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Exploration of energy surfaces and conformation of molecules and solids by utilizing a machine-learning technique

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Predicting the physical properties of novel materials requires an accurate description of atomic interactions as provided by first-principles quantum mechanical calculations. Efficient and practical calculation tools have been developed along with the progress of density functional theory (DFT). Still, however, the computational complexity associated with the quantum mechanical treatment limits their applications to systems of a few hundreds of atoms at most. Here, we present an application of the Gaussian process regression (GPR) scheme to the global optimization, conformation space annealing, and pathway optimization methods. We demonstrate that the use of GPR-based pathway optimization technique, e.g., action-derived molecular dynamics (ADMD) method, can be useful in enhancing the computational performance. We will discuss possible future applications of the GPR-based machine learning technique for the exploration of energy surfaces and conformation of molecules and solids.

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