

43. Hohenstein EG, Yu JK, **Bannwarth C**, List NH, Paul AC, Folkestad SD, Koch H, Martínez TJ; “Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Hole-Hole Tamm–Dancoff-Approximated Density Functional Theory”, *J. Chem. Theory Comput.* **2021**; 17:7120–7133.
42. Seritan S, **Bannwarth C**, Fales BS, Hohenstein EG, Isborn CM, Kokkila-Schumacher SI, Li X, Liu F, Luehr N, James W Snyder J, Song C, Titov AV, Ufimtsev IS, Wang LP, Martínez TJ; “A GPU-accelerated electronic structure package for large-scale ab initio molecular dynamics”, *WIREs Comput. Mol. Sci.* **2021**; 11:e1494.
41. **Bannwarth C**, Caldeweyher E, Ehlert S, Hansen A, Pracht P, Seibert J, Spicher S, Grimme S; “Extended tight-binding quantum chemistry methods”, *WIREs Comput. Mol. Sci.* **2021**; 11:e01493.
40. Yu JK, **Bannwarth C**, Liang R, Hohenstein EG, Martínez TJ; “Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Involving Excitations to the  $n\pi^*$  and  $\pi\pi^*$  Excited States”, *J. Am. Chem. Soc.* **2020**; 142:20680–20690.
39. Yu JK, **Bannwarth C**, Hohenstein EG, Martínez TJ; “Ab Initio Nonadiabatic Molecular Dynamics with Hole–Hole Tamm–Dancoff Approximated Density Functional Theory”, *J. Chem. Theory Comput.* **2020**; 16:5499–5511.
38. **Bannwarth C**, Yu JK, Hohenstein EG, Martínez TJ; “Hole-hole Tamm-Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation”, *J. Chem. Phys.* **2020**; 153:024110.
37. Seritan S, **Bannwarth C**, Fales BS, Hohenstein EG, Kokkila-Schumacher SI, Luehr N, Snyder JW, Song C, Titov AV, Ufimtsev IS, Martínez TJ; “TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units”, *J. Chem. Phys.* **2020**; 152:224110.
36. de Wergifosse M, **Bannwarth C**, Grimme S; “A Simplified Spin-Flip Time-Dependent Density Functional Theory Approach for the Electronic Excitation Spectra of Very Large Diradicals”, *J. Phys. Chem. A* **2019**; 123:5815–5825.
35. **Bannwarth C**, Ehlert S, Grimme S; “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.
34. Caldeweyher E, Ehlert S, Hansen A, Neugebauer H, Spicher S, **Bannwarth C**, Grimme S; “A generally applicable atomic-charge dependent London dispersion correction”, *J. Chem. Phys.* **2019**; 150:154122.
33. Hölzl-Hobmeier A, Bauer A, Silva AV, Huber SM, **Bannwarth C**, Bach T; “Catalytic deracemization of chiral allenes by sensitized excitation with visible light”, *Nature* **2018**; 564:240–243.
32. Seibert J, Pisarek J, Schmitz S, **Bannwarth C**, Grimme S; “Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB)”, *Mol. Phys.* **2019**; 117:1104–1116.
31. Brandenburg JG, **Bannwarth C**, Hansen A, Grimme S; “B97-3c: A revised low-cost variant of the B97-D density functional method”, *J. Chem. Phys.* **2018**; 148:064104.
30. Grimme S, **Bannwarth C**, Dohm S, Hansen A, Pisarek J, Pracht P, Seibert J, Neese F; “Fully Automated Quantum-Chemistry-Based Computation of Spin–Spin-Coupled Nuclear Magnetic Resonance Spectra”, *Angew. Chem. Int. Ed.* **2017**; 56:14763–14769.
29. Seibert J, **Bannwarth C**, Grimme S; “Biomolecular Structure Information from High-Speed Quantum Mechanical Electronic Spectra Calculation”, *J. Am. Chem. Soc.* **2017**; 139:11682–11685.
28. Caldeweyher E, **Bannwarth C**, Grimme S; “Extension of the D3 dispersion coefficient model”, *J. Chem. Phys.* **2017**; 147:034112.
27. Grimme S, **Bannwarth C**, Caldeweyher E, Pisarek J, Hansen A; “A general intermolecular force field based on tight-binding quantum chemical calculations”, *J. Chem. Phys.* **2017**; 147:161708.

26. Grimme S, **Bannwarth C**, Shushkov P; "A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements ( $Z=1-86$ )", *J. Chem. Theory Comput.* **2017**; 13:1989–2009.
25. Strelnik ID, Musina EI, Ignatieva SN, Balueva AS, Gerasimova TP, Katsyuba SA, Krivolapov DB, Dobrynin AB, **Bannwarth C**, Grimme S, Kolesnikov IE, Karasik AA, Sinyashin OG; "Pyridyl Containing 1,5-Diaza-3,7-diphosphacyclooctanes as Bridging Ligands for Dinuclear Copper(I) Complexes", *Z. Anorg. Allg. Chem.* **2017**; 643:895–902.
24. Burganov TI, Zhukova NA, Mamedov VA, **Bannwarth C**, Grimme S, Katsyuba SA; "Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects", *Phys. Chem. Chem. Phys.* **2017**; 19:6095–6104.
23. Jarzebski A, Tenten C, **Bannwarth C**, Schnakenburg G, Grimme S, Lützen A; "Diastereoselective Self-Assembly of a Neutral Dinuclear Double-Stranded Zinc(II) Helicate via Narcissistic Self-Sorting", *Chem. Eur. J.* **2017**; 23:12 380–12 386.
22. Struch N, **Bannwarth C**, Ronson TK, Lorenz Y, Mienert B, Wagner N, Engeser M, Bill E, Puttreddy R, Rissanen K, Beck J, Grimme S, Nitschke JR, Lützen A; "An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spin-Crossover Behavior", *Angew. Chem. Int. Ed.* **2017**; 56:4930–4935.
21. Ratzke W, Schmitt L, Matsuoka H, **Bannwarth C**, Retegan M, Bange S, Klemm P, Neese F, Grimme S, Schiemann O, Lupton JM, Höger S; "Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singlet–Triplet Emitters for Organic Light-Emitting Diodes", *J. Phys. Chem. Lett.* **2016**; 7:4802–4808.
20. Frömel S, Daniliuc CG, **Bannwarth C**, Grimme S, Bussmann K, Kehr G, Erker G; "Indirect synthesis of a pair of formal methane activation products at a phosphane/borane frustrated lewis pair", *Dalton Trans.* **2016**; 45:19 230–19 233.
19. Grimme S, **Bannwarth C**; "Ultra-fast computation of electronic spectra for large systems by tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB)", *J. Chem. Phys.* **2016**; 145:054 103.
18. Allan M, Regeta K, Gorfinkiel DJ, Mašin Z, Grimme S, **Bannwarth C**; "Recent research directions in Frimbourg: nuclear dynamics in resonances revealed by 2-dimensional EEL spectra, electron collisions with ionic liquids and electronic excitation of pyrimidine", *Eur. Phys. J. D* **2016**; 70:1–7.
17. Masnyk M, Butkiewicz A, Górecki M, Luboradzki R, **Bannwarth C**, Grimme S, Frelek J; "Synthesis and Comprehensive Structural and Chiroptical Characterization of Enones Derived from (–)- $\alpha$ -Santonin by Experiment and Theory", *J. Org. Chem.* **2016**; 81:4588–4600.
16. Grimme S, Hansen A, Brandenburg JG, **Bannwarth C**; "Dispersion-Corrected Mean-Field Electronic Structure Methods", *Chem. Rev.* **2016**; 116:5105–5154.
15. **Bannwarth C**, Seibert J, Grimme S; "Electronic Circular Dichroism of [16]Helicene With Simplified TD-DFT: Beyond the Single Structure Approach", *Chirality* **2016**; 28:365–369.
14. Musina EI, Shamsieva AV, Strelnik ID, Gerasimova TP, Krivolapov DB, Kolesnikov IE, Grachova EV, Tunik SP, **Bannwarth C**, Grimme S, Katsyuba SA, Karasik AA, Sinyashin OG; "Synthesis of novel pyridyl containing phospholanes and their polynuclear luminescent copper(I) complexes", *Dalton Trans.* **2016**; 45:2250–2260.
13. Grimme S, Brandenburg JG, **Bannwarth C**, Hansen A; "Consistent structures and interactions by density functional theory with small atomic orbital basis sets", *J. Chem. Phys.* **2015**; 143:054 107.
12. Chen GQ, Türkyilmaz F, Daniliuc CG, **Bannwarth C**, Grimme S, Kehr G, Erker G; "Enamine/butadienylborane cycloaddition in the frustrated Lewis pair regime", *Org. Biomol. Chem.* **2015**; 13:10 477–10 486.
11. Jarzebski A, **Bannwarth C**, Tenten C, Benkhäuser C, Schnakenburg G, Grimme S, Lützen A; "Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized Träger's Base Derivatives: Part III", *Synthesis* **2015**; 47:3118–3132.

10. Regeta K, **Bannwarth C**, Grimme S, Allan M; "Free electrons and ionic liquids: study of excited states by means of electron-energy loss spectroscopy and the density functional theory multireference configuration interaction method", *Phys. Chem. Chem. Phys.* **2015**; 17:15 771–15 780.
9. Yu J, Kehr G, Daniliuc CG, **Bannwarth C**, Grimme S, Erker G; "Direct synthesis of a geminal zwitterionic phosphonium/hydridoborate system - developing an alternative tool for generating frustrated Lewis pair hydrogen activation systems", *Org. Biomol. Chem.* **2015**; 13:5783–5792.
8. **Bannwarth C**, Grimme S; "Electronic Circular Dichroism of Highly Conjugated  $\pi$ -Systems: Breakdown of the Tamm–Dancoff/Configuration Interaction Singles Approximation", *J. Phys. Chem. A* **2015**; 119:3653–3662.
7. Frost JR, Huber SM, Breitenlechner S, **Bannwarth C**, Bach T; "Enantiotopos-Selective C–H Oxygenation Catalyzed by a Supramolecular Ruthenium Complex", *Angew. Chem. Int. Ed.* **2015**; 54:691–695.
6. **Bannwarth C**, Hansen A, Grimme S; "The Association of Two "Frustrated" Lewis Pairs by State-of-the-Art Quantum Chemical Methods", *Isr. J. Chem.* **2015**; 55:235–242.
5. Hansen A, **Bannwarth C**, Grimme S, Petrović P, Werlé C, Djukic JP; "The Thermochemistry of London Dispersion-Driven Transition Metal Reactions: Getting the "Right Answer for the Right Reason"", *ChemistryOpen* **2014**; 3:177–189.
4. **Bannwarth C**, Grimme S; "A simplified time-dependent density functional theory approach for electronic ultraviolet and circular dichroism spectra of very large molecules", *Comput. Theor. Chem.* **2014**; 1040–1041:45–53.
3. Gütz C, Hovorka R, Klein C, Jiang QQ, **Bannwarth C**, Engeser M, Schmuck C, Assenmacher W, Mader W, Topić F, Rissanen K, Grimme S, Lützen A; "Enantiomerically Pure  $[M_6L_{12}]$  or  $[M_{12}L_{24}]$  Polyhedra from Flexible Bis(Pyridine) Ligands", *Angew. Chem. Int. Ed.* **2014**; 53:1693–1698.
2. Hounjet LJ, **Bannwarth C**, Garon CN, Caputo CB, Grimme S, Stephan DW; "Combinations of Ethers and  $B(C_6F_5)_3$  Function as Hydrogenation Catalysts", *Angew. Chem. Int. Ed.* **2013**; 52:7492–7495.
1. Giese M, Albrecht M, **Bannwarth C**, Raabe G, Valkonen A, Rissanen K; "From attraction to repulsion: anion- $\pi$  interactions between bromide and fluorinated phenyl groups", *Chem. Commun.* **2011**; 47:8542–8544.

## Book chapters and other publications

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2. **Bannwarth C**. "Development and Application of Efficient Methods for the Computation of Electronic Spectra of Large Systems". Dissertation, Rheinische Friedrich-Wilhelms-Universität Bonn, Universitäts- und Landesbibliothek Bonn **2018**.
1. Petrović P, Djukic JP, Hansen A, **Bannwarth C**, Grimme S. "Non-covalent Stabilization in Transition Metal Coordination and Organometallic Complexes". *Non-covalent Interactions in the Synthesis and Design of New Compounds*. John Wiley & Sons, Inc, **2016**; 115–143.