From Electronic Structure Calculations to Machine Learning Models… and Back

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Electronic structure calculations have for decades been a cornerstone of physics-based modeling in chemistry. However, the high cost and unfavorable scaling of most quantum chemical approximations continue to limit their utility and application scope. However, the data generated by electronic structure calculations can be used to train surrogate models via machine learning (ML) and artificial intelligence (AI). These data-derived prediction models require only a fraction of the computational footprint, yet, they can often accurately reproduce the predictions of the corresponding physics-based models. At the same time, these AI/ML models offer new insights into structure-property relationships that may remain opaque in electronic structure calculations. AI/ML thus holds tremendous promise for the practical realization of accelerated discovery, rational design, and inverse engineering of next-generation chemistry or materials. Adapting AI/ML techniques from other application domains for the study of chemical and materials systems requires a substantial rethinking and redevelopment of the existing methods. In this presentation, we will discuss our efforts along these lines.