# 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 2020-09-08. 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 2 440 and the corresponding h-index is 23.

### 2020

[50] Y. S. Al-Hamdani, P. Nagy, **J. G. Brandenburg***, A. Tkatchenko*, *Interactions between Large Molecules: Puzzle for Reference Quantum-Mechanical Methods*, **2020**, *submitted*.

[49] B. Monserrat, **J. G. Brandenburg**, E. A. Engel, B. Cheng*, *Liquid water contains the building blocks of diverse ice phases*, **2020**, arxiv:2006.13316 *submitted*.

[48] C. Liu, **J. G. Brandenburg**, O. Valsson, K. Kremer, T. Bereau*, *Free-energy landscape of polymer-crystal polymorphism*, Soft Matter **2020**, *in press*.

[47] L. Doná, **J. G. Brandenburg**, I. J. Bush, B. Civalleri*, *Cost-effective composite methods for large-scale solid-state calculations*, Faraday Discuss. **2020**, *in press*.

[46] A. Afantitis*, G. Melagraki, P. Isigonis, A. Tsoumanis, D. D. Varsou, E. Valsami-Jones, A. Papadiamantis, L. A. Ellis, H. Sarimveis, P. Doganis, P. Karatzas, P. Tsiros, I. Liampa, V. Lobaskin, D. Greco, A. Serra, P. A. S. Kinaret, L. A. Saarimäki, R. Grafström, P. Kohonen, P. Nymark, E. Willighagen, T. Puzyn, A. Rybinska-Fryca, A. Lyubartsev, K. A. Jensen, **J. G. Brandenburg**, S. Lofts, C. Svendsen, S. Harrison, D. Maier, K. Tamm, J. Jänes, L. Sikk, M. Dusinska, E. Longhin, E. Rundén-Pran, E. Mariussen, N. E. Yamani, W. Unger, J. Radnik, A. Tropsha, Y. Cohen, J. Leszczynski, C. O. Hendren, M. Wiesner, D. Winkler, N. Suzuki, T. H. Yoon, J. Choi, N. Sanabria, M. Gulumian, I. Lynch* *Nanosolveit project: driving nanoinformatics research to develop innovative and integrated tools for in silico nanosafety assessment*, Comput. Struct. Biotechnol. J. **2020**, *18*, 583-602.

### 2019

[45] **J. G. Brandenburg***, A. Zen, D. Alfè, A. Michaelides*, *Interaction between water and carbon nanostructures: how good are current density functional approximations?*, J. Chem. Phys. **2019**, *151*, 164702.

[44] L. Doná, **J. G. Brandenburg***, B. Civalleri*, *Extending and assessing composite electronic structure methods to the solid state*, J. Chem. Phys. **2019**, *151*, 121101.

[43] A. Zen, **J. G. Brandenburg**, A. Michaelides, and D. Alfè, *A new scheme for fixed node diffusion quantum monte carlo with pseudopotentials: improving reproducibility and reducing the trial-wave function bias*, J. Chem. Phys. **2019**, *151*, 134105.

[42] R. J. Maurer, C. Freysoldt, A. M. Reilly, **J. G. Brandenburg**, O. T. Hofmann, T. Bjöorkman, S. Lebègue, A. Tkatchenko*, *Advances in Density-Functional Calculations for Materials Modeling*, Annu. Rev. Mater. Res. **2019**, *49*, 1-30.

[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.

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*[Psi-k highlight in press.]*

[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.
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[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.
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[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.

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