Replica ensemble based uncertainty estimation for NNP

This work proposes a highly efficient and atomic-resolution prediction uncertainty indicator for neural network potential (NNP) using a "replica" ensemble. Compared to previous approaches using model ensembles, the present method excels in the training speed and spatial resolution. This method is applied to simulating silicidation processes of Ni contacts in semiconductor devices, which is a highly complicated process and requires close monitoring of prediction uncertainty to judge the soundness of simulations. By analyzing the problematic structures, NNP can be improved with a repairing data set, thereby obtaining a reliable simulation up to several nanoseconds. This work was published at The Journal of Physical Chemistry Letters 2020, **11**, 6090.