MARVEL

THEOS
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Accurate and Efficient Neural Network Potentials for Atomistic Simulations

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Abstract: Simulations of realistic catalyst particles critically depend on the accurate description of the underlying potential energy surface (PES). While first-principles methods such as density-functional theory (DFT) can provide very accurate energies and forces, they are computationally too demanding to address many relevant systems. Behler-Parrinello Neural Networks (NN) trained to first-principles data have been shown to provide accurately interpolated PESs that allow to speed up simulations by many orders of magnitude compared to conventional DFT [1-3].

Here we demonstrate the capabilities of NN potentials for different classes of materials: a transition metal (copper) [3], a semi-conducting metal oxide (zinc oxide) [4], metal/oxide interfaces (a Cu cluster on ZnO) [5], and functional nanoparticles (Cu doped CeO2) [6]. To assess the accuracy of NN potentials, we compare structural energy differences, vacancy formation energies, and surface energies of different copper and zinc oxide surfaces with their DFT reference values. We then showcase how a combination of first-principles computations and large-scale Monte-Carlo simulations based on NN potentials can be employed to study the equilibrium composition and atomic ordering of bimetallic Au/Cu nanoparticles [7].

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