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Physically informed artificial neural networks for atomistic modeling of materials

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Large-scale atomistic computer simulations of materials heavily rely on interatomic potentials predicting the energy and Newtonian forces on atoms. Traditional interatomic potentials are based on physical intuition but contain few adjustable parameters and are usually not accurate. The emerging machine-learning (ML) potentials achieve highly accurate interpolation within a large DFT database but, being purely mathematical constructions, suffer from poor transferability to unknown structures. We propose a new approach that can drastically improve the transferability of ML potentials by informing them of the physical nature of interatomic bonding. This is achieved by combining a rather general physics-based model (analytical bond-order potential) with a neural-network regression. This approach, called the physically informed neural network (PINN) potential, is demonstrated by developing a general-purpose PINN potential for Al. We suggest that the development of physics-based ML potentials is the most effective way forward in the field of atomistic simulations.