Improving Spectroscopic Analysis using Machine Learning from Atomistic Simulations

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Molecular simulation is playing an increasingly important role in the modeling and interpretation of complex chemical interactions. However, major advances in the accuracy and efficiency of computational methods are needed to capture the complex chemistry of the problems encountered in analyzing the chemistry that controls events in mineral/fluid interface regions. AIMD inherently captures the dynamic spectroscopic properties that are sampled in XAS and Raman microscopies and spectroscopies and in recent years it has transformed how spectroscopic measurements from advanced light sources, such as Raman, EXAFS, CTR, XANES, etc. are analyzed. Unfortunately, AIMD simulations can quickly become prohibitive as the system sizes become larger. While advanced HPC algorithm and software development has been able to overcome many of these barriers, the computation cost of AIMD is still prohibitive for many systems and project resources. In this presentation, we will present our recent work on using machine-learned atomistic potentials based on the more rigorous AIMD simulations to improve the efficiency of AIMD/spectroscopic analysis. Our work is focused on developing machine learning methods to speed up the AIMD/spectroscopy analysis by generating and using machine-learned atomistic potentials on the fly. One of the key challenges so far has been to develop targeted features functions that can be used with modest size feed forward neural networks that can be fit in a reasonable amount of time , while maintaining the accuracy of the full AIMD analysis.