

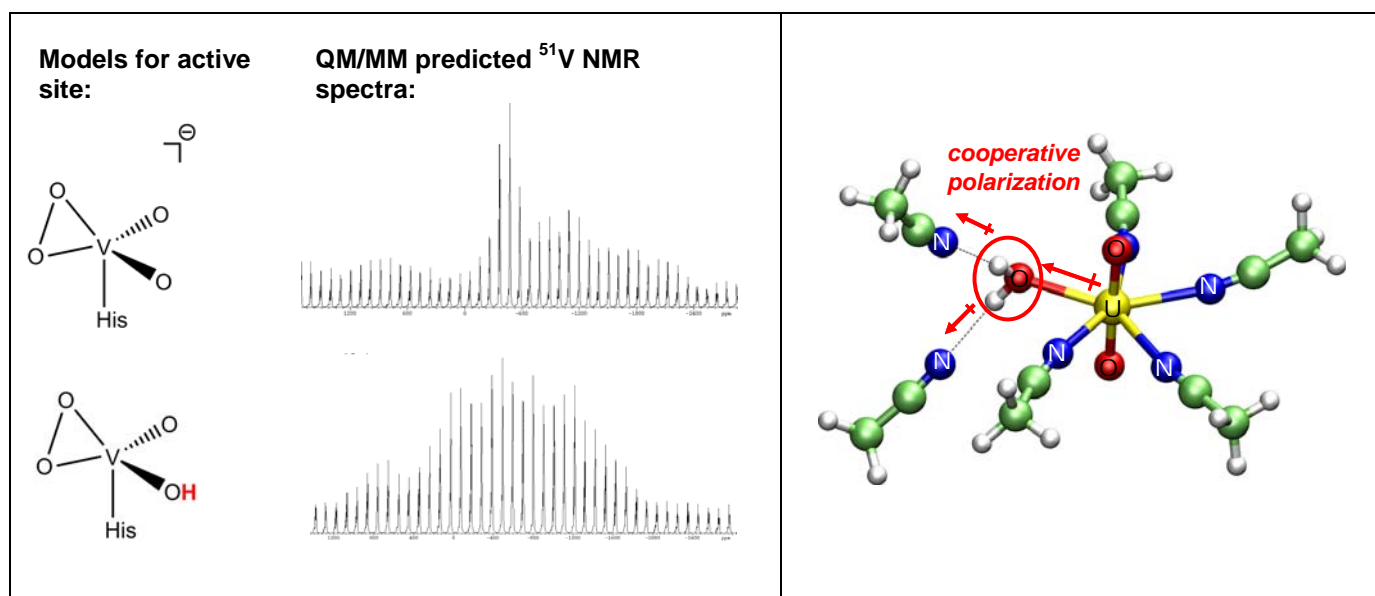
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Research Interests: computational chemistry, transition-metal complexes, homogeneous catalysis, NMR properties, first-principles molecular dynamics simulations



The ultimate goal of computational chemistry is the virtual lab, where the outcome of experiments is predicted from first principles. Due to fast computers and advanced quantum-chemical methods and program packages, such predictions have already reached a reliability that make them valuable complements to experimental techniques. In my group, suitable theoretical tools are critically validated against experiment and, subsequently, applied to a wide variety of chemical problems, mostly from the diverse and vibrant field of transition-metal and f-element chemistry. Typical targets of our investigations are structures, reactivities, and spectroscopic properties of systems ranging from simple organometallic species to complex metalloenzymes.



Solid-state ⁵¹V NMR spectra are predicted to be fingerprints for the protonation state of the active centre in a vanadium-containing haloperoxidase (ref. 5).

Analysis of computed charge distributions can give insights into the relative affinity of donor ligands toward metal centres (e.g. toward UO₂²⁺, ref. 1).

SELECTED RECENT PUBLICATIONS

1. M. Bühl, N. Sieffert, A. Chaumont, Georges Wipff, Water versus Acetonitrile Coordination to Uranyl. Density Functional Study of Cooperative Polarization Effects in Solution, *Inorg. Chem.*, **50**, 299-308 (2011).
2. N. Sieffert, M. Bühl, Hydrogen Generation from Alcohols Catalyzed by Ruthenium-Triphenylphosphine Complexes: Multiple Reaction Pathways, *J. Am. Chem. Soc.*, **132**, 8056-8070 (2010).
3. M. Bühl, G. Schreckenbach, Oxygen Exchange in Uranyl Hydroxide via Two "Non-Classical" Ions, *Inorg. Chem.*, **49**, 3821-3827 (2010).
4. R. Bjornsson, M. Bühl, Electric field gradients of transition metal complexes from density functional theory: assessment of functionals, geometries and basis sets, *Dalton Trans.*, **39**, 5319-5324 (2010).
5. K. R. Geethalakshmi, M. P. Waller, W. Thiel, M. Bühl, ⁵¹V NMR chemical shifts calculated from QM/MM models of Peroxo-forms of Vanadium Haloperoxidases, *J. Phys. Chem. B*, **113**, 4456-4465 (2009).
6. M. Kaupp, M. Bühl, NMR Parameters of Transition Metal Complexes. Methods and Applications, in: *Computational Inorganic and Bioinorganic Chemistry (Encyclopedia of Inorganic Chemistry)*, R. B. King (Ed.), Wiley, New York, pp. 91-108 (2009).
7. Z. Su, M. Bühl, W. Zhou, Dissociation of Water During Formation of Anodic Aluminium Oxide, *J. Am. Chem. Soc.*, **131**, 8697-8702 (2009).