



G. Frenking

The author presented on this page has published more than **35 articles** since 2000 in *Angewandte Chemie*, most recently:

"Synthesis and Characterization of a Two-Coordinate Manganese Complex and its Reaction with Molecular Hydrogen at Room Temperature": P. P. Samuel, K. C. Mondal, H. W. Roesky, M. Hermann, G. Frenking, S. Demeshko, F. Meyer, A. C. Stückl, J. H. Christian, N. S. Dalal, L. Ungur, L. F. Chibotaru, K. Pröpper, A. Meents, B. Dittrich, *Angew. Chem.* **2013**, 125, 12033–12037; *Angew. Chem. Int. Ed.* **2013**, 52, 11817–11821.

## Gernot Frenking

<b>Date of birth:</b>	January 23, 1946
<b>Position:</b>	Professor of Theoretical Chemistry, University of Marburg
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<b>Education:</b>	1961–1964 Chemical technician, Bayer AG 1969–1975 Undergraduate degree in chemistry, Universities of Aachen and Kyoto 1976–1979 PhD with Horst Goetz, Technische Universität (TU) Berlin 1979–1984 Habilitation, TU Berlin
<b>Awards:</b>	<b>2007</b> Elhuyar–Goldschmidt Prize of the Real Sociedad Española de Química; <b>2008</b> Fellow of the Royal Society of Chemistry; <b>2009</b> Schrödinger Medal of the WATOC (World Association of Theoretical and Computational Chemists); <b>2010</b> Hofmann Distinguished Lecture, Imperial College London; <b>2011</b> Lise Meitner Lecture, Hebrew University of Jerusalem; <b>2012</b> Hans Hellmann Research Professorship, University of Marburg
<b>Current research interests:</b>	Quantum chemical calculations of molecules with unusual bonds; analysis of chemical bonding; reaction mechanisms
<b>Hobbies:</b>	Literature, travelling, and music

**My greatest achievement has been ...** exchanging the engine of a VW Beetle on a remote countryside road in Denmark, only equipped with a simple toolbox and the book *Now I Help Myself*.

**My worst nightmare is ...** sitting in the Festspielhaus in Bayreuth and suffering a Wagner opera.  
**I lose track of time when ...** I watch children play.

**The best advice I have ever been given is ...** never give up.

**The worst advice I have ever been given was ...** never give up.

**I am most attracted by ...** my wife.

**I celebrate success by ...** becoming very quiet.

**The most amusing chemistry adventure in my career was ...** my laboratory courses in organic and inorganic chemistry, where my education as chemical assistant at Bayer AG meant that I was more skilful than my advisors.

**My favorite authors (fiction) are ...** Franz Kafka and Hermann Hesse.

**My top three films of all time are ...** *Dodesukaden* (1970; Kurosawa); *La Strada* (1954; Fellini); *Cherries* (2008; Zhang Jiabei). I also like *Berlinger* (1975; Brustellin/Sinkel) because the main figure is a chemist.

**My favorite food is ...** oysters (fines de claires) and ice-cold champagne.

**My favorite songs/pieces of music are ...** a triple: *Summertime* (Janis Joplin, Live 1969); *Les palais de nos chimères* (Charles Aznavour; Live à l'Olympia 1973); *My Funny Valentine* (Chet Baker). Beyond grading: *Le Sacre du Printemps* (Strawinsky).

**My favorite saying is ...** "Stay hungry, stay foolish".

**The most significant scientific advance of the last 100 years has been ...** quantum theory and relativity, because they stunningly show the incomprehensible limitation of sensory perception and imagination of humans.

**The biggest problem that scientists face is ...** to make people understand that the primary goal of scientific efforts is to gain knowledge but not the usability of knowledge. Science is first and foremost a cultural activity without material profit, which, particularly in chemistry, is often not recognized.

**My favorite piece of research is ...** "Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik" (W. Heitler, F. London, *Z. Phys.* **1927**, 44, 455). The birth of understanding chemical bonding, which can not be directly described in terms of particles.

**My favorite place on earth is ...** the garden of our house in the early morning of a clear spring day.

I chose chemistry as a career because ... my uncle had chosen for me an apprenticeship as a physical technician, but after I had passed the qualifying examination, the committee of Bayer AG convinced him that physics was too difficult for someone who has only an elementary school qualification and I should therefore enroll in the more simple subject of chemistry.

My secret/not-so-secret passion is ... amateur soccer.

If I were not a scientist, I would be ... a hippie in the South Seas.

My most exciting discovery to date has been ... the covalent He–C bond in  $\text{HeCCHe}^{2+}$ , which brought me an interview in the *New York Times*.

### How is chemistry research different now than at the beginning of your career?

Today it is characterized by theory and experiment being on an equal par and by interdisciplinary cooperation and the gradual disappearance of the barriers between the classical disciplines of organic, inorganic, and physical chemistry as well as between chemistry and the neighboring professions physics and biology. Chemistry as the science of understanding and transformation of the material world in molecular dimensions plays a particular

role in the treatment of the material resources at a time where we realize their limitations. This has a political dimension that must be faced by responsible scientists. Those who only understand chemistry do not even understand chemistry.

### What is the secret to publishing so many high-quality papers?

The talent for lateral thinking and a sense for scientific results that point toward unrecognized phenomena.

### My 5 top papers:

1. "Helium Chemistry: Theoretical Predictions and Experimental Challenge": W. Koch, G. Frenking, J. Gauss, D. Cremer, J. R. Collins, *J. Am. Chem. Soc.* **1987**, *109*, 5917–5934.

The light noble gases helium, neon, and argon are essentially terra incognita in chemistry. We used quantum chemical calculations to show that ion chemistry of helium features a broad spectrum of covalently bonded helium compounds.

2. "Why do the Heavy-Atom Analogues of Acetylene  $\text{E}_2\text{H}_2$  ( $\text{E} = \text{Si} - \text{Pb}$ ) Exhibit Unusual Structures?": M. Lein, A. Krapp, G. Frenking, *J. Am. Chem. Soc.* **2005**, *127*, 6290–6299.

In the years 2000–2004, the first Group 14 homologues of alkynes  $\text{REER}$  ( $\text{E} = \text{Si} - \text{Pb}$ ), which possess a *trans*-bent geometry were isolated. Much discussion in the following years focused on the questions if the molecules have a E–E triple bond and why they are bent rather than linear. The debates ignored the fact that the parent compounds  $\text{E}_2\text{H}_2$  possess completely different hydrogen-bridged equilibrium structures. The *trans*-bent geometries of  $\text{REER}$  come from the steric repulsion of the bulky substituents R. We gave an explanation for the unusual geometries and for the relative energies of all isomers, and we answered the question about the nature of the bonding and the bond orders in the molecules.

3. "Orbital Overlap and Chemical Bonding": A. Krapp, F. M. Bickelhaupt, G. Frenking, *Chem. Eur. J.* **2006**, *12*, 9196–9216.

Covalent bonding is usually discussed in textbooks in terms of interactions of electrons in bonding orbitals where the strength and the bond length are determined by the orbital overlap. In this work, we show that the crucial factor for the equilibrium distance is the Pauli repulsion, which prevents maximum overlap of the

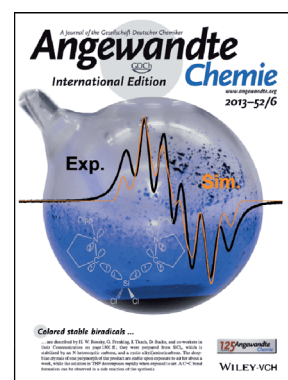
orbitals, and that the bond strength depends on three factors: orbital interactions, Pauli repulsion, and Coulomb interactions.

4. "Carbodiphosphoranes: The Chemistry of Divalent Carbon(0)": R. Tonner, F. Öxler, B. Neumüller, W. Petz, G. Frenking, *Angew. Chem.* **2006**, *118*, 8206–8211; *Angew. Chem. Int. Ed.* **2006**, *45*, 8038–8042.

This publication is the actual birth of carbenes  $\text{CL}_2$ , which are dicoordinated carbon(0) compounds with donor–acceptor bonds  $\text{L} \rightarrow \text{C} \leftarrow \text{L}$  and two lone pairs of electrons at carbon, presenting a new class of carbon compounds. They differ from carbenes  $\text{CR}_2$ , which have C–R electron-sharing bonds and only one lone pair of electrons at carbon. The work was the starting point for systematic theoretical studies of carbenes, which led to the prediction of stable carbodicarbenes  $\text{C}(\text{NHC})_2$  ( $\text{NHC} = \text{N}$ -heterocyclic carbene), which in the meantime could become synthesized. Further theoretical studies were directed toward isoelectronic boron analogues  $(\text{BH})\text{L}_2$  and the heavy Group 14 homologues  $\text{EL}_2$  ( $\text{Si} - \text{Pb}$ ), which meanwhile were also synthesized.

5. "Structures and Stabilities of Group 13 Adducts  $[(\text{NHC})(\text{EX}_3)]$  and  $[(\text{NHC})_2(\text{E}_2\text{X}_n)]$  ( $\text{E} = \text{B}$  to  $\text{In}$ ;  $\text{X} = \text{H}, \text{Cl}$ ;  $n = 4, 2, 0$ ;  $\text{NHC} = \text{N}$ -Heterocyclic Carbene) and the Search for Hydrogen Storage Systems: A Theoretical Study": N. Holzmann, A. Stasch, C. Jones, G. Frenking, *Chem. Eur. J.* **2011**, *17*, 13517–13525.

The calculation of the Group 13 complexes  $\text{E}_2(\text{NHC})_2$  led to a boron compound with a linear arrangement and a boron–boron triple bond ( $\text{NHC} \rightarrow \text{B} \equiv \text{B} \leftarrow \text{NHC}$ ), which has been isolated in the meantime. There is now a third class of compounds besides alkynes and  $\text{N}_2$  with a homoatomic classical triple bond that consists of one  $\sigma$  bond and two  $\pi$  bonds.



The work of G. Frenking has been featured on the back cover of *Angewandte Chemie*:

"Conversion of a Singlet Silylene to a Stable Biradical": K. C. Mondal, H. W. Roesky, M. C. Schwarzer, G. Frenking, I. Tkach, H. Wolf, D. Kratzert, R. Herbst-Irmer, B. Niepötter, D. Stalke, *Angew. Chem.* **2013**, *125*, 1845–1850; *Angew. Chem. Int. Ed.* **2013**, *52*, 1801–1805.

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