

Reducing the scaling of higher-order coupled cluster methods through tensor decomposition techniques

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Abstract

It is shown that the use of tensor decomposition techniques like canonical product (CP) decomposition can lead to a formal reduction in the scaling of higher-level coupled cluster methods. We take coupled cluster singles, doubles and triples (full CCSDT) as an example and illustrate how higher-scaling terms in the residual equation can be treated, with possible reduction of operation complexity, with control over the error introduced with the reduced rank of the decomposed tensor.

References

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