Differential Many-Body Cooperativity and Characterisation of Cu(I) TADF Complexes

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The differential many-body expansion [1] is applied to investigate non-additive and cooperative effects in UV/Vis spectra, singlet-triplet energy gaps and electronic energies of Cu(I) and Ag(I) halide TADF complexes. The dependence of these properties on different ligand systems is studied in terms of diphenylphosphinopyridine-type ligand system with and without halide containing arylphosphines [2,3], see Figure 1. Subsystems for the differential many-body expansion are obtained by substituting metals and halides. Properties of subsystems are described by first-order terms while second-order terms describe non-additive but pairwise contributions, and third-order - and higher-order - terms can be understood as indicator for cooperativity.

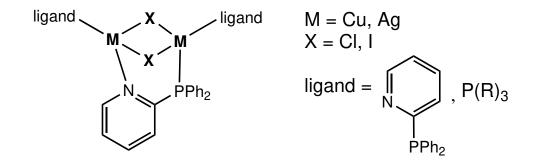


Figure 1: Schematic structure of the complexes studied.

References

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