ARTIFICIAL NEURAL NETWORKS FOR ATOMIC MIGRATION BARRIER PREDICTION

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Kinetic Monte Carlo (KMC) is a stochactic simulation method, especially suited for studying diffusion. KMC simulations require the rates of all allowed processes to be known. One way of calculating the rates for migration processes is the Arrhenius equation

$$k = \nu \times \exp\left(-\frac{E_\mathrm{b}}{k_\mathrm{B}T}\right)$$

where ν is a temperature-dependent prefactor, E_b is a process-dependent energy barrier, k_B is the Boltzmann constant and T is temperature. In some systems, millions (or billions, or more) of different processes are possible, requiring a computationally unfeasible amount of barrier calculations. One way to avoid doing some of these calculations is to train an artificial neural network (ANN) on a small calculated subset of all possible barriers, and use it to predict the rest.

ANN is a machine learning method that can be applied to find the underlying patterns and dependencies in large datasets, e.g. in computational physics, chemistry and biology. We have applied it to study surface diffusion in Cu and bulk diffusion in Ni-Cr alloy. The training dataset was calculated with the nudged elastic band method (NEB). The advantages and disadvantages of the ANN method are discussed.

(left) ANN-predicted Cu migration energy vs. exact values from NEB. Inset is an image of a migration event: blue atom jumps to position circled in red.
(right) A schematic figure of energy levels and barriers of a forward and reverse migration process.