Scientific Computing & Modelling

Quality **Software**.
Quantum **Science**.

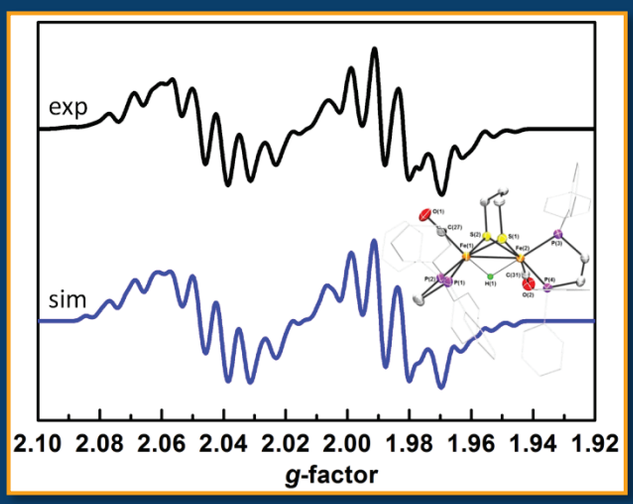
Modeling Bioinorganic Chemistry with ADF

Accurate spin states

- SSB-D, OPBE xc functionals perform well for 3d-TM
- Accurate relativistic effects (scalar, spin-orbit)
- All-electron Slater orbitals for all elements
- Broken symmetry

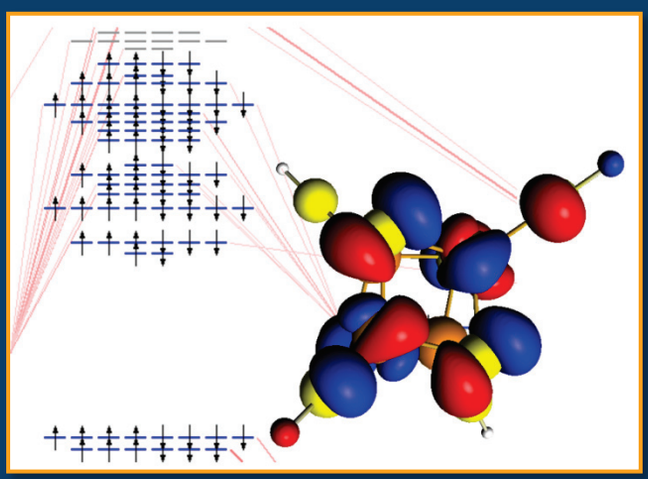
Many spectroscopic properties

- EPR/ESR (g-factor, A-tensor)
- ENDOR (Q-tensor)
- ZFS (D-tensor)
- MCD
- (paramagnetic) NMR
- IR, (resonance) Raman, VCD, VROA
- UV/VIS, CD, ORD
- X-ray absorption (XANES, NEXAFS)



Chemical Bonding Analysis

- Many charges, bond orders, (spin) density and field visualization
- Energy decomposition analysis
- ETS-NOCV: orbital interactions
- NBO, AIM, ELF, NCI, SEDD, (p)DOS



General

- Fully integrated graphical interface
- Expert staff and support
- Latest developments, functionals

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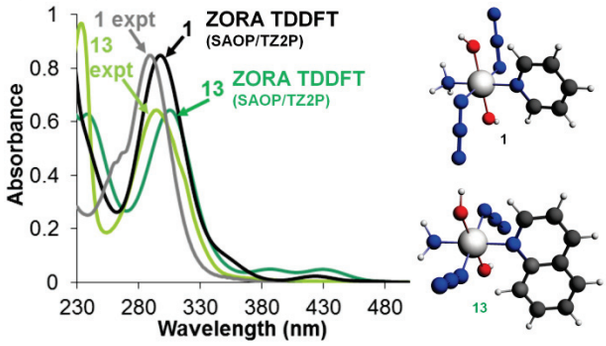
Modeling Bioinorganic Chemistry Research Highlights

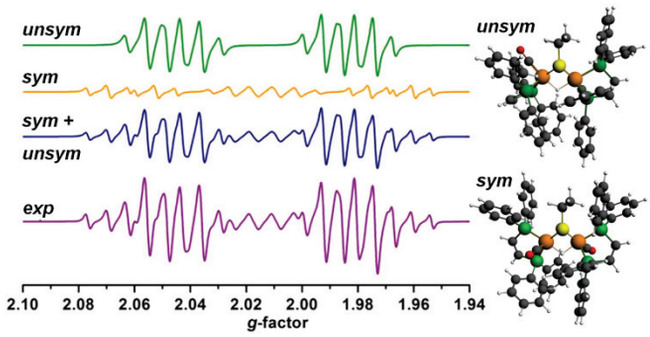
Scientific Computing & Modelling

Designing phytocytotoxic Pt complexes by tuning the absorption spectrum



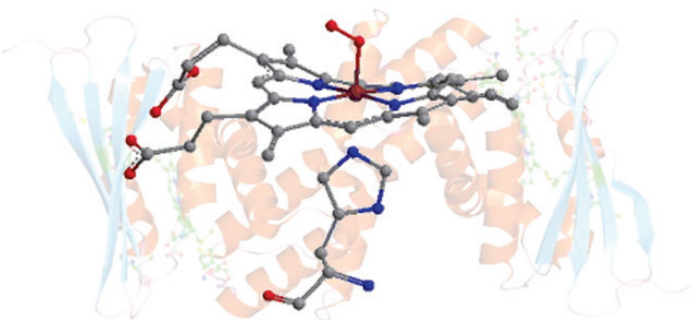
H.-C. Tai, Y. Zhao, N. J. Farrer, A. E. Anastasi, G. Clarkson, P. J. Sadler, and R. J. Deeth, *A Computational Approach to Tuning the Photochemistry of Platinum(IV) Anticancer Agents.* Chem. Eur. J. **18**, 10630 (2012)

EPR spectra of bio-mimetic hydrogen evolution catalyst: mixed-valence Fe(II)-Fe(I) hydride spectator state



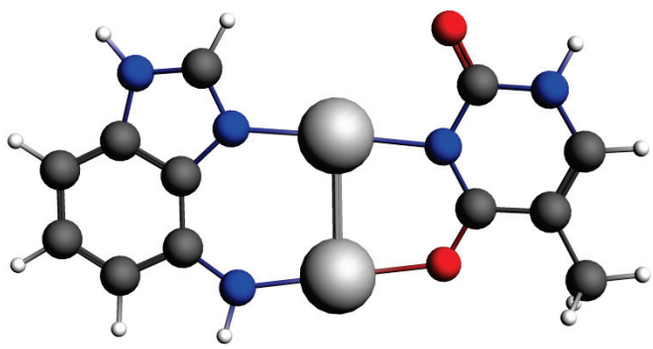
W. Wang, M. J. Nilges, T. B. Rauchfuss, and M. Stein, *Isolation of a Mixed Valence Diiron Hydride: Evidence for a Spectator Hydride in Hydrogen Evolution Catalysis* J. Am. Chem. Soc. **135**, 3633 (2013)

Heme distortion in H-NOX domains reproduced with D3 dispersion corrected DFT QM/MM calculations



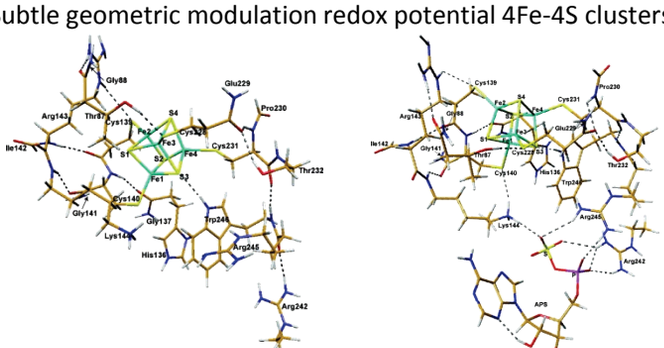
M. S. Liao, M. J. Huang, and J. D. Watts, *Factors that distort the heme structure in Heme-Nitric Oxide/OXygen-Binding (H-NOX) protein domains. A theoretical study.* J. Inorg. Biochem. **118**, 28 (2013)

DFT calculations provide insight into the structure, formation and stabilization of twofold metalated base pairs



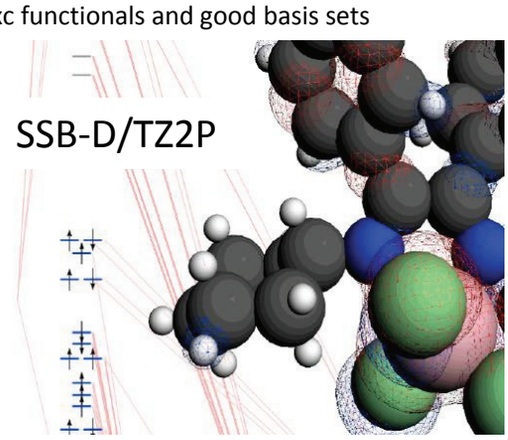
D. A. Megger, C. Fonseca Guerra, J. Hoffmann, B. Brutschy, F. M. Bickelhaupt, and J. Müller, *Contiguous Metal-Mediated Base Pairs Comprising Two AgI Ions.* Chem. Eur. J. **17**, 6533 (2011)

Subtle geometric modulation redox potential 4Fe-4S clusters



D. P. Bhave, W.-G. Han , S. Pazicni, J. E. Penner-Hahn, K. S. Carroll, and L. Noodleman, *Geometric and Electrostatic Study of the [4Fe-4S] Cluster of Adenosine-5'-Phosphosulfate Reductase from Broken Symmetry Density Functional Calculations and Extended X-ray Absorption Fine Structure Spectroscopy.* Inorganic Chem. **50**, 6610 (2011)

Spin state splittings of transition metal complexes with recent xc functionals and good basis sets



M. Swart, *Spin states of (bio)inorganic systems: Successes and pitfalls.* Int. J. Quantum Chem. **113**, 2 (2013)

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