Ten years of the Distinguishable Cluster: Past, Present and Future

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Modified coupled cluster (MCC) methods motivated by higher efficiency or superior accuracy have been developed from early days of coupled cluster theory. Already in the first publication on coupled cluster methods in quantum chemistry, [1] the linearized version has been introduced, and the connection between the ring-coupled-cluster with doubles method and the random-phase approximation has been recognized. A non-complete list of MCC methods [2] include CEPA, [3] ACP-D45,[4] ACCD,[5] ACPQ,[6] ACP-D14,[7] nCC,[8] pCCSD[9]. In 2013, we have developed a new addition to this list called the distinguishable cluster (DC) approach[10].

As many other MCC methods, DC is exact for two electrons, size extensive and invariant with respect to subspace-orbital rotations. Numerous benchmark studies over the past ten years have demonstrated higher accuracy of DC with singles and doubles (DCSD) compared to standard CCSD for description of weakly correlated systems. But the most striking aspect of DC is the qualitatively correct description of even very strongly correlated systems.

In my talk I will review the progress on DC methods, combinations of DC with other approaches and discuss potential future developments.

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