Quantum Chemistry Assisted by Machine Learning

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In my talk I will show how machine learning (ML) assists quantum chemical research in a variety of ways. First, machine learning can be used to improve the accuracy of low-level quantum chemical (QC) method either by explicitly correcting their predictions as in Δ-learning approach[1] or by improving the semiempirical QC Hamiltonian as in parameter learning technique.[2] Second, ML can be used for very accurate representation of potential energy surfaces, *e.g.* to drastically cut the number of high-level QC calculations required for predicting rovibrational spectra with spectroscopic accuracy[3] or to perform excited-state nonadiabatic dynamics simulations at very low computational cost[4-5]. For carrying out this research I develop *MLatom*[6-7] program package optimized for efficient and user-friendly use of kernel ridge regression-based ML in atomistic simulations.

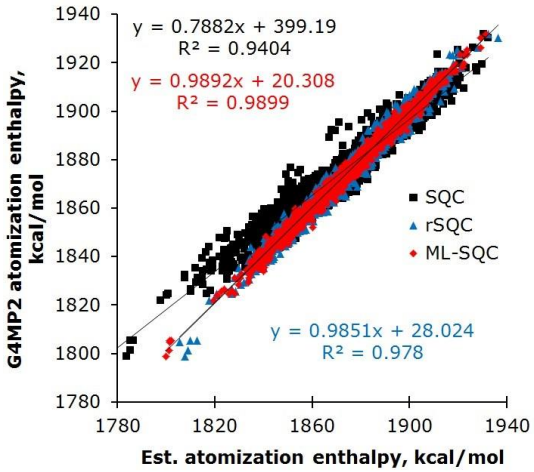

Figure 1: ML significantly improves semiempirical QC Hamiltonian.[2]

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