



H. Schwarz

The author presented here has recently published his **25th article** since 2000 in *Angewandte Chemie*: "Thermal Hydrogen-Atom Transfer from Methane: The Role of Radicals and Spin States in Oxo-Cluster Chemistry": N. Dietl, M. Schlangen, H. Schwarz, *Angew. Chem.* **2012**, 124, 5638; *Angew. Chem. Int. Ed.* **2012**, 51, 5544.

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Awards:	1990 Leibniz Prize, DFG; 1998 Liebig Medal, GDCh; 2000 Prelog Medal; 2001 F. H. Field and J. L. Franklin Award, ACS; 2003 Otto Hahn Prize, GDCh; 2011 Blaise Pascal Medal, European Academy of Sciences and Arts; 2011 Officer's Cross of the Order of Merit; 2012 Lichtenberg Medal, Göttingen Academy of Sciences and Humanities
Current research interests:	Elucidation of fundamental steps in metal-mediated bond activation; single-atom catalysis; electron-transfer processes; chemistry under extreme conditions
Hobbies:	Music and literature

A good work day begins ... now and again with the thought "Time is a strange thing" (from "Der Rosenkavalier").

My secret/not-so-secret passion is ... a deep curiosity for people.

My motto is ... "solidaire et solitaire" (united and solitary; A. Camus).

The best stage in a scientist's career is ... probably as a postdoc, as people tend to mature themselves during this period.

If I could have dinner with three famous people from history, they would be ... Nelson Mandela, James Franck, and Lise Meitner.

And I would ask them ... how can people love their enemies?

My favorite places on earth are ... Castel del Monte (Apulia) at sunset in spring, Venice in the December mist, or Jerusalem covered in snow.

My favorite food is ... Spaghetti à la Helmut, to be served with Brunello di Montalcino "Montosoli" 1968 or 2002.

A good day finishes with ... the trio "Soave sia il vento" from "Così fan tutte".

My worst nightmare is ... to forget Horst Fuhrmann's advice about how one would like to die, that is, to fall asleep and be dead when you wake up.

What was decisive for you in choosing the discipline for your doctoral thesis and later on your independent career?

My choice of career meant that I started my studies rather late (and at the beginning I was also not sure if I had chosen the right subject) and so there was only one goal: to quickly become independent! Among the many offers that I received as an undergraduate and PhD student, the research theme was not particularly important as I was fascinated by all areas of the subject (except for technical chemistry). What was decisive was the "feeling" that Ferdinand Bohlmann was the right supervisor for me and that I really could do what I wanted. He did not really promote me scientifically,

but in an exemplary manner, he selflessly supported my drive to become independent, sometimes against the opinion of the faculty. I could have not have wished for a better environment.

Why is chemistry considered as one of the most creative science disciplines?

To be creative means to bring something new into being, and chemists can do just this. They don't just discover what was already there, they also create new forms of matter. Among all the natural sciences, chemistry is the one that is most closely related to the arts and the engineering sciences. I would bet anything that if Leonardo da Vinci were alive today, he would be fascinated by chemistry.

Despite many measures to try and correct this, the reputation of chemistry is still poor. How could this be changed?

I think that the reputation of the subject was a lot worse in the past. When I talk to young people around the world, it is obvious that they do not see chemistry as being the cause of the problems that the world is currently facing. On the contrary, many of them are aware that these challenges can only be solved by better education, understanding, and reasoning and actions based on science. It is maybe typical that saturated societies, such as in Central Europe, accept changes only reluctantly, and as chemistry represents the incarnation of material changes, many people view it with suspicion. In Germany we are seeing how a long-term commitment to better scientific education, for example, supported by the Fonds der Chemischen Industrie, is beginning to pay off. Young people are interested in intellectual adventures, and chemistry can satisfy their curiosity.

Do you have any advice for choosing the “right” research projects and when and how a project should be ended?

There is probably no ideal solution. Research projects pass through various stages of maturity; when there are really no more new questions on a topic or when the answers only marginally increase our knowledge then it is time to change topic, even if you have become attached to it. Projects should also be ended when it becomes clear that the problem cannot be solved using available methods—but don’t stop too soon!

You have published more than 950 scientific papers and received more than 40 awards—what’s the secret of your success?

It is anyone’s guess if the numbers of papers and lectures are a measure of success. Looking back, I would say that I avoided the mainstream and tried to find my own path. I did not follow fashions, which are also present in science. I was always interested in questions that had a general aspect. Several examples are given in my top papers below, and I would like to add a few more. 1) In the 1930s, Linus Pauling posed the question of how small can a multiply charged molecule be before the coulombic repulsion causes it to split. This question fascinated me so much that I built up a large research program around it that had quite some influence on certain areas of physics or interstellar

chemistry. Curiosity was the driving force! 2) The question of the constitution of cyclic peptides, namely sequence or retrosequence, is not unimportant. Of course, this structural problem can be easily solved by using NMR spectroscopy, as shown by Kessler’s group. However, if only a few nanomoles of a natural product are available, this technique is not sensitive enough to solve the problem. My PhD student Klaus Eckart used fundamental mechanistic considerations combined with methodological developments (tandem mass spectrometry) to carry out a sequence analysis that was unbelievably easy. 3) Why is it so difficult to convert methane into “more useful” products in a selective, economical, and environmentally friendly way? I have worked on this subject for around 20 years (*Angew. Chem.* **2011**, 123, 10276; *Angew. Chem. Int. Ed.* **2011**, 50, 10096), and I have never learnt so much as I did when working with this seemingly simple problem, for example, the large role of relativistic effects, the theory of two-state reactivity, and a detailed understanding of ligand or cluster-size effects. Seminars were often lessons for me and my teachers were generally my students, for example, Berger, Beyer, Brönstrup, Engeser, Fiedler, Frenking, Harvey, Heinemann, Lebrilla, Koch, Koszinowski, Kretzschmar, Schall, Schlangen, Schröder, Weiske, Zhang, and Zipse! It appears there is no secret for “success”, you should simply live by the motto “work with students who are passionate about their projects”. The most important task for an academic should be to spark an intellectual fire (according to Augustine).

What do you think are Germany’s future prospects in science—particularly against the background of Asian competitors?

In the next 10–20 years, we will continue to play in the world league; there are sufficient reliable indicators that research in Germany is still very attractive. The fact that China, India, and Korea are also in the competition for first place is neither a secret nor a reason to be discouraged. Doing science is comparable to a competition and thus there are winners and losers, and promoted and demoted teams. Who cares if the faces on the “olympic podium” in Stockholm are of different colors—I for one am not bothered.

The interview questions were provided by Kirsten Zeitler (University of Regensburg).

My 5 top papers:

1. “Non-Ergodic Behavior of Excited Radical Cations in the Gas Phase”: G. Depke, C. Lifshitz, H. Schwarz, E. Tzidony, *Angew. Chem.* **1981**, 93, 824–825; *Angew. Chem. Int. Ed. Engl.* **1981**, 20, 792–793.

The Ergodic theorem, a central dogma of reaction dynamics, states that the intramolecular energy redistribution in an excited molecule is quicker than its unimolecular dissociation. We proved that this is not



The work of H. Schwarz has been featured on the inside cover of Angewandte Chemie:

“Diatomic $[\text{CuO}]^+$ and Its Role in the Spin-Selective Hydrogen- and Oxygen-Atom Transfers in the Thermal Activation of Methane”: N. Dietl, C. van der Linde, M. Schlangen, M. K. Beyer, H. Schwarz, *Angew. Chem.* **2011**, 123, 5068–5072; *Angew. Chem. Int. Ed.* **2011**, 50, 4966–4969.

- the case in the enol form of the acetone radical anion. The methyl groups, which become constitutionally equivalent by isomerization of the enol form, are eliminated at different speeds, and the newly formed methyl group quicker than that originally present. Labeling experiments, model calculations, and determination of the energy distribution in the fragments provided the first example that “larger” molecules can also display nonergodic behavior. This finding was later shown by many research groups (e.g., Houk and Carpenter) to be valid for completely different systems.
2. “The Reaction of Nitriles and Fe^+ in the Gas Phase. A Case of Remote Functionalization”: C. B. Lebrilla, C. Schulze, H. Schwarz, *J. Am. Chem. Soc.* **1987**, *109*, 98–100.

We were able to verify Breslow’s concept of a remote-controlled functionalization in a simple ion–molecule reaction. The “naked” iron was not statistically inserted into the various C–H or C–C bonds; in fact, the dominant process consists of an attachment of the cation to the functional group and a subsequent “internal” solvation to bring the distant, unactivated C–H and C–C bonds close to the metal so they can react. Later studies showed that regio- and stereoselective activation, which was dependent on the metal, the functional groups, and the length of the alkyl chain, could occur: enzyme-analogous behavior without an enzyme, and all in one simple ion–molecule reaction!

3. “Endohedral Cluster Compounds: Inclusion of Helium within C_{60}^{\oplus} and C_{70}^{\oplus} through Collision Experiments”: T. Weiske, D. K. Böhme, J. Hrušák, W. Krätschmer, H. Schwarz, *Angew. Chem.* **1991**, *103*, 898–900; *Angew. Chem. Int. Ed. Engl.* **1991**, *30*, 884–886.

“Can fullerene cavities be packed with something?” Today, after more than 20 years of fullerene chemistry, this can be carried out by elaborate chemical surgery: the cage is opened, a guest is introduced into the cavity, and the operation is completed by stitching the cage back together. If chemists or physicists had been asked in the early 1990s whether atoms could be introduced into C_{60} cavities, for example, by collision experiments, the answer would have been a resounding “no”, as these experiments involve highly excited transients that decay within picoseconds. (Incidentally, mass-spectrometry-based proteomics “lives” on these collision-induced decays!) In a breathtaking experiment, and despite strong competition with two American groups that we beat in the “race” by only a few weeks,

we succeeded the inclusion of one helium atom (and later, two atoms) in the football-shaped molecule without bursting the collision complex. Further well-designed experiments were required to convince even the hard sceptics of that the interpretation of these results, which contradicted standard textbook chemistry, was correct.

4. “Two-State Reactivity in Organometallic Gas-Phase Ion Chemistry”: S. Shaik, D. Danovich, A. Fiedler, D. Schröder, H. Schwarz, *Helv. Chim. Acta* **1995**, *78*, 1393–1407.

Spin and energy conservation laws belong to the foundations of chemical processes, and the majority of thermal reactions generally occur through one potential surface. Gas-phase experiments with “naked” FeO^+ prove that in the course of bond activation in RH ($\text{R} = \text{H}, \text{CH}_3$) a spin change from a sextet to a quartet state must occur, that is, *thermal* processes pass through *electronically excited* states. What initially was seen as a special case rapidly became established as a widespread reaction principle: Two-state reactivity (TSR) phenomena are observed in biological processes (e.g., cytochrome P450), metal-mediated polymerization, oxidation of olefins, ligand-exchange reactions, and activation of C=X bonds ($\text{X} = \text{O}, \text{S}$).

5. “Ethylenedione: An Intrinsically Short-Lived Molecule”: D. Schröder, C. Heinemann, H. Schwarz, J. N. Harvey, S. Dua, S. J. Blanksby, J. H. Bowie, *Chem. Eur. J.* **1998**, *4*, 2550–2557.

The literature is full of references to molecules that should not really exist, as these molecules cannot (yet) be “bottled in flasks”. Although samples of, for example, AuF cannot be produced, that does not mean that AuF cannot exist as an isolated molecule, in fact, quite the opposite (see *Angew. Chem.* **1994**, *106*, 223; *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 212). According to Staudinger’s postulations (*Ber. Dtsch. Chem. Ges.* **1913**, *46*, 1426), C_2O_2 also belongs to this class of “unbottleable molecules”. In this paper, we report how it might be feasible to generate the neutral molecule C_2O_2 , even if it exists for only 10^{-9} s, in the gas phase by reducing or oxidizing the well-known ions C_2O_2^{+} and C_2O_2^{-} , respectively. Once again we encounter the TSR principle, as the spin change from a triplet that resides in the energy minimum to an unbound singlet state from which the spontaneous dissociation into two CO molecules occurs.

DOI: 10.1002/anie.201202389