machine learned potential and various applications of the method that has been carried out in our group.