

Studying Atom Diffusion Behaviors in Amorphous Oxides Using Neural Network Potentials

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To clarify atom diffusion behaviors in solids, especially oxides, is important for development of novel information and energy devices. Atomistic simulations using reliable method such as the density functional theory (DFT) are powerful for this, but performing this for amorphous materials is computationally quite heavy. In this talk, I describe our attempts to construct simplified neural network (NN) interatomic potentials for efficient prediction of atom diffusion behaviors in amorphous oxides.

First, we discuss Cu diffusion in amorphous Ta₂O₅ [1]. The structures and data for the NN training are obtained using DFT. One Cu atom is inserted into the amorphous Ta₂O₅ randomly, and then the structure is optimized. The NN potential is constructed using the method proposed by Behler and Parrinello [2], but we simplify their method considering that only the Cu atom motion is important in the present case. After training using 540 samples, the mean absolute error of energy prediction is less than 0.1 eV. The calculation speed of NN potential is several orders of magnitude faster than DFT. The pathways and barrier energies for Cu diffusion calculated using the NN potential agree well with those obtained from DFT calculations.

Next, we discuss Li diffusion in amorphous Li₃PO₄ [3]. In this case, we constructed NN potentials for P and O atoms assuming preservation of P-O polyhedron structures, while individual atoms are considered for Li. The Li diffusion coefficient estimated using the obtained NN potential agrees well with the one estimated with DFT calculation.

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References

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- [2] Behler and Parrinello, Phys. Rev. Lett. 98 (2007) 146401.
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