Dr. Jan Gerit Brandenburg, Dipl.-Phys. - List of Publications

Publications most relevant for establishing independent research:

1. E. Caldeweyher and **J. G. Brandenburg***, *Simplified DFT methods for consistent structures and energies of large systems*, J. Phys.: Condens. Matter **2018**, *30*, 213001. [Ref. 35]

   Even though affordable many-body electronic structure methods emerge, we still see DFT as an irreplaceable tool for (a) the routine calculation of structures and properties of systems with medium size of about 100 atoms and (b) the electronic structure description of increasingly large systems with well above 1000 atoms. In this topical review, we presented a set of low-cost methods and mainly focused on the electronic structure part by combining compact orbital basis sets with semi-classical correction potentials. Substantial speed-ups of one to three orders of magnitude can be achieved while keeping the good DFT-D accuracy. This hierarchy of methods is well suited for the every-day calculation on systems of modest to large size and we expect a significant impact on the crystal structure prediction algorithms and on large scale material screenings in general.

2. **J. G. Brandenburg***, C. Bannwarth, A. Hansen, and S. Grimme, *B97-3c: A revised low-cost variant of the B97-D density functional method*, J. Chem. Phys. **2018**, *148*, 064104. [Ref. 33]

   Quantum chemistry meets semi-classical potentials: B97-3c combines a well-established density functional evaluated in compact orbital expansions with correction potentials yielding excellent molecular and condensed phase properties applicable to hundreds of atoms an a single computer node. B97-3c completes the hierarchy of “3c” low-cost electronic structure methods and is implemented in the program packages Crystal, Turbomole, and Orca.

3. L. Iuzzolino, P. McCabeb, S. L. Price, and **J. G. Brandenburg***, *Crystal structure prediction of flexible pharmaceutical-like molecules: Density functional tight-binding as an intermediate optimization method and for free energy estimation*, Faraday Discuss. **2018**, *211*, 275-296. [Ref. 34]

   Successful methodologies for theoretical crystal structure prediction (CSP) on flexible pharmaceutical-like organic molecules explore the lattice energy surface to find a set of plausible crystal structures. The initial search stages of CSP studies use relatively simple lattice energy approximations as hundreds of thousands of minima have to be considered. These generated crystal structures often have poor molecular geometries, as well as inaccurate lattice-energy rankings. Here, we explore how semi-empirical quantum-mechanical methods can generate reasonably accurate but computationally affordable geometries of the crystal structures generated in a search.

4. **J. G. Brandenburg***, J. Potticary, H. A. Sparkes, S. L. Price, and S. R. Hall, *Thermal expansion of carbamazepine: Systematic crystallographic measurements challenge quantum chemical calculations*, J. Phys. Chem. Lett. **2017**, *8*, 4319-4324. [Ref. 29]

   Our colleagues from Bristol challenged us by measuring the anisotropic thermal expansion of the most stable Carbamazepine polymorph, an antiepileptic, antioconvulsant, bipolar disorder treatment drug. This API is used to demonstrate how the thermal expansion can probe certain intermolecular interactions resulting in anisotropic expansion behavior. We show that most structural features can be captured by electronic structure calculations at the quasi-harmonic approximation (QHA) provided a dispersion-corrected density functional based method is employed.

5. A. Zen, **J. G. Brandenburg**, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides*, *Fast and accurate quantum Monte-Carlo for molecular crystals*, Proc. Natl. Acad. Sci. U.S.A. **2018**, *115*, 1724. [Ref. 31]

   Computational approaches based on the fundamental laws of quantum mechanics are now integral to almost all materials design initiatives in academia and industry. If computational materials science is genuinely going to deliver on its promises, then an electronic structure method with consistently high accuracy is urgently needed. We show that, thanks to recent algorithmic advances and the strategy developed in our manuscript, quantum Monte Carlo yields extremely accurate predictions for the lattice energies of materials at a surprisingly modest computational cost. It is thus no longer a technique that requires a world-leading computational facility to obtain meaningful results. While we focus on molecular crystals, the significance of our findings extends to all classes of materials.

Full list of publications:

The following list of publications in peer-reviewed international journals was generated 2019-04-02. The publication status “in press” denotes an accepted manuscript that will be printed in the next journal issue, “submitted” indicates a submitted manuscript that is currently under review, and the star indicates the corresponding author(s). According to the Google scholar database, the total number of citations is 1 505 and the corresponding h-index is 19.

2019

[42] R. J. Maurer, C. Freysoldt, A. M. Reilly, **J. G. Brandenburg**, O. T. Hofmann, T. Björkman, S. Lebègue, A. Tkatchenko*, *Advances in Density-Functional Calculations for Materials Modeling*, Annu. Rev. Mater. Res. **2019**, *49*, 3.1-3.30.

[41] **J. G. Brandenburg**, A. Zen, M. Fitzner, B. Ramberger, G. Kresse, T. Tsatsoulis, A. Grüneis, A. Michaelides, and D. Alfè* *Physisorption of water on graphene: Sub-chemical accuracy from many-body electronic structure methods*, *J. Phys. Chem. Lett.* **2019**, *10*, 358-368.

2018

[40] C. Adjiman, **J. G. Brandenburg**, D. Braun, J. Cole, C. Collins, A. I. Cooper, A. Cruz-Cabeza, G. Day, M. Dudek, A. Hare, L. Iuzzolino, D. McKay, J. Mitchell, S. Mohamed, S. Neelamraju, M. Neumann, S. N. Lill, J. Nyman, A. R. Oganov, S. L. Price, A. Pulido, S. Reutzel-Edens, I. Rietveld, M. T. Ruggiero, C. Schoön, S. Tsuzuki, J. van den Ende, G. Woollam, and Qiang Zhu, *Applications of crystal structure prediction - organic molecular structures: general discussion*, Faraday Discuss. **2018**, *211*, 493-539.

[39] M. Addicoat, C. Adjiman, M. Arhangelskis, G. Beran, D. Bowskill, **J. G. Brandenburg**, D. Braun, V. Burger, J. Cole, A. Cruz-Cabeza, G. Day, V. Deringer, R. Guo, A. Hare, J. Helfferich, J. Hoja, L. Iuzzolino, S. Jobbins, N. Marom, D. McKay, J. Mitchell, S. Mohamed, M. Neumann, S. N. Lill, J. Nyman, A. R. Oganov, P. Piaggi, S. L. Price, S. Reutzel-Edens, I. Rietveld, M. Ruggiero, M. Ryder, G. Sastre, C. Schoön, C. Taylor, A. Tkatchenko, S. Tsuzuki, J. van den Ende, S. Woodley, G. Woollam, and Qiang Zhu, *Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion*, Faraday Discuss. **2018**, *211*, 325-381.

[38] M. Addicoat, C. Adjiman, M. Arhangelskis, G. Beran, **J. G. Brandenburg**, D. Braun, V. Burger, A. Burow, C. Collins, A. Cooper, G. Day, V. Deringer, M. S. Dyer, A. Hare, K. Jelfs, J. Keupp, S. Konstantinopoulos, Y. Li, Y. Ma, N. Marom, D. McKay, C. Mellot-Draznieks, S. Mohamed, M. Neumann, S. N. Lill, J. Nyman, A. R. Oganov, S. L. Price, S. Reutzel-Edens, M. Ruggiero, G. Sastre, R. Schmid, J. Schmidt, C. Schoön, P. Spackman, S. Tsuzuki, S. Woodley, S. Yang, and Qiang Zhu, *Structure searching methods: general discussion*, Faraday Discuss. **2018**, *211*, 133-180.

[37] G. Sansone, A. Karttunen*, D. Usvyat, M. Schuetz, **J. G. Brandenburg***, L. Maschio*, *On the exfoliation and anisotropic thermal expansion of black phosphorus*, Chem. Comm. **2018**, *54*, 9793-9796.

[36] L. Wang, G. Kehr, C. G. Daniliuc, M. Brinkkötter, T. Wiegand, A.-L. Wübker, H. Eckert*, L. Liu, **J. G. Brandenburg**, S. Grimme*, and G. Erker*, *Solid state frustrated Lewis pair chemistry*, Chem. Sci. **2018**, *9*, 4859-4865.

[35] E. Caldeweyher and **J. G. Brandenburg***, *Simplified DFT methods for consistent structures and energies of large systems*, J. Phys.: Condens. Matter **2018**, *30*, 213001.
[Psi-k highlight.]

[34] L. Iuzzolino, P. McCabe, S. L. Price, and **J. G. Brandenburg***, *Crystal structure prediction of flexible pharmaceutical-like molecules: Density functional tight-binding as an intermediate optimization method and for free energy estimation*, Faraday Discuss. **2018**, *211*, s.
[Open access through RCS author choice.]

[33] **J. G. Brandenburg***, C. Bannwarth, A. Hansen, and S. Grimme, *B97-3c: A revised low-cost variant of the B97-D density functional method*, J. Chem. Phys. **2018**, *148*, 064104.
[Open access through AIP editor’s pick 2018.]

[32] M. Mortazavi, **J. G. Brandenburg**, R. J. Maurer*, and A. Tkatchenko*, *Structure and stability of molecular crystals with many body dispersion inclusive density functional tight binding*, J. Phys. Chem. Lett. **2018**, *9*, 399-405.

[31] A. Zen, **J. G. Brandenburg**, J. Klimeš, A. Tkatchenko, D. Alfè, and A. Michaelides*, *Fast and accurate quantum Monte-Carlo for molecular crystals*, Proc. Natl. Acad. Sci. U.S.A. **2018**, *115*, 1724-1729. *[Open access.]*

2017

[30] T. Jensen, J. Potticary, L. R. Terry, H. Bruce-Macdonald, **J. G. Brandenburg**, and S. R. Hall*, *Polymorphism in crystals of bis(4-bromophenyl)fumaronitrile through vapour phase growth*, CrystEngComm **2017**, *19*, 7223-7228.

[29] **J. G. Brandenburg***, J. Potticary, H. A. Sparkes, S. L. Price, and S. R. Hall, *Thermal expansion of carbamazepine: Systematic crystallographic measurements challenge quantum chemical calculations*, J. Phys. Chem. Lett. **2017**, *8*, 4319-4324.
[Open access through ACS author choice.]

[28] Y. S. Al-Hamdani, M. Rossi, D. Alfè, T. Tsatsoulis, B. Ramberger, **J. G. Brandenburg**, A. Zen, G. Kresse, A. Grüneis, A Tkatchenko, and A. Michaelides*, *Properties of the water to boron nitride interaction: from zero to two dimensions with benchmark accuracy*, J. Chem. Phys. **2017**, *147*, 044710.

[27] S. L. Price* and **J. G. Brandenburg**, *Molecular Crystal Structure Prediction*; Non-covalent interactions in Quantum Chemistry and Physics, G. DiLabio, A. Otero-de-la-Roza, Eds., Elsevier Australia, Melbourne, Australia, **2017**, *ISBN: 9780128098356*.

[26] H. Buchholz, R. K. Hylton, **J. G. Brandenburg**, A. Seidel-Morgenstern, H. Lorenz, M. Stein*, and S. L. Price*, *The thermochemistry of racemic and enantiopure molecular crystals for predicting enantiomer separation*, Cryst. Growth. Des. **2017**, *17*, 4676-4686.
[Open access through ACS editor's choice 2017.]

[25] L. Liu, **J. G. Brandenburg**, and S. Grimme*, *On the hydrogen activation by frustrated Lewis pairs in solid state: benchmark studies and theoretical insights*, Phil. Trans. A **2017**, *375* 20170006.

[24] S. A. Katsyubaa*, M. V. Vener, E. E. Zvereva, and **J. G. Brandenburg**, *The role of London dispersion interactions in strong and moderate intermolecular hydrogen bonds in the crystal and in the gas phase*, Chem. Phys. Lett. **2017**, *672*, 124-127.

2016

[23] J. Chen, A. Zen, **J. G. Brandenburg**, D. Alfè, and A. Michaelides*, *Evidence for stable square ice from quantum Monte Carlo*, Phys. Rev. B **2016**, *94*, 220102.

[22] **J. G. Brandenburg***, J. E. Bates, J. Sun, and J. P. Perdew, *Benchmark tests of a strongly constrained semilocal density functional with a long-range dispersion correction*, Phys. Rev. B **2016**, *94*, 115144.

[21] M. Cutini, B. Civalleri, M. Corno, R. Orlando, **J. G. Brandenburg**, L. Maschio, and P. Ugliengo*, *Assessment of different quantum mechanical methods for the prediction of structure and cohesive energy of molecular crystals*, J. Chem. Theory Comput. **2016**, *12*, 3340-3352.

[20] **J. G. Brandenburg***, E. Caldeweyher, and S. Grimme*, *Screened exchange hybrid density functional for accurate and efficient structures and interaction energies*, Phys. Chem. Chem. Phys. **2016**, *18*, 15519-15523.

[19] **J. G. Brandenburg*** and S. Grimme*, *Organic crystal polymorphism: A benchmark for dispersion corrected mean field electronic structure methods*, Acta Cryst. B. **2016**, *72*, 502-513.

[18] A. M. Reilly*, R. I. Cooper, C. S. Adjiman, S. Bhattacharya, D. A. Boese, **J. G. Brandenburg**, P. J. Bygrave, R. Bylsma, J. E. Campbell, R. Car, D. H. Case, R. Chadha, J. C. Cole, K. Cosburn, H. M. Cuppen, F. Curtis, G. M. Day, R. A. DiStasio Jr, A. Dzyabchenko, B. P. van Eijck, D. M. Elking, J. A. van den Ende, J. C. Facelli, M. B. Ferraro, L. Fusti-Molnar, C. Gatsiou, T. S. Gee, R. de Gelder, L. M. Ghiringhelli, H. Goto, S. Grimme, R. Guo, D. W. M. Hofmann, J. Hoja, R. K. Hylton, L. Iuzzolino, W. Jankiewicz, D. T. de Jong, J. Kendrick, N. J. J. de Klerk, H. Ko, L. N. Kuleshova, X. Li, S. Lohani, F. J. J. Leusen, A. M. Lund, J. Lv, Y. Ma, N. Marom, A. E. Masunov, P. McCabe, D. P. McMahon, H. Meekes, M. P. Metz, A. J. Misquitta, S. Mohamed, B. Monserrat, R. J. Needs, M. A. Neumann, J. Nyman, S. Obata, H. Oberhofer, A. R. Oganov, A. M. Orendt, G. I. Pagola, C. C. Pantelides, C. J. Pickard, R. Podeszwa, L. S. Price, S. L. Price, A. Pulido, M. G. Read, K. Reuter, E. Schneider, C. Schober, G. P. Shields, P. Singh, I. J. Sugden, K. Szalewicz, C. R. Taylor, A. Tkatchenko, M. E. Tuckerman, F. Vacarro, M. Vasileiadis, A. Vázquez-Mayagoitia, L. Vogt, Y. Wang, R. E. Watson, G. A. de Wijs, J. Yang, Q. Zhu, C. R. Groom, *Report on the sixth blind test of organic crystal-structure prediction methods*, Acta Cryst. B. **2016**, *72*, 439-459.
[Open access.]

2015

[17] S. Grimme*, A. Hansen, **J. G. Brandenburg**, and C. Bannwarth, *Dispersion-corrected mean-field electronic structure methods*, Chem. Rev. **2016**, *116*, 5105-5154.
[Open access through ACS author choice.]

[16] R. Sure, **J. G. Brandenburg**, and S. Grimme*, *Small atomic orbital basis set first-principles quantum chemical methods for large molecular and periodic systems*, ChemistryOpen **2016**, *5*, 94-109.
[Open access, identified by computational chemistry highlights]

[15] N. Struch, **J. G. Brandenburg**, G. Schnakenburg, N. Wagner, J. Beck, S. Grimme*, and A. Lützen*, *A case study of mechanical strain in supramolecular complexes to manipulate the spin state of iron(II) centres*, Eur. J. Inorg. Chem. **2015**, *33*, 5503-5510

[14] S. A. Katsyuba*, M. V. Vener, E. E. Zvereva, Z. Fei, R. Scopelliti, **J. G. Brandenburg**, S. Sienkevich, and P. J. Dyson, *Quantification of conventional and nonconventional charge-assisted hydrogen bonds in the condensed and gas phases*, J. Phys. Chem. Lett. **2015**, *6*, 4431–4436

[13] S. Grimme*, **J. G. Brandenburg**, C. Bannwarth, and A. Hansen, *Consistent structures and interactions by density functional theory with small basis sets for large molecules*, J. Chem. Phys. **2015**, *143*, 054107.
[Identified by computational chemistry highlights]

[*] **J. G. Brandenburg**, *Development and application of electronic structure methods for noncovalent interactions in organic solids*, Rheinische Friedrich-Wilhelms-Universität Bonn, Dissertation, **2015**, URN: nbn:de:hbz:5n-40608
[Open access through University of Bonn PhD program.]

[12] **J. G. Brandenburg**, T. Maas, and S. Grimme*, *Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs*, J. Chem. Phys. **2015**, *142*, 124104.
[Open access through JCP editor's choice 2016.]

2014

[11] **J. G. Brandenburg**, M. Hochheim, T. Bredow*, and S. Grimme*, *Low-cost quantum chemical methods for non-covalent interactions*, J. Phys. Chem. Lett. **2014**, *5*, 4275–4284.
[Open access through ACS author choice.]

[10] **J. G. Brandenburg**, G. Bender, J. Ren, A. Hansen, S. Grimme*, H. Eckert*, C. G. Daniliuc, G. Kehr, and G. Erker*, *Crystal packing induced carbon-carbon double-triple bond isomerization in a zirconocene complex*, Organometallics **2014**, *33*, 5358–5364.

[9] D. Schweinfurth, S. Demeshko, S. Hohloch, M. Steinmetz, **J. G. Brandenburg**, S. Dechert, F. Meyer, S. Grimme*, and B. Sarkar*, *Spin crossover in Fe (II) and Co (II) complexes with the same click-derived tripodal ligand*, Inorg. Chem. **2014**, *53*, 8203–8212.

[8] F. Malberg, **J. G. Brandenburg**, W. Reckien, O. Hollóczki, S. Grimme*, and B. Kirchner*, *Substitution effect and effect of axle's flexibility at (pseudo-) rotaxanes*, Beilstein J. Org. Chem. **2014**, *10*, 1299–1307.
[Open access]

[7] **J. G. Brandenburg** and S. Grimme*, *Accurate modeling of organic molecular crystals by dispersion-corrected density functional tight-binding (DFTB)*, J. Phys. Chem. Lett. **2014**, *5*, 1785–1789.

[6] **J. G. Brandenburg** and S. Grimme*, *Dispersion corrected Hartree-Fock and density functional theory for organic crystal structure prediction*, Top. Curr. Chem. **2014**, *345*, 1–23.

2013

[5] **J. G. Brandenburg** and S. Grimme*, *A Dispersion-corrected density functional theory case study on ethyl acetate conformers, dimer, and molecular crystal*, Theor. Chem. Acc. **2013**, *132*, 1399.

[4] **J. G. Brandenburg**, M. Alessio, B. Civalleri*, M. F. Peintinger, T. Bredow*, and S. Grimme*, *Geometrical correction for the inter-and intramolecular basis set superposition error in periodic density functional theory calculations*, J. Phys. Chem. A **2013**, *117*, 9282–9292.

[3] B.-H. Xu, K. Bussmann, R. Fröhlich, C. G. Daniliuc, **J. G. Brandenburg**, S. Grimme*, G. Kehr, and G. Erker*, *An enamine/HB(C_6F_5)$_2$ adduct as a dormant state in frustrated Lewis pair chemistry*, Organometallics **2013**, *32*, 6745–6725.

[2] **J. G. Brandenburg**, S. Grimme*, P. G. Jones, G. Markopoulos, H. Hopf, M. K. Cyranski, and D. Kuck*, *Unidirectional molecular stacking of tribenzotriquinacenes in the solid state: A combined x-ray and theoretical study*, Chem. Eur. J. **2013**, *19*, 9930–9938.

[1] **J. G. Brandenburg** and B. V. Fine* *Dimensionality of spin modulations in $1/8$-doped lanthanum cuprates from the perspective of NQR and μSR experiments*, J. Supercond. Nov. Magn. **2013**, *26*, 2621.

Dr. Jan Gerit Brandenburg, Dipl.-Phys. - List of Invited Talks

The following list of presentations consists of contributions to international conferences and invited seminar talks. The contributions to international conferences and workshops are separated into *invited* and *invited plenary talks*. The total number is 28, the presentation decks of all talks starting at 04/2016 (excluding non-published material) can be found at gerit-brandenburg.de.

2019

03/2019 **Seminar at the Max Planck Institute for Polymer Research** Mainz, Germany
Invited Talk on *"Towards the design of molecular materials: Improved quantum mechanical methods for structure and stability prediction"*

01/2019 **MARVEL Mini Series** École Polytechnique Fèdèrale de Lausanne, Switzerland
Invited talk on *"Towards the design of molecular materials"*

01/2019 **Seminar at the Chemistry Department** in Zürich, Switzerland
Invited talk on *"Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods"*

2018

07/2018 **Faraday discussions: Methods and applications of crystal structure prediction** in Cambridge, UK
Invited talk on *"Crystal structure prediction of flexible pharmaceutical-like molecules: DFTB as an intermediate optimization method and for free energy estimation"*

07/2018 **Properties of water at molecular scale workshop** at National Graphene Institute in Manchester, UK
Invited talk on *"Benchmarking the interaction strength between water and graphene"*

06/2018 **Seminar on Special Problems in Quantum Chemistry** at Mulliken Center for Theoretical Chemistry in Bonn, Germany
Invited talk on *"Excitation vs. projection techniques: Towards sub-chemical accuracy for large noncovalent systems"*

05/2018 **Theoretical Chemical Physics Workshop** in Engelberg, Switzerland
Invited talk on *"Many-body electronic structure methods: Sub-chemical accuracy for noncovalent interactions of large systems?"*

03/2018 **EPS Condensed Matter Division and German Physical Society (CMD/DPG) Spring Meeting** in Berlin, Germany
Invited talk on *"Control and prediction of molecular crystal properties by multilevel strategies"*

03/2018 **Thomas Young Center Colloquium** in London, UK
Invited talk on *"Crystal structure prediction of pharmaceutical-like molecules: Fast optimization methods and high-level energies"*

02/2018 **Berufungsverfahren 530** at the Technical University Darmstadt, Germany
Invited talk on *"Control and prediction of molecular & crystal properties by multilevel strategies"*

2017

11/2017 **Seminar at the Solid State Chemistry Center** at the University of Turin, Italy
Invited talk on *"Many-body electronic structure theory: Is Quantum Monte-Carlo affordable for molecular crystals?"*

11/2017 **SFB on *N*-heterocycles as functional materials** in Heidelberg, Germany
Invited talk on *"Predicting properties of molecular crystals by multilevel strategies"*

10/2017 **Alexander von Humboldt foundation network meeting** in Bielefeld, Germany
Invited talk on *"Highly accurate stability prediction at surprisingly modest cost: On the capabilities of quantum Monte-Carlo for molecular crystals"*

06/2017 **Seminar at the Fritz-Haber-Institute of the Max-Planck Society** in Berlin, Germany
Invited talk on *"Molecular crystal polymorph prediction via multilevel strategies"*

05/2017 **Seminar at the Physical Chemistry Institute of the University of Göttingen** in Göttingen, Germany
Invited talk on *"Molecular crystal polymorph prediction via multilevel strategies"*

04/2017 **Alexander von Humboldt foundation network meeting** in Dresden, Germany
Invited talk on *"Towards a new paradigm in molecular crystal polymorph prediction"*

02/2017 **International Sanibel Symposium** in St. Simons Island, Gorgia, USA
Invited plenary talk on *"Density functional theory including van der Waals interaction"*

01/2017 **Seminar at the STFC Rutherford Appleton Laboratory** in Harwell Oxford, UK
Invited talk on *"Thermal properties of organic solids from the quasi-harmonic approximation: Constrasting ab inito phonon spectra with inelastic neutron scattering"*

2016

12/2016 **Seminar at the University Society Bonn council** in Bonn, Germany
Invited talk on *"Vom Gecko bis zur Aspirintablette: Weiterentwicklung von Elektronenstrukturmethoden zur effizienten Modellierung"*

11/2016 **Seminar at the Solid State Chemistry Center** at the University of Turin, Italy
Invited talk on *"Implementation of density functional approximations of screened exchange hybrid and tight-binding types evaluated in local atomic orbitals within CRYSTAL14"*

11/2016 **Seminar at the MPI for Condensed Matter and Materials Physics** in Stuttgart, Germany
Invited talk on *"Development and application of 'low-cost' dispersion corrected density functional methods"*

10/2016 **Seminar at the Centre for Condensed Matter and Materials Physics** at Queen Mary University London, UK
Invited talk on *"Organic crystal modeling: On the importance of accurate London dispersion interactions"*

04/2016 **Thomas Young Center Colloquium** in London, UK
Invited talk on *"Organic crystal modeling: A hierarchy of quantum chemical methods"*

2015

10/2015 **Workshop on Crystal Structure Prediction** in Cambridge, UK
Invited talk on *"The 6^{th} blind test of organic crystal structure prediction: Bridging the gap from FF to DFT"*

07/2015 **International School on Ab initio Modelling of Solids** in Regensburg, Germany
Invited Talk on *"Dispersion-corrected mean-field electronic structure methods"*

07/2015 **GDCh introduces young researcher** in Bonn, Germany
Invited talk on *"Electronic structure methods for organic crystals"*

2014

12/2014 **Theoretical Chemistry Colloquia** in Bochum, Germany
Invited talk on *"Low-cost quantum chemical methods for noncovalent interactions"*

07/2014 **International Conference on Computational and Mathematical Methods in Science and Engineering** in Cádiz, Spain
Invited talk on *"Electronic structure modeling of organic molecular crystals"*