AI for learning across chemical space and quantum chemical methods

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Abstract

Our work focuses on using AI to accelerate and improve the accuracy of molecular simulations at the quantum chemical level. We developed a range of methods, most of which can make predictions faster and more accurately than popular DFT approaches such as B3LYP/6-31G* without needing to be trained, i.e., they can be directly used as DFT approaches across the chemical space. The first successful example of such an approach is the AIQM1 method[1] approaching CCSD(T)/CBS accuracy at the semi-empirical cost. AIQM1 was proven efficient for simulations ranging from accurate ground-state geometry optimizations, thermochemical calculations, and dynamics to excited-state property predictions. We have developed a series of the successors of AIQM1 collected in the universal and updatable AI-enhanced quantum mechanical (UAIQM) models.[2] These models mark the paradigm change in computational chemistry towards auto-selection of the best approach for the given time budget with the capability to be continuously improved with more usage. We also introduced many more novel approaches for learning across different quantum chemical levels, e.g., DFT ensembles[3] and all-in-one models[4]. Our methods are available in the MLatom[5] package for AI-enhanced computational chemistry.

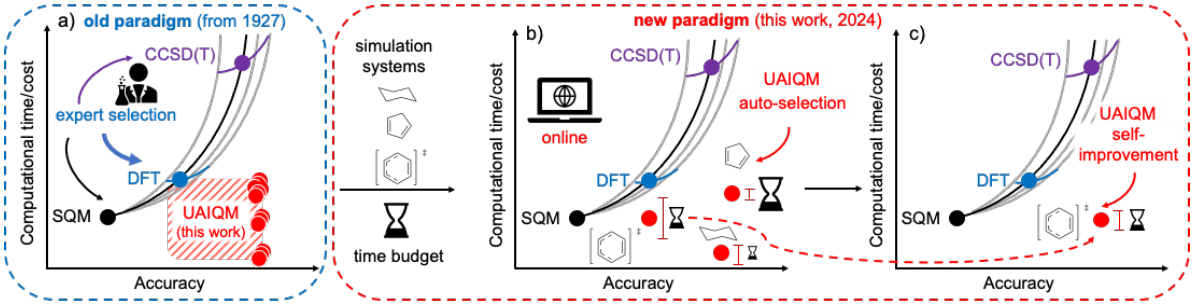

Figure 1. The introduced paradigm change in computational chemistry.[2]

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