

Modern DFT Trend

Modern DFT functionals are favoring flexibility in the energy fitting over physical rigor, which differs from the trend before the 2000s where theorists were working towards achieving the exact energy functionals without sacrificing much in empirical methods. This new trend was not tested that it will improve the functionals along with their energies.

This study tested 128 energy-minimizing electron densities for atomic species DFT functionals, and compared their "normalized error". The study shows that modern DFT functionals on average are drifting away from the exact functional. Functionals that were constructed with the minimum amount of empiricism did produce more accurate electron densities than highly empirical ones. Also, little empirical functionals were found to get more accuracy as their complexity of the density functional increases.