# Implementation of spin-orbit coupling effects in partially contracted Quasi-Degenerate N-electron Valence Perturbation Theory

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Spin-orbit interactions play a major role in understanding the magnetic properties of matter and describing the hyperfine structure of molecules and atoms. Accurate theoretical treatment of these effects has garnered significant interest, especially in modelling single-molecule magnets and molecular spintronic devices. Though significant progress has been made in simulating the spin-orbit interactions of molecular systems, accurate and efficient description of spin-orbit coupling for heavy metal compounds including electron correlation effects is still lacking. In this poster, I will present the implementation of spin-orbit mean field approximation (SOMF) in partially contracted quasi-degenerate N-electron valence perturbation theory (QD-NEVPT2) and demonstrate the capabilities and shortcomings of the implementation for several systems of interest. I will present a benchmark of spin-orbit coupling splitting in diatomic and triatomic radicals along with my results for 3d and 4d transition metal ions. Finally, I will present results for several transition metal complexes where spin-orbit coupling effects are crucial to understanding their electronic structure.