Applying a Well-Defined Energy Density for Machine-Learned Density Functionals

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Abstract

The recent integration of machine learning techniques in density functional theory (DFT) has established a powerful framework for developing next generation density functionals. While robust modelling of the exchange-correlation requires a well-defined energy density, conventional training sets usually rely on global quantities. We propose the application of the local slope in the non-interacting limit of the adiabatic connection approach in DFT [1]. The talk will elucidate the methods for an efficient implementation of this quantity, with a focus on its spin-resolved components and its regularized version. Furthermore, we will highlight the potential of this strategy in paving the way for the next generation of machine-learned local dynamic hybrid functionals. Our results show a marked improvement in the prediction of observables while also maintaining computational efficiency.

References

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