# Bernd Engels

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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|---|---|---|---|
| 259 papers | 7,102 citations | 43 h-index | 69 g-index |
| 267 ext. papers | 7,827 ext. citations | 5.8 avg, IF | 5.98 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 259 | Excitation localization in a trimeric perylenediimide macrocycle: Synthesis, theory, and single molecule spectroscopy.. *Journal of Chemical Physics*, **2022**, 156, 044304 | 3.9 | |
| 258 | Wave packet dynamics in an harmonic potential disturbed by disorder: Entropy, uncertainty, and vibrational revivals.. *Journal of Chemical Physics*, **2022**, 156, 054303 | 3.9 | 0 |
| 257 | Accurate Polarization-Resolved Absorption Spectra of Organic Semiconductor Thin Films Using First-Principles Quantum-Chemical Methods: Pentacene as a Case Study.. *Journal of Physical Chemistry Letters*, **2022**, 3726-3731 | 6.4 | 1 |
| 256 | 2-Sulfonylpyrimidines as Privileged Warheads for the Development of Sortase A Inhibitors.. *Frontiers in Molecular Biosciences*, **2021**, 8, 804970 | 5.6 | 1 |
| 255 | Anionic Boron- and Carbon-Based Hetero-Diradicaloids Spanned by a -Phenylene Bridge. *Journal of the American Chemical Society*, **2021**, 143, 3687-3692 | 16.4 | 8 |
| 254 | Fragmentation of isocyanic acid, HNCO, following core excitation and ionization. *Journal of Chemical Physics*, **2021**, 154, 114302 | 3.9 | 1 |
| 253 | Isolation of Neutral, Mono-, and Dicationic B P Rings by Diphosphorus Addition to a Boron-Boron Triple Bond. *Angewandte Chemie - International Edition*, **2021**, 60, 13661-13665 | 16.4 | 4 |
| 252 | Isolierung neutraler, mono- und dikationischer B2P2-Ringe durch Addition eines Diphosphans an eine Bor-Bor-Dreifachbindung. *Angewandte Chemie*, **2021**, 133, 13774-13779 | 3.6 | 1 |
| 251 | Femtosecond dynamics of diphenylpropynylidene in ethanol and dichloromethane. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 254, 119606 | 4.4 | |
| 250 | Reduction and Rearrangement of a Boron(I) Carbonyl Complex. *Angewandte Chemie - International Edition*, **2021**, 60, 2963-2968 | 16.4 | 11 |
| 249 | Isolierung und Reaktivit□eines s-Block-Metall-Antiaromaten. *Angewandte Chemie*, **2021**, 133, 3856-3863 | 3.6 | 5 |
| 248 | Twisting versus Delocalization in CAAC- and NHC-Stabilized Boron-Based Biradicals: The Roles of Sterics and Electronics. *Chemistry - A European Journal*, **2021**, 27, 5160-5170 | 4.8 | 11 |
| 247 | Isolation and Reactivity of an Antiaromatic s-Block Metal Compound. *Angewandte Chemie - International Edition*, **2021**, 60, 3812-3819 | 16.4 | 11 |
| 246 | Reduktion und Umlagerung eines Bor(I)-Carbonylkomplexes. *Angewandte Chemie*, **2021**, 133, 3000-3005 | 3.6 | 4 |
| 245 | Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. *Chemistry - A European Journal*, **2021**, 27, 3407-3419 | 4.8 | 6 |
| 244 | Unexpected formation of a dodecanuclear {CoII6CuII6} nanowheel under ambient conditions: magneto-structural correlations. *Dalton Transactions*, **2021**, 50, 12430-12434 | 4.3 | 2 |
| 243 | Twisting versus Delocalization in CAAC- and NHC-Stabilized Boron-Based Biradicals: The Roles of Sterics and Electronics. *Chemistry - A European Journal*, **2021**, 27, 5056 | 4.8 | |

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| 242 | One- and two-electron reduction of triarylborane-based helical donor-acceptor compounds. *Chemical Science*, **2021**, 12, 11864-11872 | 9.4 | 3 |
| 241 | A Long Residence Time Enoyl-Reductase Inhibitor Explores an Extended Binding Region with Isoenzyme-Dependent Tautomer Adaptation and Differential Substrate-Binding Loop Closure. *ACS Infectious Diseases*, **2021**, 7, 746-758 | 5.5 | 0 |
| 240 | Taming the Antiferromagnetic Beast: Computational Design of Ultrashort Mn-Mn Bonds Stabilized by N-Heterocyclic Carbenes. *Chemistry - A European Journal*, **2021**, 27, 12126-12136 | 4.8 | 2 |
| 239 | Fluorovinylsulfones and -Sulfonates as Potent Covalent Reversible Inhibitors of the Trypanosomal Cysteine Protease Rhodesain: Structure-Activity Relationship, Inhibition Mechanism, Metabolism, and In Vivo Studies. *Journal of Medicinal Chemistry*, **2021**, 64, 12322-12358 | 8.3 | 3 |
| 238 | The Dimethylbismuth Cation: Entry Into Dative Bi-Bi Bonding and Unconventional Methyl Exchange. *Angewandte Chemie - International Edition*, **2021**, 60, 24388-24394 | 16.4 | 2 |
| 237 | Methylbismuth: an organometallic bismuthinidene biradical. *Chemical Science*, **2020**, 11, 7562-7568 | 9.4 | 17 |
| 236 | Oxidation, Coordination, and Nickel-Mediated Deconstruction of a Highly Electron-Rich Diboron Analogue of 1,3,5-Hexatriene. *Angewandte Chemie*, **2020**, 132, 15847-15855 | 3.6 | 2 |
| 235 | Boranediyl- and Diborane(4)-1,2-diyl-Bridged Platinum A-Frame Complexes. *Chemistry - A European Journal*, **2020**, 26, 8518-8523 | 4.8 | 6 |
| 234 | Predicting F NMR Chemical Shifts: A Combined Computational and Experimental Study of a Trypanosomal Oxidoreductase-Inhibitor Complex. *Angewandte Chemie - International Edition*, **2020**, 59, 12669-12673 | 16.4 | 6 |
| 233 | Highly Conjugated Systems Arising from Cannibalistic Hexadehydro-Diels-Alder Couplings: Cleavage of C-C Single and Triple Bonds. *Chemistry - A European Journal*, **2020**, 26, 15989-16000 | 4.8 | 6 |
| 232 | Functionalization of N via Formal 1,3-Haloboration of a Tungsten(0) Dinitrogen Complex. *Chemistry - A European Journal*, **2020**, 26, 16019-16027 | 4.8 | 8 |
| 231 | Predicting 19F NMR Chemical Shifts: A Combined Computational and Experimental Study of a Trypanosomal Oxidoreductase Inhibitor Complex. *Angewandte Chemie*, **2020**, 132, 12769-12773 | 3.6 | 2 |
| 230 | Diborane(4) Azides: Surprisingly Stable Sources of Transient Iminoboranes. *Angewandte Chemie - International Edition*, **2020**, 59, 15480-15486 | 16.4 | 2 |
| 229 | New Cysteine Protease Inhibitors: Electrophilic (Het)arenes and Unexpected Prodrug Identification for the Protease Rhodesain. *Molecules*, **2020**, 25, | 4.8 | 9 |
| 228 | Naphthoquinones as Covalent Reversible Inhibitors of Cysteine Proteases-Studies on Inhibition Mechanism and Kinetics. *Molecules*, **2020**, 25, | 4.8 | 14 |
| 227 | Geometry relaxation-mediated localization and delocalization of excitons in organic semiconductors: A quantum chemical study. *Journal of Chemical Physics*, **2020**, 153, 224104 | 3.9 | 4 |
| 226 | cAAC-Stabilized 9,10-diboraanthracenes-Acenes with Open-Shell Singlet Biradical Ground States. *Angewandte Chemie - International Edition*, **2020**, 59, 19338-19343 | 16.4 | 24 |
| 225 | Spatial Anisotropy of Charge Transfer at Perfluoropentacene-Pentacene (001) Single-Crystal Interfaces and its Relevance for Thin Film Devices. *ACS Applied Materials & Interfaces*, **2020**, 12, 53547-53556 | 8.5 | 4 |

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| 224 | Tuneable reduction of cymantrenylboranes to diborenes or borylene-derived boratafulvenes. *Chemical Communications*, **2020**, 56, 14809-14812 | 5.8 | 2 |
| 223 | Role of Intermolecular Interactions in the Excited-State Photophysics of Tetracene and 2,2?-Ditetracene. *Journal of Physical Chemistry C*, **2020**, 124, 19435-19446 | 3.8 | 2 |
| 222 | cAAC-stabilisierte 9,10-Diboraanthracene offenschalige Singulettbiradikale. *Angewandte Chemie*, **2020**, 132, 19502-19507 | 3.6 | 8 |
| 221 | Oxidation, Coordination, and Nickel-Mediated Deconstruction of a Highly Electron-Rich Diboron Analogue of 1,3,5-Hexatriene. *Angewandte Chemie - International Edition*, **2020**, 59, 15717-15725 | 16.4 | 8 |
| 220 | Lewis-Base Stabilization of the Parent Al(I) Hydride under Ambient Conditions. *Journal of the American Chemical Society*, **2019**, 141, 16954-16960 | 16.4 | 28 |
| 219 | Bond-Strengthening Backdonation in Aminoborylene-Stabilized Aminoborylenes: At the Intersection of Borylenes and Diborenes. *Angewandte Chemie - International Edition*, **2019**, 58, 12893-12897 | 16.4 | 5 |
| 218 | Pentadiynylidene and Its Methyl-Substituted Derivates: Threshold Photoelectron Spectroscopy of R-C-R Triplet Carbon Chains. *Journal of Physical Chemistry A*, **2019**, 123, 2008-2017 | 2.8 | 10 |
| 217 | A time-resolved photoelectron imaging study on isolated tolane: observation of the biradicalic A state. *Physical Chemistry Chemical Physics*, **2019**, 21, 13157-13164 | 3.6 | 4 |
| 216 | Bindungsstkende Rkbindung in Aminoborylen-stabilisierten Aminoborylenen: an der Grenze zwischen Borylenen und Diborenen. *Angewandte Chemie*, **2019**, 131, 13025-13029 | 3.6 | 1 |
| 215 | Excited-State Dynamics in Perylene-Based Organic Semiconductor Thin Films: Theory Meets Experiment. *Journal of Physical Chemistry C*, **2019**, 123, 27561-27572 | 3.8 | 12 |
| 214 | Tuning the Product Spectrum of a Glycoside Hydrolase Enzyme by a Combination of Site-Directed Mutagenesis and Tyrosine-Specific Chemical Modification. *Chemistry - A European Journal*, **2019**, 25, 6533-6541 | 4.8 | 9 |
| 213 | Structural and chemical insights into the covalent-allosteric inhibition of the protein kinase Akt. *Chemical Science*, **2019**, 10, 3573-3585 | 9.4 | 30 |
| 212 | Inhibitor-Induced Dimerization of an Essential Oxidoreductase from African Trypanosomes. *Angewandte Chemie - International Edition*, **2019**, 58, 3640-3644 | 16.4 | 16 |
| 211 | Eine neue Strukturklasse neutraler borhaltiger Diradikale verbrkt ber zwei Kohlenstoffatome. *Angewandte Chemie*, **2019**, 131, 1857-1861 | 3.6 | 7 |
| 210 | Inhibitor-induzierte Dimerisierung einer essentiellen Oxidoreduktase aus afrikanischen Trypanosomen. *Angewandte Chemie*, **2019**, 131, 3679-3683 | 3.6 | 2 |
| 209 | A New Class of Neutral Boron-Based Diradicals Spanned by a Two-Carbon-Atom Bridge. *Angewandte Chemie - International Edition*, **2019**, 58, 1842-1846 | 16.4 | 17 |
| 208 | Nitrogen fixation and reduction at boron. *Science*, **2018**, 359, 896-900 | 33.3 | 632 |
| 207 | Comparison of the periodic slab approach with the finite cluster description of metal-organic interfaces at the example of PTCDA on Ag(110). *Journal of Computational Chemistry*, **2018**, 39, 844-852 | 3.5 | 9 |

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|---|---|---|---|
| 206 | The ortho-benzyne cation is not planar. *Physical Chemistry Chemical Physics*, **2018**, 20, 3988-3996 | 3.6 | 11 |
| 205 | Isolation of diborenes and their 90°-twisted diradical congeners. *Nature Communications*, **2018**, 9, 1197 | 17.4 | 41 |
| 204 | Mechanistical Insights into the Bioconjugation Reaction of Triazolinediones with Tyrosine. *Journal of Organic Chemistry*, **2018**, 83, 10248-10260 | 4.2 | 8 |
| 203 | A model hamiltonian tuned toward high level ab initio calculations to describe the character of excitonic states in perylenebisimide aggregates. *Journal of Computational Chemistry*, **2018**, 39, 1979-1989 | 3.5 | 9 |
| 202 | Unravelling the Dramatic Electrostructural Differences Between N-Heterocyclic Carbene- and Cyclic (Alkyl)(amino)carbene-Stabilized Low-Valent Main Group Species. *Journal of the American Chemical Society*, **2018**, 140, 12580-12591 | 16.4 | 23 |
| 201 | Product-oriented chemical surface modification of a levansucrase (SacB) an ene-type reaction. *Chemical Science*, **2018**, 9, 5312-5321 | 9.4 | 14 |
| 200 | Isolation and Characterization of Crystalline, Neutral Diborane(4) Radicals. *Angewandte Chemie - International Edition*, **2018**, 57, 10752-10755 | 16.4 | 8 |
| 199 | Selective one- and two-electron reductions of a haloborane enabled by a π-withdrawing carbene ligand. *Chemical Communications*, **2018**, 54, 9015-9018 | 5.8 | 7 |
| 198 | Electronic Structure and Excited-State Dynamics of an Arduengo-Type Carbene and its Imidazolone Oxidation Product. *Chemistry - A European Journal*, **2017**, 23, 3084-3090 | 4.8 | 6 |
| 197 | The dimer-approach to characterize opto-electronic properties of and exciton trapping and diffusion in organic semiconductor aggregates and crystals. *Physical Chemistry Chemical Physics*, **2017**, 19, 12604-12619 | 3.6 | 42 |
| 196 | Atomistic Approach To Simulate Processes Relevant for the Efficiencies of Organic Solar Cells as a Function of Molecular Properties. II. Kinetic Aspects. *Journal of Physical Chemistry C*, **2017**, 121, 26-51 | 3.8 | 16 |
| 195 | The electronic character of PTCDA thin films in comparison to other perylene-based organic semi-conductors: ab initio-, TD-DFT and semi-empirical computations of the opto-electronic properties of large aggregates. *Physical Chemistry Chemical Physics*, **2017**, 19, 2434-2448 | 3.6 | 20 |
| 194 | On the applicability of time-dependent density functional theory (TDDFT) and semiempirical methods to the computation of excited-state potential energy surfaces of perylene-based dye-aggregates. *International Journal of Quantum Chemistry*, **2017**, 117, e25337 | 2.1 | 24 |
| 193 | Vibrational Spectroscopy of a Low-Band-Gap Donor–Acceptor Copolymer and Blends. *Journal of Physical Chemistry C*, **2017**, 121, 19543-19547 | 3.8 | 2 |
| 192 | Structure–Property Relationships from Atomistic Multiscale Simulations of the Relevant Processes in Organic Solar Cells. I. Thermodynamic Aspects. *Journal of Physical Chemistry C*, **2017**, 121, 4-25 | 3.8 | 24 |
| 191 | Benchmarking singlet and triplet excitation energies of molecular semiconductors for singlet fission: Tuning the amount of HF exchange and adjusting local correlation to obtain accurate functionals for singlet–triplet gaps. *Chemical Physics*, **2017**, 482, 319-338 | 2.3 | 36 |
| 190 | QM/MM calculations combined with the dimer approach on the static disorder at organic-organic interfaces of thin-film organic solar cells composed of small molecules. *Journal of Physical Organic Chemistry*, **2017**, 30, e3740 | 2.1 | 4 |
| 189 | Theoretical investigation of the interactions between the π-systems of molecular organic semiconductors and an analysis of the contributions of repulsion and electrostatics. *International Journal of Quantum Chemistry*, **2016**, 116, 1138-1152 | 2.1 | 5 |

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| 188 | Quantum Chemical-Based Protocol for the Rational Design of Covalent Inhibitors. *Journal of the American Chemical Society*, **2016**, 138, 8332-5 | 16.4 | 47 |
| 187 | Experimental and theoretical investigations into the stability of cyclic aminals. *Beilstein Journal of Organic Chemistry*, **2016**, 12, 2280-2292 | 2.5 | 15 |
| 186 | Influence of a polarizable surrounding on the electronically excited states of aggregated perylene materials. *Journal of Computational Chemistry*, **2016**, 37, 1601-10 | 3.5 | 11 |
| 185 | A theoretical description of charge reorganization energies in molecular organic P-type semiconductors. *Journal of Computational Chemistry*, **2016**, 37, 1335-44 | 3.5 | 19 |
| 184 | New Algorithms for Global Optimization and Reaction Path Determination. *Methods in Enzymology*, **2016**, 578, 145-67 | 1.7 | 1 |
| 183 | Dipeptidyl Nitroalkenes as Potent Reversible Inhibitors of Cysteine Proteases Rhodesain and Cruzain. *ACS Medicinal Chemistry Letters*, **2016**, 7, 1073-1076 | 4.3 | 31 |
| 182 | Charge carrier mobilities in organic semiconductor crystals based on the spectral overlap. *Journal of Computational Chemistry*, **2016**, 37, 2146-56 | 3.5 | 7 |
| 181 | Comparison of different rate constant expressions for the prediction of charge and energy transport in oligoacenes. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 694-720 | 7.9 | 36 |
| 180 | Macrocyclic cis-Indolenine Squaraine Dyes as Efficient Near Infrared Emitters. *Journal of Physical Chemistry C*, **2015**, 119, 6174-6180 | 3.8 | 7 |
| 179 | Vinyl sulfone building blocks in covalently reversible reactions with thiols. *New Journal of Chemistry* , **2015**, 39, 5841-5853 | 3.6 | 14 |
| 178 | Structure–Property Relationships for Exciton and Charge Reorganization Energies of Dipolar Organic Semiconductors: A Combined Valence Bond Self-Consistent Field and Time-Dependent Hartree-Fock and DFT Study of Merocyanine Dyes. *Journal of Physical Chemistry C*, **2015**, 119, 17602-17611 | 3.8 | 20 |
| 177 | Electron Delocalization in Reduced Forms of 2-(BMes2)pyrene and 2,7-Bis(BMes2)pyrene. *Journal of the American Chemical Society*, **2015**, 137, 6750-3 | 16.4 | 118 |
| 176 | Novel dengue virus NS2B/NS3 protease inhibitors. *Antimicrobial Agents and Chemotherapy*, **2015**, 59, 1100-9 | 5.9 | 80 |
| 175 | Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). *New Journal of Chemistry*, **2015**, 39, 1628-1633 | 3.6 | 10 |
| 174 | Phenylene ethynylene-tethered perylene bisimide folda-dimer and folda-trimer: investigations on folding features in ground and excited states. *Chemistry - A European Journal*, **2015**, 21, 615-30 | 4.8 | 32 |
| 173 | A general ansatz for constructing quasi-diabatic states in electronically excited aggregated systems. *Journal of Chemical Physics*, **2015**, 143, 084106 | 3.9 | 23 |
| 172 | Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. *Journal of Physical Chemistry A*, **2015**, 119, 12876-91 | 2.8 | 22 |
| 171 | Structure–property relationships for 1,7-diphenoxy-perylene bisimides in solution and in the solid state. *Chemical Science*, **2014**, 5, 608-619 | 9.4 | 78 |

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| 170 | Photoisomerization among ring-open merocyanines. II. A computational study. *Journal of Chemical Physics*, **2014**, 140, 224311 | 3.9 | 15 |
| 169 | Theoretical analysis of the relaxation dynamics in perylene bisimide dimers excited by femtosecond laser pulses. *Journal of Physical Chemistry A*, **2014**, 118, 1403-12 | 2.8 | 34 |
| 168 | Nonthermally activated exciton transport in crystalline organic semiconductor thin films. *Physical Review B*, **2014**, 89, | 3.3 | 19 |
| 167 | Singlet Exciton Diffusion in Organic Crystals Based on Marcus Transfer Rates. *Journal of Chemical Theory and Computation*, **2014**, 10, 1242-55 | 6.4 | 49 |
| 166 | CAST: a new program package for the accurate characterization of large and flexible molecular systems. *Journal of Computational Chemistry*, **2014**, 35, 1801-7 | 3.5 | 5 |
| 165 | Multidimensional spectroscopy of photoreactivity. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 4764-9 | 11.5 | 46 |
| 164 | Identification of ultrafast relaxation processes as a major reason for inefficient exciton diffusion in perylene-based organic semiconductors. *Journal of the American Chemical Society*, **2014**, 136, 9327-37 | 16.4 | 45 |
| 163 | Photoisomerization among ring-open merocyanines. I. Reaction dynamics and wave-packet oscillations induced by tunable femtosecond pulses. *Journal of Chemical Physics*, **2014**, 140, 224310 | 3.9 | 25 |
| 162 | Effects of characteristic length scales on the exciton dynamics in rubrene single crystals. *Physical Review B*, **2014**, 90, | 3.3 | 10 |
| 161 | Photoinduced Electron Transfer Dynamics in Triarylamine□Naphthalene Diimide Cascades. *Journal of Physical Chemistry C*, **2014**, 118, 27698-27714 | 3.8 | 12 |
| 160 | Anisotropy of singlet exciton diffusion in organic semiconductor crystals from ab initio approaches. *Journal of Chemical Physics*, **2014**, 140, 024503 | 3.9 | 33 |
| 159 | Protocol for rational design of covalently interacting inhibitors. *ChemPhysChem*, **2014**, 15, 3226-35 | 3.2 | 16 |
| 158 | Cation-□interactions: accurate intermolecular potential from symmetry-adapted perturbation theory. *Journal of Physical Chemistry B*, **2013**, 117, 10093-102 | 3.4 | 34 |
| 157 | Solvent Controlled Energy Transfer Processes in Triarylamine-Triazole Based Dendrimers. *Journal of Physical Chemistry C*, **2013**, 117, 19816-19831 | 3.8 | 18 |
| 156 | Benchmark Study for the Cysteine-Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. *Journal of Chemical Theory and Computation*, **2013**, 9, 1765-77 | 6.4 | 33 |
| 155 | Similarities and differences in the optical response of perylene-based hetero-bichromophores and their monomeric units. *ChemPhysChem*, **2013**, 14, 1413-22 | 3.2 | 7 |
| 154 | The electronic structure of pyracene: a spectroscopic and computational study. *Physical Chemistry Chemical Physics*, **2013**, 15, 8151-61 | 3.6 | 17 |
| 153 | Structure-property relationship of perylene bisimide macrocycles probed by atomic force microscopy and single-molecule fluorescence spectroscopy. *ACS Nano*, **2013**, 7, 5064-76 | 16.7 | 32 |

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| 152 | Ultrafast Exciton Self-Trapping upon Geometry Deformation in Perylene-Based Molecular Aggregates. *Journal of Physical Chemistry Letters*, **2013**, 4, 792-6 | 6.4 | 110 |
| 151 | PathOpt--a global transition state search approach: outline of algorithm. *Journal of Computational Chemistry*, **2013**, 34, 1810-8 | 3.5 | 7 |
| 150 | St□prozesse in organischen Solarzellen. *Chemie in Unserer Zeit*, **2013**, 47, 142-142 | 0.2 | |
| 149 | Clarification on the decarboxylation mechanism in KasA based on the protonation state of key residues in the acyl-enzyme state. *Journal of Physical Chemistry B*, **2013**, 117, 8095-104 | 3.4 | 6 |
| 148 | A New Tabu-Search-Based Algorithm for Solvation of Proteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 814-21 | 6.4 | 11 |
| 147 | Force field-based conformational searches: efficiency and performance for peptide receptor complexes. *Molecular Physics*, **2013**, 111, 2489-2500 | 1.7 | 2 |
| 146 | Multiple reduction of 2,5-bis(borolyl)thiophene: isolation of a negative bipolaron by comproportionation. *Angewandte Chemie - International Edition*, **2013**, 52, 12852-5 | 16.4 | 57 |
| 145 | Can Experimental Electron-Density Studies be Used as a Tool to Predict Biologically Relevant Properties of Low-Molecular Weight Enzyme Ligands?. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2013**, 639, 1905-1921 | 1.3 | 9 |
| 144 | The structure of 5-cyanoindole in the ground and the lowest electronically excited singlet states, deduced from rotationally resolved electronic spectroscopy and ab initio theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 10266-70 | 3.6 | 27 |
| 143 | Oligo(borolyl)benzenes--synthesis and properties. *Chemistry - A European Journal*, **2012**, 18, 14292-304 | 4.8 | 30 |
| 142 | Comparison of the electronic structure of different perylene-based dye-aggregates. *Journal of Computational Chemistry*, **2012**, 33, 1544-53 | 3.5 | 52 |
| 141 | First-principles calculations of anisotropic charge-carrier mobilities in organic semiconductor crystals. *Physical Review B*, **2011**, 83, | 3.3 | 103 |
| 140 | Challenging Problems in Charge Density Determination: Polar Bonds and Influence of the Environment. *Structure and Bonding*, **2011**, 47-97 | 0.9 | 14 |
| 139 | Theoretical and spectroscopic studies on the conformational equilibrium of 9-oxabispidines in solution. *Journal of Molecular Structure*, **2011**, 1005, 178-185 | 3.4 | 9 |
| 138 | Assessment of TD-DFT- and TD-HF-based approaches for the prediction of exciton coupling parameters, potential energy curves, and electronic characters of electronically excited aggregates. *Journal of Computational Chemistry*, **2011**, 32, 1971-81 | 3.5 | 64 |
| 137 | Efficiency of tabu-search-based conformational search algorithms. *Journal of Computational Chemistry*, **2011**, 32, 2245-53 | 3.5 | 22 |
| 136 | The pentaphenylborole-2,6-lutidine adduct: a system with unusual thermochromic and photochromic properties. *Angewandte Chemie - International Edition*, **2011**, 50, 2833-6 | 16.4 | 85 |
| 135 | Paracyclophanes as model compounds for strongly interacting □ systems. Part 2: mono-hydroxy[2.2]paracyclophane. *Physical Chemistry Chemical Physics*, **2011**, 13, 11076-82 | 3.6 | 19 |

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| 134 | Accurate Intermolecular Potentials with Physically Grounded Electrostatics. *Journal of Chemical Theory and Computation*, **2011**, 7, 1791-803 | 6.4 | 58 |
| 133 | Paracyclophanes as model compounds for strongly interacting π-systems, part 3: influence of the substitution pattern on photoabsorption properties. *Journal of Physical Chemistry A*, **2011**, 115, 3583-91 | 2.8 | 12 |
| 132 | A clear correlation between the diradical character of 1,3-dipoles and their reactivity toward ethylene or acetylene. *Journal of the American Chemical Society*, **2010**, 132, 7631-7 | 16.4 | 84 |
| 131 | Paracyclophanes as model compounds for strongly interacting pi-systems. Part 1. Pseudo-ortho-dihydroxy[2.2]paracyclophane. *Physical Chemistry Chemical Physics*, **2010**, 12, 9339-46 | 3.6 | 23 |
| 130 | Predicting the tautomeric equilibrium of acetylacetone in solution. I. The right answer for the wrong reason?. *Journal of Computational Chemistry*, **2010**, 31, 665-70 | 3.5 | 16 |
| 129 | Theoretical study of weak CC double bond coordination in a gold (I) catalyst precursor. *Computational and Theoretical Chemistry*, **2010**, 957, 21-25 | | 29 |
| 128 | Mechanistic study of the reaction of thiol-containing enzymes with alpha,beta-unsaturated carbonyl substrates by computation and chemoassays. *ChemMedChem*, **2010**, 5, 869-80 | 3.7 | 26 |
| 127 | Interaction of (benzylidene-hydrazono)-1,4-dihydropyridines with beta-amyloid, acetylcholine, and butyrylcholine esterases. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 2049-59 | 3.4 | 37 |
| 126 | Density-functional study on the migration of Cd and Te adsorbates on the (001) surface of CdTe. *Physica Status Solidi (B): Basic Research*, **2010**, 247, 937-944 | 1.3 | 2 |
| 125 | 1-Phenyl-1,2-cyclohexadiene: astoundingly high enantioselectivities on generation in a Doering-Moore-Skattebøl reaction and interception by activated olefins. *Chemistry - A European Journal*, **2009**, 15, 11266-72 | 4.8 | 15 |
| 124 | Stable five-membered-ring allenes with second-row elements only: not allenes, but zwitterions. *Angewandte Chemie - International Edition*, **2009**, 48, 1538-9; author reply 1540-2 | 16.4 | 52 |
| 123 | What controls the reactivity of 1,3-dipolar cycloadditions?. *Angewandte Chemie - International Edition*, **2009**, 48, 7968-70 | 16.4 | 81 |
| 122 | Rational design of improved aziridine-based inhibitors of cysteine proteases. *Journal of Physical Chemistry B*, **2009**, 113, 5282-9 | 3.4 | 19 |
| 121 | Origin of the reactivity differences of substituted aziridines: CN vs CC bond breakages. *Journal of Organic Chemistry*, **2009**, 74, 5244-9 | 4.2 | 27 |
| 120 | Tabu search based strategies for conformational search. *Journal of Physical Chemistry A*, **2009**, 113, 11692-705 | 2.8 | 18 |
| 119 | Understanding ground- and excited-state properties of perylene tetracarboxylic acid bisimide crystals by means of quantum chemical computations. *Journal of the American Chemical Society*, **2009**, 131, 15660-8 | 16.4 | 94 |
| 118 | Environmental effects on charge densities of biologically active molecules: do molecule crystal environments indeed approximate protein surroundings?. *Journal of Physical Chemistry B*, **2009**, 113, 5072-82 | 3.4 | 34 |
| 117 | Tautomeric equilibria of 3-formylacetylacetone: low-temperature NMR spectroscopy and ab initio calculations. *Journal of Organic Chemistry*, **2009**, 74, 4878-81 | 4.2 | 10 |

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