Efficient Implementation of Density Cumulant Theory. Application to Transition Metal Compounds

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Density cumulant theory (DCT) [1] has recently emerged as an attractive *ab initio* method for the treatment of electron correlation. In its orbital-optimized formulation [2], DCT has been shown to provide highly accurate results for a variety of challenging chemical systems [3, 4]. Among the attractive properties of DCT are size-consistency and size-extensivity, as well as the efficient computation of the molecular properties and analytic gradients. In this work, we present a new implementation of DCT that takes advantage of spin adaptation and the density-fitting approximation (DF-DCT). For the S22 database, our new DF-DCT implementation is more efficient than the conventional DCT with ~10-fold speed-up. We demonstrate the capabilities of DF-DCT in a study of transition metal compounds, which require high levels of electron correlation treatment.

References:

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