Dr. Andreas Hansen

Personal Data

Title	Dr.
First name	Andreas
Name	Hansen
Current position	Akademischer Oberrat (A14)
Current institution(s)/site(s), country	Clausius-Institute of Physical and Theoretical Chemistry, Rheinische Friedrich-Wilhelms-University Bonn, Germany
Identifiers/ORCID	orcid.org/0000-0003-1659-8206

Qualifications and Career

Stages	Periods and Details	
Degree programme	Diploma in Chemistry, 2007, University of Bonn, Germany	
Doctorate	2012	Mentor: F. Neese, MPI for Chemical Energy Conversion, Mülheim a. d. Ruhr, Germany
Stages of academic/professional career	Since 2016	Akademischer Oberrat, Mulliken Center for Theoretical Chemistry, University of Bonn, Germany: Prof. Dr. Stefan Grimme (parental leave 2017 and 2019)
	2013 – 2016	Akademischer Rat, Mulliken Center for Theoretical Chemistry, University of Bonn, Germany: Prof. Dr. Stefan Grimme
	2012 – 2013	Postdoctoral researcher, Mulliken Center for Theoretical Chemistry, University of Bonn, Germany: Prof. Dr. Stefan Grimme

Supplementary Career Information

2 children (*2016, *2018)

Activities in the Research System

Committee involvement & activities in the field of academic self-governance:

2022 – 2023	Temporary chair replacement (sabbatical Prof. Dr. Stefan Grimme), Mulliken Center for Theoretical Chemistry, University of Bonn
2022 – 2024	Senator of the University of Bonn
2021 – 2023	Member of the Steering Committee of TRA Matter, University of Bonn
Since 2021	Digitalization Manager of the Department of Chemistry, University of Bonn
2020 – 2024	Tenure Track Commission, Faculty of Mathematics and Natural Sciences, University of Bonn
2018 – 2024	Member of the Senate Commission for Early Career Scientists, University of Bonn
Since 2015	Safety Representative of the Clausius-Institute of Physical and Theoretical Chemistry, University of Bonn
Since 2014	Room manager and lecture program coordinator of the Department of Chemistry, University of Bonn

Academic Distinctions: Poster Award at the 16th ICQC Congress, Menton, France (2018); NRW Certificate "Professional Teaching Competence for the University" (2016); Ernst-Haage Award of the MPI for Chemical Energy Conversion (2012); Job offer from BASF, Ludwigshafen, Germany (declined) (2012).

Scientific Results

Citations: 16006, h-index: 42, i10-index: 60 (Google Scholar, 21.03.2024)

Category A (* corresponding author)

1. T. Gasevic, M. Bursch*, Q. Ma, S. Grimme, H.-J. Werner*, **A. Hansen*** "The p-block challenge: assessing quantum chemistry methods for inorganic heterocycle dimerizations" *Phys. Chem. Chem. Phys.* **2024**, 26, 13884–13908. DOI: 10.1039/D3CP06217A.
2. C. Plett, S. Grimme, **A. Hansen*** "Conformational energies of biomolecules in solution: Extending the MPCONF196 benchmark with explicit water molecules" *J. Comput. Chem.* **2024**, 45, 419–429. DOI: 10.1002/jcc.27248.
3. H. Neugebauer, H.T. Vuong, J.L. Weber, R.A. Friesner, J. Shee*, **A. Hansen*** "Toward Benchmark-Quality *Ab Initio* Predictions for 3d Transition Metal Electrocatalysts: A Comparison of CCSD(T) and ph-AFQMC" *J. Chem. Theory Comput.* **2023**, 19, 6208–6225. DOI: 10.1021/acs.jctc.3c00617.
4. H.-J. Werner*, **A. Hansen*** "Accurate Calculation of Isomerization and Conformational Energies of Larger Molecules Using Explicitly Correlated Local Coupled Cluster Methods in Molpro and ORCA" *J. Chem. Theory Comput.* **2023**, 19, 7007–7030. DOI: https://doi.org/10.1021/acs.jctc.3c00270.
5. S. Ehlert, S. Grimme, **A. Hansen*** "Conformational Energy Benchmark for Longer *n*-Alkane Chains" *J. Phys. Chem. A* **2022**, 126, 3521–3535. DOI: 10.1021/acs.jpca.2c02439.
6. S. Spicher, C. Plett, P. Pracht, **A. Hansen**, S. Grimme* "Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods" *J. Chem. Theory Comput.* **2022**, 18, 3174–3189. DOI: 10.1021/acs.jctc.2c00239.
7. J. Gorges, S. Grimme, **A. Hansen*** "Reliable prediction of association (free) energies of supramolecular complexes with heavy main group elements – the HS13L benchmark set" *Phys. Chem. Chem. Phys.* **2022**, 24, 28831–28843. DOI: 10.1039/D2CP04049B.
8. J. Gorges, S. Grimme, **A. Hansen***, P. Pracht* "Towards understanding solvation effects on the conformational entropy of non-rigid molecules" *Phys. Chem. Chem. Phys.* **2022**, 24, 12249–12259. DOI: 10.1039/D1CP05805C.
9. L.R. Maurer, M. Bursch, S. Grimme, **A. Hansen*** "Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions" *J. Chem. Theory Comput.* **2021**, 17, 6134–6151. DOI: 10.1021/acs.jctc.1c00659.
10. **A. Hansen**, D.G. Liakos, F. Neese* "Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals" *J. Chem. Phys.* **2011**, 135, 214102. DOI: doi.org/10.1063/1.3663855.

Category B

Publications

1. M. Bursch*, S. Grimme*, **A. Hansen*** “Influence of Steric and Dispersion Interactions on the Thermochemistry of Crowded (Fluoro)alkyl Compounds” *Acc. Chem. Res.* **2024**, 57, 153–163. DOI: 10.1021/acs.accounts.3c00634.
2. M. Bursch*, J.-M. Mewes*, **A. Hansen***, S. Grimme* “Best-Practice DFT Protocols for Basic Molecular Computational Chemistry” *Angew. Chem. Int. Ed.* **2022**, 61, e202205735. DOI: 10.1002/anie.202205735.
3. C. Bannwarth*, E. Caldeweyher, S. Ehlert, **A. Hansen**, P. Pracht, J. Seibert, S. Spicher, S. Grimme* “Extended tight-binding quantum chemistry methods” *WIREs Comput. Mol. Sci.* **2021**, 11, e1493. DOI: 10.1002/wcms.1493.
4. M. Bursch, E. Caldeweyher, **A. Hansen**, H. Neugebauer, S. Ehlert, S. Grimme* “Understanding and Quantifying London Dispersion Effects in Organometallic Complexes” *Acc. Chem. Res.* **2019**, 52, 258–266. DOI: 10.1021/acs.accounts.8b00505.
5. S. Grimme*, **A. Hansen**, J.G. Brandenburg, C. Bannwarth “Dispersion-Corrected Mean-Field Electronic Structure Methods” *Chem. Rev.* **2016**, 116, 5105–5154. DOI: 10.1021/acs.chemrev.5b00533.
6. F. Neese*, **A. Hansen**, F. Wennmohs, S. Grimme “Accurate Theoretical Chemistry with Coupled Pair Models” *Acc. Chem. Res.* **2009**, 42, 641–648. DOI: 10.1021/ar800241t.

Software

1. U. Becker, D. Bykov, D. Ganyushin, **A. Hansen**, R. Izsak, D.G. Liakos, C. Kollmar, S. Kossmann, D.A. Pantazis, T. Petrenko, C. Reimann, C. Riplinger, M. Roemelt, B. Sandhöfer, I. Schapiro, K. Sivalingam, Frank Wennmohs, B. Wezisla, F. Neese “ORCA 2.9” (and other versions). Max-Planck-Institut für Kohlenforschung. https://www.kofo.mpg.de/en/research/services/orca.

   Generic Reference for ORCA:
   F. Neese* “The ORCA program system“ *WIREs Comput. Mol. Sci.* **2012**, 2, 73–78. DOI: 10.1002/wcms.81.