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Author Profile

Angewandte
International Edition Chemie

S. Grimme

The author presented on this page has published more than ***25 articles*** *since 2000 in Angewandte Chemie, most recently:*
"Facile Carbon Monoxide Reduction at Intramolecular Frustrated Phosphane/Borane Lewis Pair Templates": M. Sajid, L.-M. Elmer, C. Rosorius, C. G. Daniliuc, S. Grimme, G. Kehr, G. Erker, *Angew. Chem.* **2013**, *125*, 2299–2302; *Angew. Chem. Int. Ed.* **2013**, *52*, 2243–2246.

Stefan Grimme

Date of birth:	September 4, 1963
Position:	Professor of Theoretical Chemistry, Mulliken Center for Theoretical Chemistry, Institute for Physical and Theoretical Chemistry of the University of Bonn
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Education:	1986–1989 studies in chemistry, Technische Universität (TU) Braunschweig 1989–1991 PhD thesis under the supervision of Prof. Herbert Dreeskamp, TU Braunschweig 1992–1999 Postdoc in the group of Prof. Sigrid D. Peyerimhoff at the University ofBonn 1997 Habilitation
Awards:	**2010** Lise Meitner Lectureship Award of the Lise Meitner–Minerva Center; **2013** Schrödiger Medal of the World Association of Theoretical and Computational Chemists
Current research interests:	Electronic structure theory for large systems, quantum chemistry, density functional theory, development of functionals (double hybrids), perturbation theory (SCS-MP*n*), electronically excited states, electronic spectroscopy, mass spectrometry, circular dichroism, theoretical thermochemistry, applications in (bio)chemistry and organometallic chemistry, frustrated Lewis pairs, dispersion corrections (DFT-D), noncovalent interactions, protein–ligand interactions, supramolecular chemistry, molecular crystals
Interests:	Tennis, running, mountain biking, playing the guitar

My greatest achievement has been … finishing a marathon run in reasonable time.

Guaranteed to make me laugh is … Loriot (German humorist).

I can never resist … a bag of Haribo sweets.

I would have liked to have discovered … a chemical element.

The downside of my job … does not exist.

The most significant scientific advance of the last 100 years has been … the development of quantum mechanics.

What I look for first in a publication is … an original idea.

My favorite place on earth is … at home.

I chose chemistry as a career because … (theoretical) chemistry is fun.

My best investment was … a BMW motorbike.

If I were not a scientist, I would be … a taxi driver.

My most exciting discovery to date has been … that mass spectra can be computed by quantum chemistry.

How has your approach to chemistry research changed since the start of your career?

Our general ways of doing quantum chemistry have evolved enormously in the last 20 years or so, owing to the extreme development of computer hardware, while my personal approach has changed little. When I started theoretical research, calculations were often deeply planned because of missing resources, and, for example, the structure of the considered molecule was first analyzed by pencil and paper. Thinking about and reflecting on the actual problems is nowadays at least partially in the hands of the computer, and many theoreticians perform computational experiments rather than formulating theories. This evolution has certain positive aspects (omission of empty-headed routine work, emergence of totally new research areas), but in the worst case can lead to an intellectual impoverishment in our field.

How do you think your field of research will evolve over the next 10 years?

On one hand, quantum chemistry will increasingly be established as a standard research tool in chemistry and certainly get a strong and permanent position in addition to for example experimental spectroscopy. Even today, many experimental papers in chemical journals contain DFT calculations for relatively simple problems like structures or energetics. Although the quality of such treatments sometimes leaves much to be desired, this altogether positive trend will definitely continue. Further progress in soft- and hardware development in the next years will allow more robust and accurate calculations for systems of increasing size and complexity. On the other hand, there are ongoing fundamental methodical and theoretical developments that will foster and broaden the fields of quantum-chemical applications. The interpretation of some special spectroscopic techniques even by now depend solely on the combined application of experiment and quantum chemistry, and this will improve further. Slower paths of consolidation are expected for some very hard and challenging problems like the explicit computation of solvent effects, the inclusion of entropy, or in the field of strongly correlated electronic systems.

My 5 top papers:

1. "Improved second-order Møller–Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies": S. Grimme, *J. Chem. Phys.* **2003**, *118*, 9095–9102.
   The accurate calculation of the electronic correlation energy is a fundamental problem in quantum chemistry and its account is essential in order to obtain so-called "chemical accuracy" in practical calculations. This paper shows that by using a clever scaling of the fundamentally different electron pair correlation energies ("same-spin" and "opposite-spin"), a significantly improved accuracy without increased computational effort can be obtained. The introduced SCS-MP2 method is still applied as a standard quantum chemical method, even ten years after its development, and furthermore has opened a new field of "spin-component-scaled" wave-function-based methods (e.g., SCS(MI)-MP2, SCS-CC2).
2. "Semiempirical hybrid density functional with perturbative second-order correlation": S. Grimme, *J. Chem. Phys.* **2006**, *124*, 034108.
   Hybrid density functionals like the famous B3LYP provide limited accuracy because the correlation energy (opposed to the exchange energy) is computed merely by semilocal expressions from the electron density. The paper introduces an efficient functional called B2PLYP from the fifth rung of the so-called "Jacobs ladder" in DFT in which the correlation energy is computed by an MP2-type expression from the KS determinant and is combined with a "normal" hybrid functional. The method represents the prototype of the so-called double-hybrid functionals, which still belong to the most accurate DFT methods developed to date. Meanwhile it is known that the two scaling parameters used can be derived theoretically and that B2PLYP and variants represent a class of nowadays intensively investigated virtual-orbital-dependent DFT methods (of the "RPA"-type). The application of double-hybrids in the framework of time-dependent DFT produces also good results for electronic excitations.
3. "Seemingly Simple Stereoelectronic Effects in Alkane Isomers and the Implications for Kohn–Sham Density Functional Theory": S. Grimme, *Angew. Chem.* **2006**, *118*, 4571–4575; *Angew. Chem. Int. Ed.* **2006**, *45*, 4460–4464.
   Almost all standard functionals in DFT give dramatically wrong results for the simplest organic isomerization reactions. For example, the branched alkane 2,2,3,3-tetramethylbutane is experimentally, and according to highly accurate wave-function theory, more stable by 2 kcal mol^{-1} than its linear isomer *n*-octane. A standard functional like B3LYP does not only give the qualitatively wrong result but in addition an extremely large error of around 10 kcal mol^{-1} for two electronically simple molecules! The problem that has attracted a lot of interest in the theoretical research community and its origin are analyzed and explained in detail in this work. The effect, which is at the heart of chemists' "steric interactions", is attributed to the "medium-range" correlation energy that is insufficiently described in most functionals. Since the appearance of this paper, new DFT methods are tested for this rather general phenomenon. It is strongly related to the poorly described London dispersion interactions in many approximate functionals.
4. "A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H–Pu": S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.
   The account of long-ranged London dispersion interactions is a very active research field because these forces are ubiquitous in large or condensed systems. The papers introduces the third version of our atom-pairwise dispersion correction in which all important quantities (dispersion coefficients) are computed with ab initio methods and can be combined with almost any standard density functional by simple adjustment of the short-ranged parts. The method (DFT-D3) provides very robust accuracy with errors typically less than 5–10% for very many molecular as well as periodic systems, and is used worldwide as a standard tool in quantum chemistry.
5. "Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory": S. Grimme, *Chem. Eur. J.* **2012**, *18*, 9955–9964.
   The nonempirical calculation of binding affinities (i.e., free enthalpies of association) of host–guest systems is very challenging because various energy, entropy, and solvation components have to be computed accurately, and favorable error compensations are not at work. This paper shows the nonempirical reproduction of experimental affinity values in a ΔG range of 0 to -20 kcal mol^{-1} for 12 realistic supramolecular complexes (S12L-set). The combined DFT-D3 and COSMO-RS solvation approaches achieve an average error of only around 2 kcal mol^{-1} and in addition always calculate relative affinities quantitatively. The methods can be applied routinely to complexes containing of about 300 atoms and can furthermore provide detailed insight about binding motifs and energy–entropy relationships.

DOI: 10.1002/anie.201301621