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Investigating the impact of high electric field on the surface of metals using artificial neural networks along with molecular dynamics

The effect of high electric fields on the surface of metals can be severe and problematic leading to tip formation and vacuum breakdown. Since these effects relate to electric dipole and polarizability of the surface, they should be studied based on first-principle methods. On the other hand, these methods are computationally demanding and do not scale up to realistic times and dimensions. In this regard, Machine learning (ML) can establish a useful bridge between high-accuracy ab-initio calculations and high-efficient molecular dynamics. Since the effect of electric field is confined to only a few layers in the surface, a model based on artificial neural networks is proposed to calculate these surface effects, while the bulk of material is being treated classically by molecular dynamics. To make the surface interactions accurate, the input for training were prepared by density functional theory (DFT) and overall 500 frames were prepared for a 6-layer Tungsten slab between temperatures 0-2500 K. After training the deep neural network model, there was a good correlation between the forces predicted by ML and DFT. The model then coupled with LAMMPS code to predict surface effects simultaneously and feed them to classical force fields.

Type of contribution

Poster

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