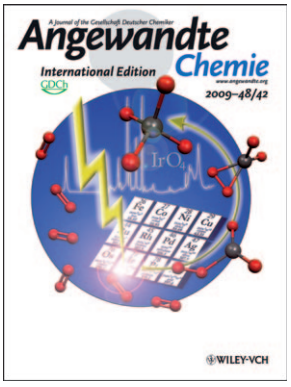
M. Kaupp

*The author presented on this page has recently published his **10th article** since 2000 in Angewandte Chemie, which was also featured on the Inside Cover*: "Formation and Characterization of the Iridium Tetraoxide Molecule with Iridium in the Oxidation State +VIII": Y. Gong, M. Zhou, M. Kaupp, S. Riedel, *Angew. Chem.* **2009**, *121*, 8019–8023; *Angew. Chem. Int. Ed.* **2009**, *48*, 7879–7883.



Martin Kaupp

Date of birth:	July 7, 1962
Position:	Professor of Theoretical Chemistry, Universität Würzburg (Germany)
Education:	1982–1986 and 1987–1989 Universität Stuttgart (Germany) 1986–1987 University of Cincinnati (USA) 1989–1992 PhD with P. von R. Schleyer, Erlangen (Germany) 1992–1993 Postdoc with H. G. von Schnering, MPI Stuttgart 1993–1994 Postdoc with D. Salahub, Montreal (Canada) 1994–1997 Habilitation, Universität Stuttgart 1997–1999 Docent, Universität Stuttgart 1999–Present Professor, Universität Würzburg
Awards:	**1989** Procter & Gamble Award, **1991** Hoechst Award, **1994** Heinz Mayer-Leibnitz Award (BMFG), **1997** Heisenberg Fellowship (DFG), **1998** Dozentenstipendium (FCI), **2001** Dirac Medal (WATOC)
Current research interests:	Computational quantum chemistry, density functional theory (development of local hybrid functionals, perturbation theory for properties, ReSpect and Turbomole program development), computation and understanding of spin-orbit and other relativistic effects, calculation and interpretation of NMR and EPR parameters, magnetic and electronic properties of metalloenzymes and bioradicals, various aspects of chemical bonding and of bond analysis methods, periodic trends, organometallic and bioinorganic catalysis, mixed-valence systems, spectroscopy and electronic structure of π aggregates, non-innocent ligands, ab initio molecular dynamics for property calculations
Hobbies:	Music, sports, and reading

In a nutshell, my research involves … understanding how molecules work.

The biggest challenge facing scientists is … securing sufficient renewable energy resources.

My favorite subjects at school were … chemistry and music.

When I was eighteen I wanted to be … a scientist.

If I could be anyone for a day, I would be … Oscar Peterson in his younger days.

If I could have dinner with three famous scientists from history, they would be … Einstein, Bohr, and Woodward.

The most exciting thing about my research is … to learn new things every day.

In ten years time I will be … still a scientist (hopefully).

The part of my job which I enjoy the most is … discussing science with my co-workers and colleagues.

The most groundbreaking discovery in science in the past 100 years has been … quantum mechanics and relativity.

My biggest motivation is … to learn new things every day and then to teach them.

A good work day begins with … a new idea.

My favorite book is … Neal Stephenson's "The Baroque Cycle".

My 5 top papers:

1. "Local Hybrid Functionals: An Assessment for Thermochemical Kinetics": M. Kaupp, H. Bahmann, A. V. Arbuznikov, *J. Chem. Phys.* **2007**, *127*, 194102.
2. "Mercury is a Transition Metal: The First Experimental Evidence for HgF_4": X. Wang, L. Andrews, S. Riedel, M. Kaupp, *Angew. Chem.* **2007**, *119*, 8523–8527; *Angew. Chem. Int. Ed.* **2007**, *46*, 8371–8375.
3. "Non-VSEPR Structures and Bonding in d^0 Systems": M. Kaupp, *Angew. Chem.* **2001**, *113*, 3642–3677; *Angew. Chem. Int. Ed.* **2001**, *40*, 3534–3565.
4. "How Do Spin–Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin–Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds": M. Kaupp, O. L. Malkina, V. G. Malkin, P. Pyykkö, *Chem. Eur. J.* **1998**, *4*, 118–126.
5. "Ab Initio Study of Structures and Stabilities of Substituted Lead Compounds. Why is Inorganic Lead Chemistry Dominated by Pb^{II} but Organolead Chemistry by Pb^{IV}?": M. Kaupp, P. von R. Schleyer, *J. Am. Chem. Soc.* **1993**, *115*, 1061–1073.

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