



# Dr. Stefan Knecht

## Curriculum Vitae

### Personal Information

Date of Birth 31.10.1979  
Nationality German  
Civil Status married, two children (\* 2013, \* 2018)

### Professional Experience

#### Current position

since 08.2018 **Senior Scientist**, *Group of Prof. M. Reiher*, ETH Zürich.

#### Previous Positions

- 2013-2018 **Habilitand**, *Group of Prof. M. Reiher*, ETH Zürich.  
Title of Habilitationsschrift: Electronic structure theory for the whole periodic table of the elements.
- 2010–2013 **Postdoctoral Researcher**, *Group of Prof. H. J. Aa. Jensen*, SDU Odense.  
Development of parallel range-separated density functional theory multiconfiguration methods.
- 2009–2010 **Postdoctoral Researcher**, *Group of Prof. T. Saue*, U Strasbourg.  
Development of relativistic exact two-component Hamiltonians.
- 2005–2009 **Research Assistant**, *Group of Prof. C. M. Marian*, U Düsseldorf.  
Developing exercise materials and being responsible for student tutorials.

### Education

- 2005–2009 **Dr. rer. nat. (Chemistry)**, *Theoretical Chemistry*, U Düsseldorf, “*summa cum laude*”.  
Thesis: Parallel relativistic multiconfiguration methods: new powerful tools for heavy-element electronic-structure studies. Advisers: Prof. T. Fleig and Prof. C. M. Marian
- 2000–2005 **Dipl.-Chem.**, *Theoretical Chemistry*, U Heidelberg, “*very good*”.  
Thesis: Investigation of the ionization spectra and electronic decay processes in alkali iodides by means of the four-component propagator method. Adviser: Prof. L. S. Cederbaum

### Fellowships, Awards and Funding

- 2017 Professeur invité (NEXT program) (CNRS/Université Toulouse III)
- 2017 Named external partner for actipNMR project funded by the ANR (France)
- 2015 Named external partner for MCFUNEX project funded by the ANR (France)
- 2010 Postdoctoral fellowship by the Danish research council for natural sciences (FNU), 224 kEuro
- 2007 EU Marie Curie research fellow (project NANOQUANT)
- 1999 School student's award in chemistry from the Fonds der Chemischen Industrie

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## Supervision of Theses

### Co-supervision of PhD Theses

2013-2016 Sebastian Keller (ETH Zürich)

### Co-supervision of Master Theses

2014 Stefano Battaglia (ETH Zürich)

2011–2012 Morten Nørby Pedersen (SDU Odense), Frank Heiden (SDU Odense)

### Co-supervision of Semester Theses

Stefan Heinen (ETH Zürich, 2013), Stefano Battaglia (ETH Zürich, 2014),

Leonard Floryan (ETH Zürich, 2014), Eno Paernuk (ETH Zürich, 2016)

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## Co-supervision of Postdoctoral Projects

2015- Dr. Leon Freitag (ETH Zürich)

2014-2016 Dr. Erik D. Hedegaard (ETH Zürich)

2013-2016 Dr. Yingjin Ma (ETH Zürich)

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## Teaching Experience

### Lecturer

- "Advanced Quantum Chemistry" (ETH Zürich, fall term 2014, 2015, 2016, 2017 and 2018)
- "Quantum Chemistry" (ETH Zürich, spring term 2016 and 2017)
- "Statistical Physics and Computer Simulations" (ETH Zürich, spring term 2016, 2017 and 2018)
- 15th European Summerschool in Quantum Chemistry (Sicily, 09/2015)
- 30th Winter School in Theoretical Chemistry (U Helsinki, 12/2014)
- PhD school "Introduction to relativistic quantum chemistry" (U Corrientes, 09/2012)
- "Introduction to molecular modeling" (SDU Odense, spring and fall term 2011)

### Tutor

- "Statistical Physics and Computer Simulations" (ETH Zürich, spring term 2015, 2016 and 2017)
- 15th European Summerschool in Quantum Chemistry (Sicily, 09/2015)
- "Advanced Quantum Chemistry" (ETH Zürich, fall term 2013 and 2014)
- 14th European Summerschool in Quantum Chemistry (Sicily, 09/2013)
- 11th Sostrup summer school (Himmelbjerget, 06/2010)
- "Advanced Quantum Chemistry" (U Düsseldorf, summer term 2008)
- "Mathematical Methods in Chemistry" (U Düsseldorf, summer term 2007)
- "Group Theory" (U Düsseldorf, summer term 2006)
- "Introduction to Quantum Chemistry" (U Düsseldorf, winter term 2005 and summer term 2009)

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## Scientific Publications and Conference Contributions

- 50 articles published/accepted;  
for further bibliometric statistics see <http://www.researcherid.com/rid/H-5282-2012>
- More than 36 oral communications at international conferences including 17 invited lectures;  
for further information see <http://stefanknecht.xyz>
- Leading author for Theoretical Chemistry in the section "Notizen aus der Chemie" for the GDCh journal "Nachrichten aus der Chemie".

## List of Invited Lectures

### upcoming

20. MPI Dresden (Germany), Tensor product methods and entanglement optimization for ab initio quantum chemistry (TPMQC-2020), March 2020
19. Heidelberg (Germany), June 30 – July 5, 2019, The 9th Molecular Quantum Mechanics (MQM)
18. RIKEN R-CCS, Kobe (Japan), January 15-17 2019, International Workshop on Massively Parallel Programming for Quantum Chemistry and Physics 2019

### past

17. New developments for matrix-product state wave functions, Strasbourg (France), June 24-27 2018, Strasbourg satellite meeting to the 16th ICQC: Strong correlation in electronic structure theory
16. New developments for matrix-product state wave functions, New Orleans (USA), March 18-22, 2018, ACS National Meeting
15. Spin-orbit coupling approaches based on matrix-product-state wave functions: Exploring magnetic properties of f-elements, Marburg (Germany), Sep 2-6, 12th International Conference on relativistic effects in heavy-element chemistry and physics (REHE2017)
14. New developments for matrix-product state wave functions, Shropshire (UK), July 11-14, ESCMQC 2017
13. The electron correlation problem in the lower part of the periodic table, Tokyo (Japan), Sep 25-28, 2016, Current Trends and Future Directions in Relativistic Many Electron Theories (RMET 2016)
12. The electron correlation problem in the lower part of the periodic table, Grand Forks, ND (USA), July 17-22, 2016 ISTCP IX
11. The electron correlation problem in the lower part of the periodic table, Uppsala (Sweden), June 26 - July 1, 2016 The 8th Molecular Quantum Mechanics (MQM)
10. Towards large-scale quantum chemistry with second-generation DMRG, Lugano (Switzerland), 13.06.2016, ADAC workshop, CSCS/Università della Svizzera italiana
9. DMRG in quantum chemistry, Altavilla Milicia, Sicily (Italy), 06.-19.09.2015, 15th European Summer school in quantum chemistry (ESQC)
8. The electron correlation problem in the lower part of the periodic table, Middelfart, (Denmark), 24.-26.08.2015, Open shells, open questions
7. The electron correlation problem in the lower part of the periodic table, Beijing, (China), 13.-16.06.2015, New frontiers of relativistic quantum chemistry, ICQC satellite meeting
6. The electron correlation problem in the lower part of the periodic table, Mariapfarr, (Austria), 22-27.02.2015, VIIIth Workshop on Modern Methods in Quantum Chemistry
5. Calculation of excitation energies for heavy-element systems (3 lectures), U Helsinki (Finland), 30th Winter School in Theoretical Chemistry: Theoretical *f*-Element Chemistry, 15.-18.12.2014
4. Relativistic density matrix renormalization group, Smolenice Castle (Slovakia), 20.-24.9.2014, 11th International Conference on relativistic effects in heavy-element chemistry and physics (REHE2014)

3. On the electron correlation problem in quantum chemistry, Paris (France), 14.-18.4.2014, Workshop - Numerical methods for high-dimensional problems, Ecole des Ponts Paristech
2. Mössbauer spectroscopy for heavy elements, Corrientes (Argentina), September 2012, 10th International Conference on relativistic effects in heavy-element chemistry and physics (REHE2012)
1. Parallelization of the Spin-Orbit-Free GASCI-Program LUCITA - Application to the (RbBa)<sup>+</sup> molecule ion, Puhäjärvä (Estonia), December 8-10 2006, Nanoquant Young Researcher's Meeting

## Organization of scientific meetings

- 2015 Co-organizer of the symposium "Open shells, open questions" in honor of Hans Jørgen Aagaard Jensen, Middelfart, (Denmark)
- 2012 Co-organizer of the PhD school "Introduction to relativistic quantum chemistry" (U Corrientes, Argentina)

## Reviewer Activities

- Grants ERC Starting Grant 2018, section "Physical and Analytical Chemical Sciences"
- Journals Chemical Reviews, Journal of Chemical Theory and Computation, Physical Chemistry Chemical Physics, Journal of Chemical Physics, Organometallics, Journal of Physical Chemistry A/B, Molecular Physics, Chemical Physics Letters, Theoretical Chemistry Accounts, Chemical Physics

## Co-Authorship of Quantum Chemical Software

- Contributing author to the non-profit relativistic quantum chemistry program suite Dirac, 2008–2016 releases. <http://diracprogram.org>.
- Contributing author to the non-profit quantum chemistry program suite Dalton, 2011–2016 releases. <http://daltonprogram.org>.
- Contributing author to the non-profit relativistic quantum chemistry program suite ReSpect, 2013–2016 releases. <http://rel-qchem.sav.sk>
- Contributing author to the quantum chemistry program suite Molcas. <http://molcas.org>

## Memberships

- Bunsen Gesellschaft (Arbeitsgemeinschaft Theoretische Chemie)
- Gesellschaft Deutscher Chemiker
- Schweizerische Chemische Gesellschaft
- Deutsche Physikalische Gesellschaft

## Languages

- native German
- excellent English
- fluent Danish, French

## Active International Collaborations

- Prof. T. Saue (U Toulouse)
- Prof. H. J. Aa. Jensen (SDU Odense)
- Prof. B. Mennucci (U Pisa)
- Prof. E. Fromager (U Strasbourg)
- Prof. L. Visscher (VU Amsterdam)
- Prof. R. Lindh (U Uppsala)
- Prof. L. Gonzalez (U Vienna)
- Prof. J. Autschbach (U Buffalo)
- Prof. J. Neugebauer (U Münster)
- Prof. C. Angeli (U Ferrara)
- Dr. M. Repisky (U Tromsø)

## References

- Prof. M. Reiher (current employer)  
Laboratory of Physical Chemistry, ETH Zürich  
8093 Zürich, Switzerland  
phone: +41 446334308, email: markus.reiher@phys.chem.ethz.ch
- Prof. T. Saue (postdoc adviser)  
Laboratoire de Chimie et Physique Quantiques, U Toulouse III  
31062 Toulouse, France  
phone: +33 561556031, email: trond.saue@irsamc.ups-tlse.fr
- Prof. H. J. Aa. Jensen (postdoc adviser)  
Department of Physics, Chemistry and Pharmacy, SDU Odense  
5230 Odense M, Denmark  
phone: +45 65502512, email: hjj@sdu.dk
- Prof. C. M. Marian (PhD supervisor)  
Institute of Theoretical Chemistry, HHU Düsseldorf  
40225 Düsseldorf, Germany  
phone: +49 2118113209, email: christel.marian@hhu.de
- Prof. J. Neugebauer (collaborator)  
Organic Chemistry Institute, WWU Münster  
48149 Münster, Germany  
phone: +49 251 83-33241, email: j.neugebauer@uni-muenster.de

Zürich, December 5, 2018