Prof. Dr. Stefan Grimme

Personal Data

Title	Prof. Dr.
First name	Stefan
Name	Grimme
Current position	Full Professor (W3)
Current institution(s)/site(s), country	Mulliken Center for Theoretical Chemistry, Clausius-Institute of Physical and Theoretical Chemistry, Rheinische Friedrich-Wilhelms-University Bonn, Beringstr. 4, 53115 Bonn, Germany
Identifiers/ORCID	orcid.org/0000-0002-5844-4371

Qualifications and Career

Stages	Periods and Details	
Degree programme	Diploma in Chemistry, 1984 – 1989, Technical University of Braunschweig, Germany	
Doctorate	1989 – 1991	Mentor: H. Dreeskamp, PhD in Physical Chemistry, Technical University of Braunschweig, Germany
Stages of academic/professional career	Since 2011	Full Professor (W3), Theoretical Chemistry, University of Bonn, Germany
	2000 – 2011	Full Professor (C4), Theoretical Organic Chemistry, University of Münster, Germany
	1999 – 2000	Hochschuldozent, University of Bonn, Germany, Germany
	1996 – 1999	Assistant lecturer, University of Bonn, Germany
	1992 – 1996	Habilitand, University of Bonn (S.D. Peyerimhoff), Germany

Activities in the Research System

Committee involvement & activities in the field of academic self-governance:

To date	Editorial board member: *J. Comp. Chem.*, *Theor. Chem. Acc.*, *J. Chem. Theory Comput.*, *Phys. Chem. Chem. Phys.*, *Interdis. Rev. Comput. Mol. Sci.*
2015 – 2021	Member of the Kuratorium *Angew. Chem.*
2015 – 2016	Chairman of the Chemistry Department, University of Bonn
Since 2013	Board member AG Theoretische Chemie
2012 – 2019	Elected member, Review Board Chemistry DFG (Fachforum Chemie)
2010	Chair of the annual symposium for Theoretical Chemistry
2010 – 2013	Vice-chairmen of the SFB 858 (University of Münster)
2000 – 2011	Director of the Organic Chemistry Institute, University of Münster

Academic Distinctions: van der Waals Prize for Senior Scientist from the International Advisory Board (IAB) of the International Conferences on Noncovalent Interactions (ICNIs, 2024); Mulliken Lecture and Visiting Professor, University of Georgia, Athens (2020); Max-Plank Fellow, MPI für Kohlenforschung, Mülheim (2019); Member of the German National Academy of Science Leopoldina (2018); Honorary member of the Israel Chemical Society (2017); Gottfried-Wilhelm-Leibniz-Prize (2015); Ziegler Lecture of the MPI für Kohlenforschung, Mülheim (2015); Highly cited researcher by Thomson Reuters, WOS (2014 – 2023); Elected member, International Academy of Quantum Molecular Science (2013); Schrödinger Medal of WATOC (2013); Member of the Academy of Sciences and Arts of North Rhine Westphalia (2011); "Bennigsen"-Award of North Rhine Westphalia (1998); Dozentenstipendium, Fond of the Chemical Industry of Germany (1998); PhD-Fellowship, Fond of the Chemical Industry (VCI) (1989).

Scientific Results

Citations: 174841, h-index: 136, i10-index: 605 (Google Scholar, 21.03.2024)

Category A (* corresponding author)

1. **S. Grimme*** "Towards First Principles Calculation of Electron Impact Mass Spectra of Molecules" *Angew. Chem. Int. Ed.* **2013**, 52, 6306–6312. DOI: 10.1002/anie.201300158.
2. **S. Grimme*** "A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules" *J. Chem. Phys.* **2013,** 138, 244104. DOI: 10.1063/1.4811331.
3. **S. Grimme***, C. Bannwarth, S. Dohm, A. Hansen, J. Pisarek, P. Pracht, J. Seibert, F. Neese "Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra" *Angew. Chem. Int. Ed.* **2017**, 56, 14763–14769. DOI: 10.1002/anie.201708266.
4. C. Bannwarth, S. Ehlert, **S. Grimme*** "GFN2-xTB – An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions" *J. Chem. Theory Comput.* **2019**, 15, 1652–1671. DOI: 10.1021/acs.jctc.8b01176.
5. **S. Grimme*** "Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations" *J. Chem. Theory Comput.* **2019**, 5, 2847–2862. DOI: 10.1021/acs.jctc.9b00143.
6. E. Caldeweyher, S. Ehlert, A. Hansen, H. Neugebauer, S. Spicher, C. Bannwarth, **S. Grimme*** "A generally applicable atomic-charge dependent London dispersion correction" *J. Chem. Phys.* **2019**, 150, 154122. DOI: 10.1063/1.5090222.
7. S. Spicher, **S. Grimme*** "Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems" *Angew. Chem. Int. Ed.* **2020**, 59, 15665–15673. DOI: 10.1002/anie.202004239.
8. **S. Grimme***, F. Bohle, A. Hansen, P. Pracht, S. Spicher, M. Stahn "Efficient quantum chemical calculation of structure ensembles and free energies for nonrigid molecules" *J. Phys. Chem. A* **2021**, 125, 4039–4054. DOI: 10.1021/acs.jpca.1c00971.
9. M. Bursch*, J.-M. Mewes*, A. Hansen*, **S. Grimme*** "*Best-Practice DFT Protocols for Basic Molecular Computational Chemistry*" *Angew. Chem. Int. Ed.* **2022,** 61, e202205735. DOI: 10.1002/anie.202205735.

10. M. Müller, A. Hansen, **S. Grimme*** “ωB97X-3c: A composite range-separated hybrid DFT method with a molecule-optimized polarized valence double-ζ basis set” *J. Chem. Phys* **2023**, 158, 014103. DOI: 10.1063/5.0133026.

Category B

Freely available open-source quantum chemistry software:

1. **Grimme** lab “Semiempirical Extended Tight-Binding Program Package” [Source code]. https://github.com/grimme-lab/xtb.
2. Crest lab “CREST” [Source code]. https://github.com/crest-lab/crest.
3. **Grimme** lab “stda program for computing excited states and response functions via simplified TD-DFT methods” [Source code]. https://github.com/grimme-lab/stda.
4. **Grimme** lab “QCxMS” [Source code]. https://github.com/grimme-lab/QCxMS.