Improving Density Functional Theory Simulations: M11plus Implementation in the open PySCF package

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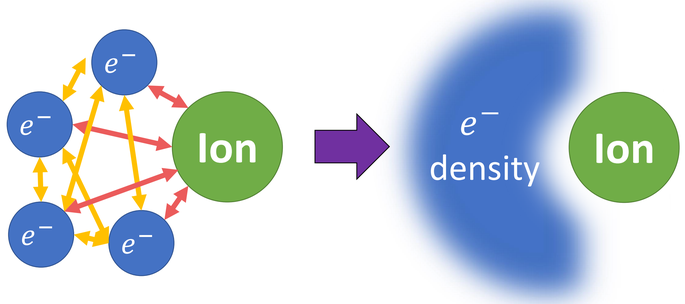
Introduction

- Density Functional Theory (DFT) is a method for simulating molecules by approximating electron densities

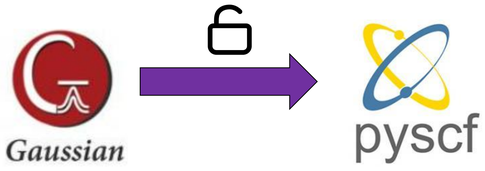


- DFT expresses total energy as the sum of different components such as exchange-correlation (XC) term; accuracy depends on this "piece".

- M11plus is one such functional that adds a new part called the **Rung-3.5 correlation** to the exchange-correlation functional M11, increasing simulation efficiency and accuracy.

Problem

Use of the M11plus functional is presently restricted to an unreleased version of the DFT software Gaussian, and unavailable to the public.



M11plus Flowchart

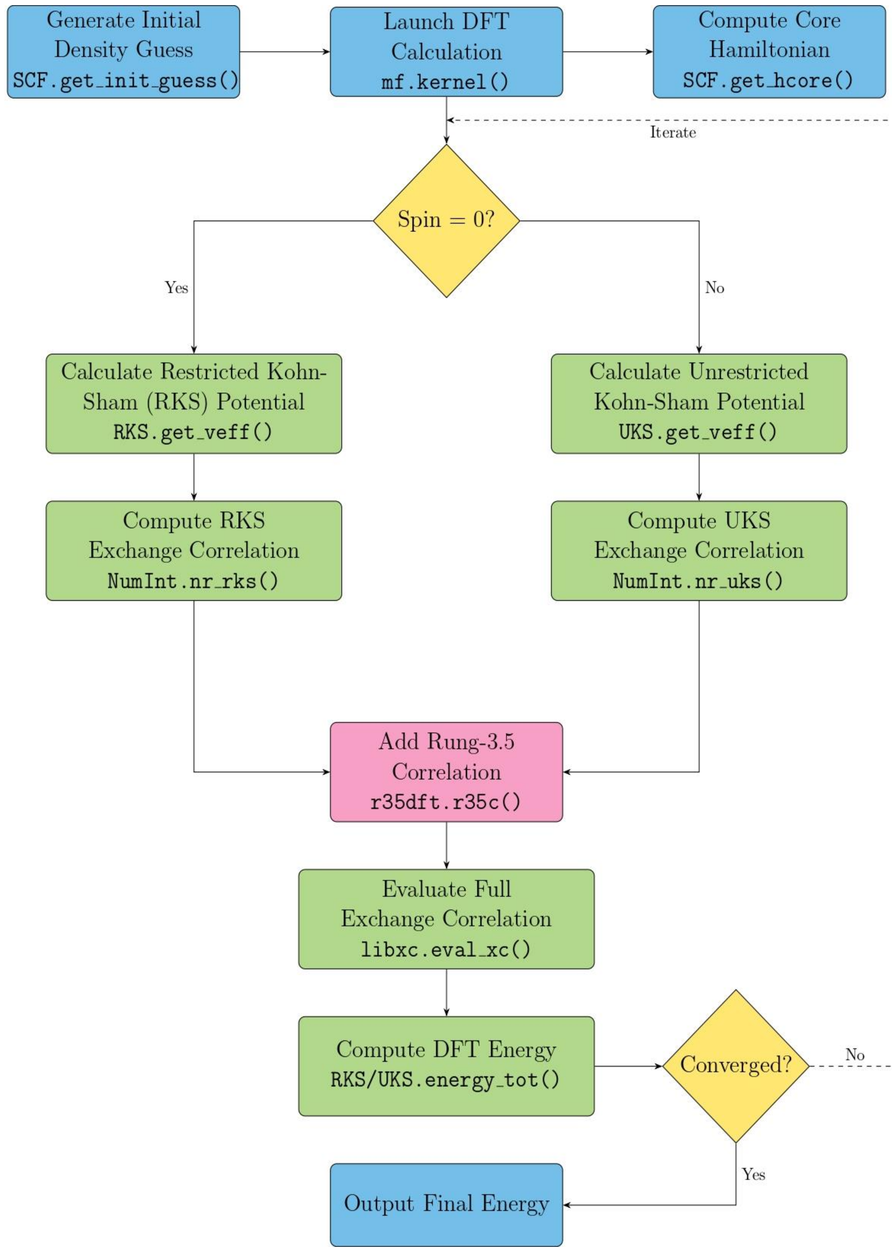


Figure 1. Key computational steps in a PySCF DFT calculation. The diagram distinguishes SCF setup (blue), exchange-correlation calculations with spin-dependent branches for RKS and UKS (green), and the Rung-3.5 correlation (pink), which this work implements.

M11plus Metrics

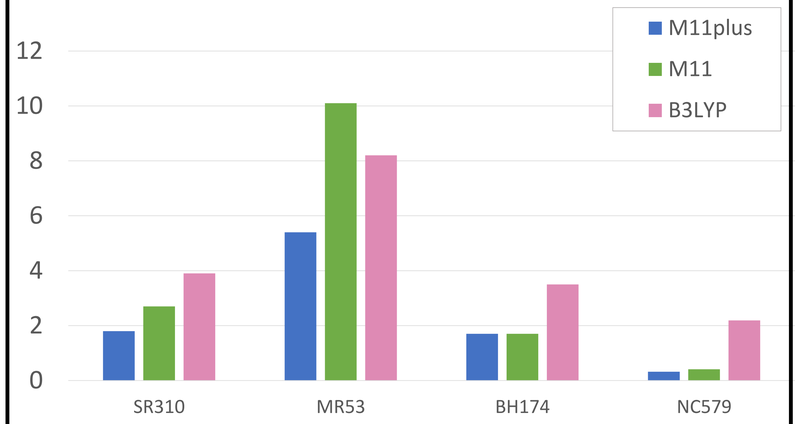


Figure 2. Mean Unsigned Errors (kcal/mol) of three DFT functionals on four chemical databases of energies[a]

Future Work

- Refit M11plus parameters on wider chemical databases
- Publish as an open-source PySCF extension

References

M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. Pragya Verma, Benjamin G. Janesko, Ying Wang, Xiao He, Giovanni Scalmani, Michael J. Frisch, and Donald G. Truhlar
Journal of Chemical Theory and Computation **2019** *15* (9), 4804-4815
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