Structure and function.
Fundamental principles and case studies with transition metal compouds.

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The computation of electronic structures of transition metal complexes has been developed in recent years to an extent where a large variety of spectroscopic properties and reactivities of mono- and oligonuclear transition metal compounds can be efficiently and reliably computed and interpreted with ab-initio quantum-chemical and DFT-based methods. These are often based on known structural data, and the interpretation of the electronic structures usually involves the comparison of computed with experimentally observed spectra, stabilities and/or reactivities. The prediction of molecular properties, which eventually may lead to a rational design of novel complexes with given properties, requires as an important additional step a reliable structure prediction. The identification of factors which influence molecular structures of transition metal complexes and the ensuing approaches for a reliable structure optimization are an important basis for electronic structure calculations. In many cases these can and must be based on efficient and accurate molecular-mechanics-based methods, and electronic structure calculations are in some important examples best done with ligand-field-based approaches. Apart from the fundamental principles and possible pitfalls, various case studies from our lab will be discussed, and these may include (i) the Cu^{II} chemistry of natural cyclic peptides and their possible biological function; (ii) the oxidation catalysis of high-valent nonheme iron model systems; (iii) the design, synthesis and characterization of single molecule magnets; (iv) the design, synthesis and characterization of enzyme model systems such as catecholase, catechol oxygenase, carboanhydrase, and purple acid phosphatase.