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High-dimensional neural network potentials for metal surfaces: A prototype study for copper

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The atomic environments at metal surfaces differ strongly from the bulk, and, in particular, in case of reconstructions or imperfections at "real surfaces," very complicated atomic configurations can be present. This structural complexity poses a significant challenge for the development of accurate interatomic potentials suitable for large-scale molecular dynamics simulations. In recent years, artificial neural networks (NN) have become a promising new method for the construction of potential-energy surfaces for difficult systems. In the present work, we explore the applicability of such high-dimensional NN potentials to metal surfaces using copper as a benchmark system. A detailed analysis of the properties of bulk copper and of a wide range of surface structures shows that NN potentials can provide results of almost density functional theory (DFT) quality at a small fraction of the computational costs.

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