Curriculum Vitae

Dr. Christoph Bannwarth

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Research interests

Electronic structure theory, Semiempirical methods, Multi-level quantum chemical approaches, Machine-learning models, Photophysics & photochemistry, Electronic circular dichroism, Noncovalent interactions, Catalysis

Postdoctoral research experience

Since 01/2021	**RWTH Aachen University**, Germany Assistant professor (*Juniorprofessor*) for "Theoretical Physical Chemistry of Large Molecules" (since 05/2021) RWTH Junior Principal Investigator (01/2021 – 04/2021) Research focus: Development and application of multi-level simulation techniques for soft energy storage and energy conversion materials.
08/2018 – 12/2020	**Stanford University** and **SLAC National Accelerator Laboratory**, CA, USA Advisor: *Todd J. Martínez* Leopoldina Postdoctoral Research Fellow (11/2018 – 04/2020) Research focus: a) Development of efficient electronic structure methods for photochemistry simulations (publications [40–42]). b) Acceleration of exchange and density matrix builds in semiempirical calculations with graphics processing units (GPUs).
03/2018 – 08/2018	**University of Bonn**, Germany Advisor: *Stefan Grimme* Research focus: Development of a semiempirical extended tight-binding method with multipole electrostatics, which is designed for structural sampling and computation of noncovalent interaction energies (publication [35]).

Education

01/2013 – 03/2018	**University of Bonn**, Germany Dr. rer. nat., Theoretical Chemistry (*summa cum laude*) "Development and Application of Efficient Methods for the Computation of Electronic Spectra of Large Systems" Advisor: *Stefan Grimme*
10/2009 – 09/2012	**RWTH Aachen University**, Germany Master of Science, Chemistry (final grade: 1.3)* "Computational Investigation of Charge Transfer in the α-helix and its Contribution to Circular Dichroism" (grade: 1.0)* Advisors: *Gerhard Raabe*, *Robert W. Woody* (Colorado State University, CO, USA)
10/2006 – 09/2009	**RWTH Aachen University**, Germany Bachelor of Science, Chemistry (final grade: 1.9)* "Stability und Catalytic Activity of Ruthenium Nanoparticles in the Presence of Acidic Additives" (grade: 1.3)* Advisor: *Marcel Liauw*
08/1997 – 06/2006	**Gymnasium der Stadt Frechen**, Germany Abitur/high school graduation (grade 1.6)*

*On a scale from 1.0 (best grade) to 4.0 (worst satisfactory grade)

Summarized teaching experience

	RWTH Aachen University
04/2021 – 07/2021	*Lecturing* in the BSc Chemistry course "Computational Chemistry"
10/2007 – 02/2010	*Teaching assistant* "General Chemistry 1": tutoring
	Stanford University
09/2018 – 01/2020	*Postdoc Teaching Certificate* Elective workshops and classes on teaching: 70 h in-class time Lecturing with originally designed content (on "Basis sets and mean-field theories", "Chemistry in industry and chirality" and "The DFT/MRCI method"): 5.5 h in-class time
	University of Bonn
04/2015 – 09/2017	*Supervision* of six students, resulting in publications [28], [29], [32], and [34]
04/2014 – 10/2017	*Teaching assistant* "Quantum Chemistry I + II": tutoring, practical courses

Awards, research grants, and scholarships

08/2020	Nomination for the **NRW Returning Scholars Program ("NRW-Rückkehrerprogramm")** to establish an independent research group (∼1,250,000 €, duration: 5 years)
07/2020	**RWTH Junior Principal Investigator Fellowship** to support early career researchers
11/2019	**CIC Advancement Award for Computational Chemistry** by the German Chemical Society (GDCh) for an exceptional dissertation
11/2018	**Postdoctoral Research Fellowship** (∼63,000 €) funded by the German National Academy of Sciences Leopoldina for an 18 months research project at the Stanford University
12/2017	**DAAD travel scholarship** (1,300 €) for an invited talk at the Stanford University, CA, USA
06/2016	**Poster award** at *The* 8^{th} *Molecular Quantum Mechanics* conference in Uppsala, Sweden
09/2015	**Poster award** at the 51^{st} *Symposium on Theoretical Chemistry* in Potsdam, Germany
11/2013	**Friedrich Wilhelm Prize** (RWTH Aachen University) for an outstanding Master's thesis
04/2012	**PROMOS scholarship** (2,375 €) of the DAAD for the Master's thesis abroad (USA)

Participation in workshops and training courses (including own contributions)

07/2014	**Sostrup Summerschool: Quantum Chemistry and Molecular Properties** in Ry, Denmark (*poster*)
12/2013	**29th Winter School in Theoretical Chemistry** in Helsinki, Finland (*poster*)
09/2013	**European Summerschool in Quantum Chemistry** in Altavilla Milicia, PA, Italy (*poster*)

Long-term stays abroad

08/2018 – 12/2020	Postdoctoral research at the Stanford University in Stanford, CA, USA
09/2011 – 03/2012	Research stay (Master's thesis) at the Colorado State University in Fort Collins, CO, USA
08/2003 – 02/2004	High school exchange program in Beausejour, MB, Canada

Professional memberships or affiliations

Since 2017	American Chemical Society (ACS)
Since 2019	German Chemical Society (GDCh)
Since 2020	Arbeitsgemeinschaft Theoretische Chemie (AGTC)

Peer review for scientific journals

J. Chem. Phys. ($6\times$), Phys. Chem. Chem. Phys. ($4\times$), RSC Adv. ($2\times$), Nucleic Acids Res. ($2\times$), J. Org. Chem. ($2\times$), J. Chem. Inf. Model. ($1\times$), Sci. Bull. ($1\times$), PeerJ Physical Chemistry ($1\times$)

Languages

German (native), English (proficient), French (basic), Turkish (basic)

Scientific software contributions

ORCA quantum chemstry program (in C++): sTDA/sTD-DFT excited state methods; Composite DFT methods PBEh-3c and B97-3c; Analytical D3 gradients

GPU-accelerated quantum chemistry program **TeraChem** (in C++/CUDA): Spherical basis set handling; Semiempirical integral library; hh-TDA method; D2 and D3 dispersion corrections; Density matrix purification

Semiempirical extended tight-binding code **xtb** (in Fortran): GFN2-xTB method including multi-pole contributions; Coordination number-dependent terms (energies and gradients), Molden file printout

Simplified TD-DFT code **stda** (in Fortran): sTD-DFT method; A+B/2 correction for ECD intensities with simplified Tamm-Dancoff approximation (sTDA); OMP parallelization; Interface to other codes via Molden file

Conference contributions and external seminar talks (selection from a total of 21)

07/2020 *Contributed talk* at the **Virtual Conference on Theoretical Chemistry 2020**: "Hole-hole Tamm-Dancoff-approximated density functional theory: a highly efficient electronic structure method incorporating dynamic and static correlation"

11/2019 *Invited talk* at the **15th German Conference on Cheminformatics** in Mainz, Germany: "Computation of Electronic Spectra of Large Molecular Systems with Efficient Electronic Structure Methods"

09/2019 *Contributed talk* at the **55th Symposium on Theoretical Chemistry** in Rostock, Germany: "GPU-accelerated semiempirical electronic structure methods for photochemical studies of large systems"

08/2019 *Contributed talk* at the **258th ACS National Meeting** in San Diego, CA, USA: "Towards non-adiabatic dynamics simulations using semiempirical extended tight-binding (xTB) methods"

12/2017 *Invited talk* at the **Stanford University** in Stanford, CA, USA: "A New Robust and Accurate Tight-Binding Method for Structures and Noncovalent Interactions of Large Molecular Systems"

08/2017 *Contributed talk* at the **254th ACS National Meeting** in Washington, DC, USA:
"Simplified Methods for the Computation of Electronic Absorption and Circular Dichroism Spectra"

06/2017 *Invited talk* at the **Karlsruhe Institute of Technology** in Karlsruhe, Germany:
"Simplified Methods for the Computation of Electronic Absorption and Circular Dichroism Spectra"

03/2017 *Invited talk* at the **CUP XVII** in Santa Fe, NM, USA:
"A robust and accurate tight-binding method for structures and non-covalent interaction energies"

01/2017 *Invited talk* at the **Interdisciplinary Center for Scientific Computing** in Heidelberg, Germany:
"Simplified Methods for the Computation of Electronic Absorption and Circular Dichroism Spectra"

07/2016 *Invited talk* at the **GDCh Kolloquium** in Bonn, Germany:
"Calculation of electronic excitation spectra with simplified TD-DFT methods" (in German)

09/2015 *Invited talk* at the **Graduate Talks on Chemistry@Spin Centers** in Trier, Germany:
"Electronic absorption and circular dichroism spectra of large closed-shell and open-shell systems by simplified TD-DFT methods"

09/2015 *Contributed talk* at the **15th International Conference on Chiroptical Spectroscopy** in Sapporo, Japan: "Computation of Electronic Circular Dichroism Spectra and Optical Rotation by Simplified Time-Dependent Density Functional Theory"

05/2015 *Invited talk* at the **Max-Planck-Institut für Chemical Energy Conversion** in Mülheim an der Ruhr, Germany: "Simplified Time-Dependent DFT: Theory, Application and Recent Developments"

09/2014 *Contributed talk* at the **50th Symposium on Theoretical Chemistry** in Vienna, Austria:
"The simplified TD-DFT and TDA approaches: Excited states and spectra for very large systems"