Developing Accurate and Transferable Artificial Neural Network Potentials for Li-Si Alloys[1] BERK ONAT, EKIN DOGUS CUBUK, BRAD MALONE, EFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Investigation of the lithiation and delithiation of Si anode in Li-ion batteries using realistic simulations is important and requires large numbers of atoms and long time scales which is generally inaccessible with first-principle approaches. These simulations can be carried out using interatomic potentials that can capture the dependence of structure on chemical composition. Compared with the fixed functional form of empirical potentials, a promising approach to construct the potential energy surface is using artificial neural networks (ANN) that extends the time scales of simulations without sacrificing the accuracy and transferability. Using ab-initio density functional theory data for training, we developed an environment-dependent high-dimensional ANN potential for Li-Si alloys. Our calculations based on the geometry optimizations and molecular dynamic simulations show that the developed potential can accurately predict total energies and equilibrium structures of Li, Si and Li-Si alloys. Using several training databases that include different concentrations of Li in the alloy, we investigated the range of the validity of the ANN potential. Our results show that ANN potentials are widely transferable to Li-Si alloys with various concentrations of Li.

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