DIRK BAKOWIES

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CURRICULUM VITAE

Personal	Citizenship	Swiss and German
	Languages	German (native), English (near-native proficiency), Italian (good knowledge)
	Degree	Dr. phil.
Employment	2021-	Senior Scientist (Univ. Vienna)
	2016-2020	Senior Scientist (Univ. Basel)
	2008-2016	Privatdozent (ETH Zürich)
	2004-2008	Oberassistent / Staff Scientist (ETH Zürich)
	1998-2004	Postdoc (Prof. van Gunsteren, ETH Zürich)
	1995-1998	Postdoc (Prof. Kollman, UCSF, San Francisco)
	1989-1994	Research assistant (Prof. Thiel, Univs. Wuppertal and Zürich)
Experience	***Research***	Computational chemistry and physics
		Chemical space exploration & quantum machine learning
		Ab initio thermochemistry
		Biomolecular simulation
		Quantum chemistry and quantum/classical embedding
		Efficient models & algorithms for computational chemistry
	Programming	Extensive programming and scripting experience
		Expert knowledge of FORTRAN
		GPU and parallel programming
		High-performance computing
		Contributions to major scientific codes (MNDO, GROMOS)
	Compute services	Linux system administration (scientific compute environments)
	Teaching	Lectures in Chemistry and in Computational Science curricula
		Co-supervision of several semester, master, and Ph.D students

Academic	2008	**Habilitation in Physical Chemistry,** ETH Zürich. *Ab Initio Thermochemistry: Models, Methods, and Perspectives*
	1994	**Dr. phil. in Chemistry,** Univ. Zürich, *summa cum laude*. *Hybrid Models for Combined Quantum Mechanical and Molecular Mechanical Approaches*
	1989	**Diploma in Chemistry,** Univ. Wuppertal, *summa cum laude*. *Semiempirical Calculations on Carbon Clusters*
Student awards	1995	Research scholarship of the German Science Foundation (DFG)
	1991	Award for exceptional graduate research, Hoechst AG, Frankfurt a.M., Germany
	1990	Second prize for best thesis (diploma) across all disciplines and all levels (diploma, Ph.D., habilitation), awarded by the Society of the Friends of the University of Wuppertal, Germany (GFBU)
Publications		Over 35 articles in high-impact journals, several single-author publications, average citation count >80, *h*-index 22 (ISI Web of Science)
Memberships in scientific societies		American Chemical Society German Chemical Society (GDCh)

Peer reviewing services

Chem. Phys. Lett.	J. Mol. Struct.: THEOCHEM
Comput. Geosci.	J. Phys. Chem. (A & B)
Eur. Biophys. J.	Opt. Mater. Express
FEBS Lett.	Org. Lett.
J. Chem. Eng. Data	Proteins
J. Chem. Inf. Model.	Dutch Science Foundation
J. Chem. Phys.	Polish National Science Ctr.
J. Chem. Theory Comput.	HPC programs (CSCS, PRACE)

Compute grants

Swiss National Supercomputing Center:

2018-	- *user project* "Exploring chemical space: The small molecule universe (SMU)"
2016-2018	- *small user project* "Efficient and accurate ab initio thermochemistry of large molecules"
2011-2016	- *development project* "CUDA accelerated classical MD simulations"
2004-2010	- *large user project* "Atomization energies from ab initio calculations without empirical corrections"

Computer management	2017-	Planning, installation, system administration, and maintenance of scientific compute cluster (> 1000 cores) at University of Basel
	2001-2007	Planning, acquisition, installation, system administration, and maintenance of student computer facilities for chemistry serving more than 1000 students over 7 years (ETH Zürich)
Lecturing: Courses	2018-2019	PC IV: Molecular Dynamics and Electronic Structure (Univ. Basel)
	2012-2016	Empirical and Quantum Interaction Models in Molecular Simulation (ETH Zürich)
	2005-2008	Statistical Physics and Computer Simulation (ETH Zürich)
	2001-2005	Computer Oriented Statistical Mechanics (ETH Zürich)

Current Research Activity (Executive Summary)

Chemical space exploration for machine learning

Chemical compounds may be thought of as collections of atoms, connected by bonds that define their structure. An impressive number of them, on the order of 100 million different compounds, have been made in the lab since the early days of chemical synthesis. This number is still dwarfed by serious estimates of how many different molecules are conceivable and small enough to have drug-like structure, a number thought to exceed an astronomical 10^{60}. Clearly, experiment alone cannot explore any significant percentage of this space.

Computational approaches, and accurate quantum chemistry in particular, allow one to predict properties of unknown molecules, but machine learning is needed to expand the collected knowledge and so turn expensive property calculations into inexpensive property queries, needed for any serious attempt to cover significant portions of chemical space.

Our work focuses on the exploration of the “Small Molecule Universe”, a chemical space we define to contain all molecules with up to 8 first-row atoms (C, N, O, F) and hydrogen. Procedures have been devised to enumerate Lewis-valence structure space exhaustively and to generate high-level, reliable reference data from quantum chemistry that so far are largely unavailable. More than a billion semiempirical (lower level) calculations were used for prescreening, and high-level calculations have been performed for millions of molecules. Generated data include thermochemical (ATOMIC-2; protocol developed in refs. 32-35, 37-39), spectroscopic (IR, UV/VIS, NMR), and other properties. The assembly of the database and the design of tools for efficient queries will satisfy growing needs in chemical information and quantum machine learning and it is expected that it marks a major leap forward compared to existing alternatives, both in coverage and data quality. Preliminary results indicate that there exist many experimentally unknown molecules that are more stable thermodynamically than well-known isomers.

Past Research Activity (published)

A. **Semiempirical calculations on large fullerenes**, focusing on aspects of stability and on spectroscopic predictions to aid experimental identification, in an area which at the time emerged as a new branch of chemistry (1-10).

B. **Development of combined quantum/classical (QM/MM) approaches**, focusing on aspects of coupling the "quantum mechanical" regions (QM, electronically important parts of a molecule) with the "classical" or "molecular mechanical" regions (MM, molecular environment) (PhD thesis, 12-13). Such approaches have now become standard tools in computational chemistry.

C. **Development of a graphical molecule editor**, exploiting molecular symmetry to facilitate the definition of suitable starting geometries for complex molecules (appendix to PhD thesis).

D. **Biomolecular simulations**, addressing, e.g., solvent effects on chemical reactivity (14-16), principles of peptide folding, structural properties of membranes, and questions of solvent mobility in large protein cavities (19-21, 24-27, reviews in 17-18, 22-23, 29).

E. **Development of analysis techniques for molecular simulation,** such as a computational geometry based procedure to capture solvent exchange between protein cavities and the environment, and application to fatty acid binding protein (19-20).

F. **Biomolecular simulation software development**, including shared-memory parallel implementations and design of improved pair-list techniques (28) and of GPU force kernels.

G. **High level *ab initio* thermochemistry**, developing procedures to extrapolate correlation energies to complete basis set limits (30-31), designing computationally efficient protocols for thermochemical data that retain high accuracy through *ab initio* isodesmic corrections (ATOMIC, 32-35), developing realistic estimates of model bias and uncertainty (37-38), and introducing further refinements in both accuracy and computational efficiency (ATOMIC-2, 39-40). Applications to larger molecules have identified a surprisingly large number of cases where experiment is likely in error and heats of formation should be revised (38).

List of Publications

Manuscripts

(2) Bakowies, D.; von Lilienfeld, O. A.,
"Enumerating Lewis valence structure space: I. Principles and accurate quantum-chemical data for molecules with up to six first-row atoms (C, N, O, F)"
to be published.

(1) Bakowies, D.; Kohlhoff, K. J.; Yang, E.; Watson, I.; Riley, P. F.; von Lilienfeld, O. A.,
"Quantum properties for 4 million conformers of all stable Lewis graphs with up to seven CNOF atoms: The Small Molecule Universe"
to be published.

Publications

(40) Bakowies, D.,
"ATOMIC-2 protocol for thermochemistry"
J. Chem. Theory Comput. **2022**, *18*, 4142-4163.

(39) Bakowies, D.; von Lilienfeld, O. A.,
"Density functional geometries and zero-point energies in ab initio thermochemical treatments of compounds with first-row atoms (H, C, N, O, F)"
J. Chem. Theory Comput. **2021**, *17*, 4872-4890.

(38) Bakowies, D.,
"Estimating systematic error and uncertainty in ab initio thermochemistry: II. ATOMIC(hc) enthalpies of formation for a large set of hydrocarbons"
J. Chem. Theory Comput. **2020**, *16*, 399-426.

(37) Bakowies, D.,
"Estimating systematic error and uncertainty in ab initio thermochemistry. I. Atomization energies of hydrocarbons in the ATOMIC(hc) protocol"
J. Chem. Theory Comput. **2019**, *15*, 5230-5251.

(36) Tahchieva, D. N.; Bakowies, D.; Ramakrishnan R.; von Lilienfeld, O. A.,
"Torsional potentials of glyoxal, oxalyl halides, and their thiocarbonyl derivatives: Challenges for popular density functional approximations"
J. Chem. Theory Comput. **2018**, *14*, 4806-4817.

(35) Bakowies, D.,
"Simplified wave function models in thermochemical protocols based on bond-separation reactions"
J. Phys. Chem. A, **2014**, *118*,11811-11827.

(34) Bakowies, D.,
"Assessment of density functional theory for thermochemical approaches based on bond separation reactions"
J. Phys. Chem. A **2013**, *117*, 228-243.

(33) Bakowies, D.,
"Ab initio thermochemistry with high-level isodesmic corrections: Validation of the ATOMIC protocol for a large set of compounds with first-row atoms (H, C, N, O, F)"
J. Phys. Chem. A **2009**, *113*, 11517-11534.

(32) Bakowies, D.,
"Ab initio thermochemistry using optimal-balance models with isodesmic corrections: The ATOMIC protocol"
J. Chem. Phys. **2009**, *130*, 144113/1-21.

(31) Bakowies, D.,
"Accurate extrapolation of electron correlation energies from small basis sets"
J. Chem. Phys. **2007**, *127*, 164109/1-12.

(30) Bakowies, D.,
"Extrapolation of electron correlation energies to finite and complete basis set targets"
J. Chem. Phys. **2007**, *127*, 084105/1-23.

(29) van Gunsteren, W. F.; Bakowies, D.; Baron, R. *et al.*,
"Biomolecular modeling: Goals, problems, perspectives"
Angew. Chem. Int. Ed. **2006**, *45*, 4064-4092, *Angew. Chem.* **2006**, *118*, 4168-4198.

(28) Christen, M.; Hünenberger, P. H.; Bakowies, D. *et al.*,
"The GROMOS software for biomolecular simulation: GROMOS05"
J. Comput. Chem. **2005**, *26*, 1719-1751.

(27) Chandrasekhar, I.; Bakowies, D.; Glättli, A.; Hünenberger, P.; Pereira, C.; van Gunsteren, W. F.,
"Molecular dynamics simulation of lipid bilayers with GROMOS96: Application of surface tension"
Mol. Simul. **2005**, *31*, 543-548.

(26) Baron, R.; Bakowies, D.; van Gunsteren, W. F.,
"Principles of carbopeptoid folding: A molecular dynamics simulation study"
J. Peptide Sci. **2005**, *11*, 74-84.

(25) Baron, R.; Bakowies, D.; van Gunsteren, W. F.,
"Carbopeptoid folding: Effects of stereochemistry, chain length, and solvent"
Angew. Chem. Int. Ed. **2004**, *43*, 4055-4059, *Angew. Chem.* **2004**, *116*, 4147-4151.

(24) Daura, X.; Bakowies, D.; Seebach, D.; Fleischhauer, J.; van Gunsteren, W. F.; Krüger, P.,
"Circular dichroism spectra of β-peptides: Sensitivity to molecular structure and effects of motional averaging"
Eur. Biophys. J. **2003**, *32*, 661-670.

(23) Bakowies, D.,
"Biomolecular reality simulations"
Nachr. Chem. **2003**, *51*, 788-793.

(22) Bakowies, D.,
"Trend reports in theoretical chemistry, 2002: Force fields for biomolecular simulations“
Nachr. Chem. **2003**, *51*, 325-327.

(21) Baron, R.; Bakowies, D.; van Gunsteren, W. F.; Daura, X.,
"β-peptides with different secondary-structure preferences: How different are their conformational spaces?"
Helv. Chim. Acta **2002**, *85*, 3872-3882.

(20) Bakowies, D.; van Gunsteren, W. F.,
"Water in protein cavities: A procedure to identify internal water and exchange pathways and application to fatty acid binding protein"
Proteins **2002**, *47*, 534-545.

(19) Bakowies, D.; van Gunsteren, W. F.,
"Simulations of *apo* and *holo*-fatty acid binding protein: Structure and dynamics of protein, ligand and internal water"
J. Mol. Biol. **2002**, *315*, 713-736.

(18) van Gunsteren, W. F.; Bakowies, D.; Bürgi, R. *et al.*,
"Molecular dynamics simulation of biomolecular systems"
Chimia **2001**, *55*, 856-860.

(17) van Gunsteren, W. F.; Bakowies, D.; Damm, W.; Hansson, T; Stocker, U.; Daura, X.,
"Practical aspects of simulation studies of biomolecular systems"
in *Dynamics, structure and function of biological macromolecules*, edited by Jardetzky, O. and Finucane, M., NATO ASI Series A315, IOS Press, Amsterdam, **2001**, pp. 1-26.

(16) Kollman, P. A.; Kuhn, B.; Donini, O.; Peräkylä, M.; Stanton, R.; Bakowies, D.,
"Elucidating the nature of enzyme catalysis utilizing a new twist on an old methodology: Quantum mechanical - free energy calculations on chemical reactions in enzymes and in aqueous solution"
Acc. Chem. Res. **2001**, *34*, 72-79.

(15) Bakowies, D.; Kollman, P. A.,
"Theoretical study of base-catalyzed amide hydrolysis: Gas and aqueous phase hydrolysis of formamide"
J. Am. Chem. Soc. **1999**, *121*, 5712-5726.

(14) Stanton, R. V.; Peräkylä, M.; Bakowies, D.; Kollman, P. A.,
"Combined ab initio and free energy calculations to study reactions in enzymes and solution: Amide hydrolysis in trypsin and aqueous solution"
J. Am. Chem. Soc. **1998**, *120*, 3448-3457.

(13) Bakowies, D.; Thiel, W.,
"Hybrid models for combined quantum mechanical and molecular mechanical approaches"
J. Phys. Chem. **1996**, *100*, 10580-10594.

(12) Bakowies, D.; Thiel, W.,
"Semiempirical treatment of electrostatic potentials and partial charges in combined quantum mechanical and molecular mechanical approaches"
J. Comput. Chem. **1996**, *17*, 87-108.

(11) Bakowies, D.; Bühl, M.; Patchkovskii, S.; Thiel, W.,
"Theoretical studies on giant fullerenes and on endohedral fullerene complexes"
in *Fullerenes: Recent advances in the physics and chemistry of fullerenes and related materials*, Vol. 3, edited by Ruoff, R. S. and Kadish, K. M., The Electrochemical Society, Pennington, NJ, **1996**, pp. 901-910.

(10) Bakowies, D.; Bühl, M.; Thiel, W.,
"A density functional study on the shape of C_{180} and C_{240} fullerenes"
Chem. Phys. Lett. **1995**, *247*, 491-493.

(9) Bakowies, D.; Bühl, M.; Thiel, W.,
"Can large fullerenes be spherical?"
J. Am. Chem. Soc. **1995**, *117*, 10113-10118.

(8) Slanina, Z.; François, J.-P.; Kolb, M.; Bakowies, D.; Thiel, W.,
"Calculated relative stabilities of C_{84}"
Fullerene Sci. Techn. **1993**, *1*, 221-230.

(7) Slanina, Z.; François, J.-P.; Bakowies, D.; Thiel, W.,
"Fullerene C_{78} isomers: Temperature dependence of their calculated relative stabilities"
J. Mol. Struct.: THEOCHEM **1993**, *279*, 213-216.

(6) Bakowies, D.; Kolb, M.; Thiel, W.; Richard, S.; Ahlrichs, R.; Kappes, M. M.,
"Quantum chemical study of C_{84} fullerene isomers"
Chem. Phys. Lett. **1992**, *200*, 411-417.

(5) Bakowies, D.; Gelessus, A.; Thiel, W.,
"Quantum chemical study of C_{78} fullerene isomers"
Chem. Phys. Lett. **1992**, *197*, 324-329.

(4) Slanina, Z.; Adamowicz, L.; Bakowies, D.; Thiel, W.,
"Fullerene C_{50} isomers: Temperature-induced interchange of relative stabilities"
Thermochim. Acta **1992**, *202*, 249-254.

(3) Bakowies, D.; Thiel, W.,
"Theoretical study of Buckminsterfullerene derivatives $C_{60}X_n$ (X=H, F; n = 2, 36, 60)"
Chem. Phys. Lett. **1992**, *192*, 236-242.

(2) Bakowies, D.; Thiel, W.,
"MNDO study of large carbon clusters"
J. Am. Chem. Soc. **1991**, *113*, 3704-3714.

(1) Bakowies, D.; Thiel, W.,
"Theoretical infrared spectra of large carbon clusters"
Chem. Phys. **1991**, *151*, 309-321.

Technical Reports

(3) Bakowies, D.,
"Ab initio thermochemistry of large molecules"
Scientific Report of the Swiss National Supercomputing Centre, **2008**, 32-35.

(2) Bakowies, D.,
"Atomization energies from ab initio calculations without empirical corrections"
Scientific Report of the Swiss National Supercomputing Centre, **2005**, 14-17.

(1) Bakowies, D.,
"Analyzing solvent in protein cavities: Methods and application to fatty acid binding protein"
Annual Report of the Competence Center for Computational Chemistry, ETH Zürich **2003**, 24-43.