Photodissociation of vinylbromide: a non-adiabatic molecular dynamics and machine learning study

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This work presents our efforts in utilizing machine learning (ML) techniques to accelerate non-adiabatic molecular dynamics (NAMD) simulations. NAMD plays a crucial role in the computational modeling of various photo-induced processes, such as photosynthesis, DNA damage/stability, phototherapy, and photovoltaics. Recent advancements in ML have shown great promise in the field of computational (quantum) chemistry, offering the potential for significantly faster calculations compared to traditional methods while maintaining comparable accuracy[1].

In this study, we explore the applicability of a kernel ridge regression technique, implemented in MLatom[2], as a potential tool for accelerating NAMD simulations involving non-adiabatic and spin-orbital couplings. We investigated the dynamics of vinyl bromide, a small molecule with a heavy bromine atom, which serves as an appropriate test system for NAMD simulations incorporating these couplings using Newton-X[3]. Figure 1a displays scatter plots comparing the ML predictions with reference values, demonstrating the performance of the ML models. Our analysis indicates that active learning should be employed in specific regions, as can be seen from Figure 1b, which shows the difference between two ML models and reference values.

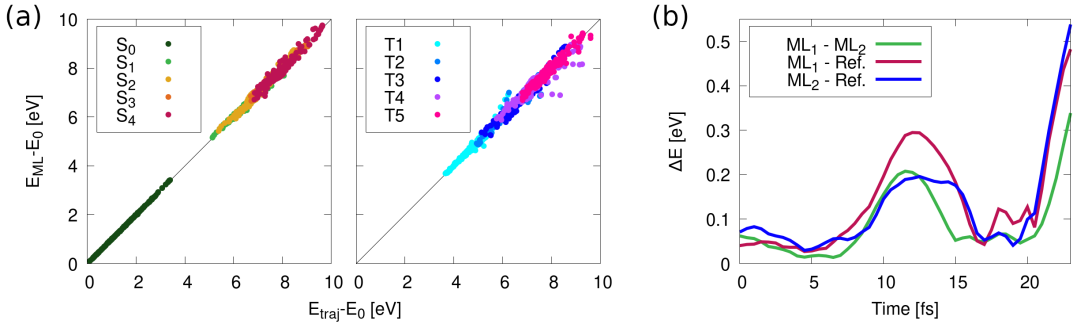

Figure 2: (a) Scatter plots comparing ML predictions to reference values can be used to analyze the accuracy of ML models. (b) Difference between ML predictions and references indicating the extrapolation regime.

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