

# Analysis of the Green's function approach for obtaining isotropic exchange couplings of 3d transition metal complexes

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Computation of magnetic exchange coupling constants is important for a growing number of areas, including spintronics, magnetic memory storage, and novel molecular magnet design. Determining exchange coupling for high-nuclearity complexes is not possible experimentally, and thus, computational methods are needed to make predictions. The most widely used methods compute the differences in total energies of a set of magnetic configurations, but the cost and difficulty increase steeply as more centers are added. Thus, it is desirable to have a black-box method that involves only a single state. Recent work[1] has adapted the use of approximate Green's functions from the solid-state community for use on molecules. The Green's function approach provides a far more efficient route to calculate isotropic magnetic exchange couplings, as it only requires the calculation of one state. However, large-scale tests have not yet been performed. Thus, we assess the ability of the Green's function approximation for exchange coupling calculations to reproduce the standard broken-symmetry energy difference approach for transition metal complexes. To accomplish this, we have selected a variety of heterodinuclear, homodinuclear and polynuclear systems containing 3d transition metal centers and computed the couplings with both the Green's function and energy difference methods.

## References

- [1] Steenbock, T.; Tasche, J.; Lichtenstein, A. I.; Herrmann, C., *J. Chem. Theory Comput.*, **2015**, *11*, 5651-5664.