**Atom Dynamics in Solids Studied by Machine-Learning Techniques**

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Development of novel information and energy devices demands deeper understanding on atom dynamics in solids, such as diffusion and vibration. First-principles calculations within the density functional theroy (DFT) is powerful to meet the demand. In practice, however, DFT often requires too heavy computations to tackle with atom dynamics in solids. In this context, interatomic potentials constructed with machine-learning technique and DFT calculation data have attracted much attention recently. In the prensent talk, we will describe our recent works on interatomic potentials constructed with one of machine-learning techniques, neural network (NN).

Our NN potentials are based on the method proposed by Behler and Parrinello [1]. We discuss NN potentials to examine diffusion behaviors of Cu in amorphous Ta2O5 [2] and Li in Li3PO4 [3]. The results agree well with DFT calculations, showing the high reliability of the constructed NN potentials. For Li in Li3PO4, the NN potential trained in a small supercell is successfully applied to calulations in much larger supercells, which suggests good transferability. We will also discuss (i) atom dynamics under electric fields, (ii) structures of metal/solid-electrolyte interfaces, and (iii) phonon bands and thermal transport, with describing our prelimienary results.

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