Development of molecular structure search method with Bayesian optimization

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In the search for molecular structures on the potential energy surface (PES), energies and energy gradients by quantum chemical calculations have been used. Replacing energy calculations with measurements on Quantum computers, smooth PES cannot be drawn due to errors in the predictions, that is the conventional structure search cannot be applied. Thus, the method without energy gradients, Bayesian optimization has drawn much attention. In molecular structure search, Bayesian optimization is a method of predicting the energy with Gaussian process regression model and obtaining the structure with the maximum value of the acquisition function repeatedly. Although it is essential to design an appropriate acquisition function to search for structures on PES using Bayesian optimization, the guideline is still unknown. In this study, we developed molecular structure search method with Bayesian optimization, and searched for the global minimum on the ground state(S0) and the most stable conical intersection between S0 and the singlet excited state (S1). Using formaldehyde and ethylene as examples, we searched for the target structures and succeeded in obtaining the desired structure with high accuracy.