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Development of Interatomic Potential Energy Surfaces Based on ab initio Electronic Structure Methods and Neural Networks for Molecular Dynamics Simulations

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Molecular simulations play an important role in the fundamental understanding of chemical reactions and materials properties. These simulations provide crucial insights into various mechanisms operational at the atomistic level which ultimately gives rise to chemical, mechanical, and electronic properties of materials. Results from these simulations often complement and guide further advancements in the experimental field. Central to molecular simulations is the interatomic potential which describes the interactions between atoms. A common approach relies on the development of empirical potential energy functions, which are relatively faster to evaluate. Such functions make it feasible to consider a few million atoms in the simulation. Although, empirical potential functions provide a simple and physically interpretable description for the interatomic interactions their accuracy is limited by the underlying functional form. An accurate description of interatomic interactions can be obtained by using ab initio electronic structure methods, but these calculations are also much more computationally expensive compared to empirical functions.

This work combines the accuracy of ab initio electronic structure methods with function approximation capabilities of neural networks without relying on a priori assumption about the functional form. During training of the neural networks, both the functional form as well as the parameters are optimized simultaneously. This approach is further extended by incorporating concepts of many-body expansions and moiety energy approximation to develop Generalized Potential Energy Surfaces. Each of the M-body terms in the expansion is represented using a neural network and all the network parameters are trained simultaneously to preserve the coupled nature of the M-body expansion terms. Generalized Potential Energy Surfaces can accurately characterize different bonding states of the system and provides a greater flexibility for investigating chemical reaction dynamics and phase transformations. This approach expedites the design and development of new materials and obtaining structure-property relationships.

This neural networks-based method is implemented for the prediction of higher-level electronic structure energies using atomic configuration coordinates and lower-level electronic structure energies. This method offers an approach for conducting electronic structure calculations at the accuracy of a higher-level electronic structure methods using a larger basis set, while keeping the computational time requirements corresponding to that of a lower-level method.