

## Open-Shell Systems & Relativistic Effects

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The talk focuses on calculations for open-shell systems, and on relativistic effects, often in combination, covering selected topics from our on-going research projects: (i) Calculation of magnetic-field induced circular dichroism (MCD) of electronic transitions in complexes with transition metals and actinides. (ii) Theory and calculation of magneto-chiral dichroism (MChD) for the complex  $[\text{Ni}(\text{en})_3]^{2+}$ , where en = ethylenediamine. Unlike MCD, MChD is a chiroptical effect, that is, it has opposite sign for the enantiomers of a chiral compound. (iii) Natural transition orbitals (NTOs) for spin-forbidden transitions, obtained from multiconfigurational SCF wavefunctions and state-interaction treatment of the spin-orbit coupling. (iv) DFT calculations for radicals that have been assigned 'non-aufbau' configurations, and the conditions in closed-shell precursors for a SOMO - HOMO energy inversion (SHI) to take place upon ionization.