Title:

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

Abstract:

Density Functional Theory (DFT) is a method for simulating molecules by approximating their electron densities, with various functionals available to model these systems. M11plus is one such functional, a range-separated hybrid meta functional that combines long-range non-local Hartree–Fock exchange with the non-local Rung 3.5 correlation, which has demonstrated effectiveness across a broad range of chemical databases. This work implements the M11plus functional into the PySCF open-source Python library and reparametrizes necessary fitting constants.