Bernd Engels

List of Publications by Citations

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	Nitrogen fixation and reduction at boron. *Science*, **2018**, 359, 896-900	33.3	632
258	Exciton trapping in pi-conjugated materials: a quantum-chemistry-based protocol applied to perylene bisimide dye aggregates. *Journal of the American Chemical Society*, **2008**, 130, 12858-9	16.4	258
257	New algorithms for an individually selecting MR-CI program. *Chemical Physics*, **1997**, 225, 197-202	2.3	146
256	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
255	Si-E (E = N, O, F) bonding in a hexacoordinated silicon complex: new facts from experimental and theoretical charge density studies. *Journal of the American Chemical Society*, **2004**, 126, 5563-8	16.4	114
254	Ultrafast Exciton Self-Trapping upon Geometry Deformation in Perylene-Based Molecular Aggregates. *Journal of Physical Chemistry Letters*, **2013**, 4, 792-6	6.4	110
253	First-principles calculations of anisotropic charge-carrier mobilities in organic semiconductor crystals. *Physical Review B*, **2011**, 83,	3.3	103
252	S=N versus S+-N-: an experimental and theoretical charge density study. *Journal of the American Chemical Society*, **2004**, 126, 1781-93	16.4	103
251	Temporary anions - calculation of energy and lifetime by absorbing potentials: the resonance. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1998**, 31, 4107-4122	1.3	98
250	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
249	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
248	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
247	What controls the reactivity of 1,3-dipolar cycloadditions?. *Angewandte Chemie - International Edition*, **2009**, 48, 7968-70	16.4	81
246	Novel dengue virus NS2B/NS3 protease inhibitors. *Antimicrobial Agents and Chemotherapy*, **2015**, 59, 1100-9	5.9	80
245	On the Accuracy of Theoretically and Experimentally Determined Electron Densities of Polar Bonds. *Journal of Physical Chemistry A*, **2004**, 108, 9442-9452	2.8	80
244	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
243	Recent Developments in Configuration Interaction and Density Functional Theory Calculations of Radical Hyperfine Structure.. *Advances in Quantum Chemistry*, **1996**, 27, 297-369	1.4	77

242	Contribution of Surface Resonances to Scanning Tunneling Microscopy Images: (110) Surfaces of III-V Semiconductors. *Physical Review Letters*, **1996**, 77, 2997-3000	7.4	76
241	Assessment of quantum chemical methods and basis sets for excitation energy transfer. *Chemical Physics*, **2008**, 346, 275-285	2.3	68
240	Comparison between ab initio theory and scanning tunneling microscopy for (110) surfaces of III-V semiconductors. *Physical Review B*, **1998**, 58, 7799-7815	3.3	68
239	A Theoretical Comparison of Two Competing Diradical Cyclizations in Enyne-Allenes: The Myers–Saito and the Novel C2–C6 Cyclization. *Journal of the American Chemical Society*, **1998**, 120, 6356-6361	16.4	67
238	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
237	"Knock-out" analogues as a tool to quantify supramolecular processes: a theoretical study of molecular interactions in guanidiniocarbonyl pyrrole carboxylate dimers. *Journal of the American Chemical Society*, **2005**, 127, 11115-24	16.4	63
236	A comparative ab initio study of the Si2C4, Si3C3, and Si4C2 clusters. *Journal of Chemical Physics*, **1994**, 101, 6790-6799	3.9	60
235	Computational assessment of the electronic structures of cyclohexa-1,2,4-triene, 1-oxacyclohexa-2,3,5-triene (3delta(2)-pyran), their benzo derivatives, and cyclohexa-1,2-diene. An experimental approach to 3delta(2)-pyran. *Journal of the American Chemical Society*, **2002**, 124, 287-97	16.4	59
234	Accurate Intermolecular Potentials with Physically Grounded Electrostatics. *Journal of Chemical Theory and Computation*, **2011**, 7, 1791-803	6.4	58
233	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
232	Two Novel Thermal Biradical Cyclizations of Enyne-Ketenimines: Theory, Experiment, and Synthetic Potential. *Angewandte Chemie - International Edition*, **1998**, 37, 1562-1564	16.4	55
231	Two Novel Thermal Biradical Cyclizations in Theory and Experiment: New Synthetic Routes to 6H-Indolo[2,3-b]quinolines and 2-Aminoquinolines from Enyne-Carbodiimides. *Angewandte Chemie - International Edition*, **1998**, 37, 2371-2373	16.4	53
230	Aziridide-based inhibitors of cathepsin L: synthesis, inhibition activity, and docking studies. *ChemMedChem*, **2006**, 1, 1126-41	3.7	53
229	Theoretical studies about the influence of different ring substituents on the nucleophilic ring opening of three-membered heterocycles and possible implications for the mechanisms of cysteine protease inhibitors. *Journal of Organic Chemistry*, **2005**, 70, 233-7	4.2	53
228	Comparison of the electronic structure of different perylene-based dye-aggregates. *Journal of Computational Chemistry*, **2012**, 33, 1544-53	3.5	52
227	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
226	The importance of the ene reaction for the C(2)-C(6) cyclization of enyne-allenes. *Journal of the American Chemical Society*, **2001**, 123, 5557-62	16.4	52
225	Calculation of hyperfine coupling constants. *Molecular Physics*, **1987**, 62, 109-127	1.7	52

224	Model Calculations about the Influence of Protic Environments on the Alkylation Step of Epoxide, Aziridine, and Thiirane Based Cysteine Protease Inhibitors. *Journal of Physical Chemistry A*, **2004**, 108, 7691-7701	2.8	51
223	On the origin of the stabilization of the zwitterionic resting state of cysteine proteases: a theoretical study. *Journal of the American Chemical Society*, **2008**, 130, 8696-705	16.4	50
222	Singlet Exciton Diffusion in Organic Crystals Based on Marcus Transfer Rates. *Journal of Chemical Theory and Computation*, **2014**, 10, 1242-55	6.4	49
221	Quantum Chemical-Based Protocol for the Rational Design of Covalent Inhibitors. *Journal of the American Chemical Society*, **2016**, 138, 8332-5	16.4	47
220	Multidimensional spectroscopy of photoreactivity. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 4764-9	11.5	46
219	Study of influences of various excitation classes onab initio calculated isotropic hyperfine coupling constants. *Theoretica Chimica Acta*, **1993**, 86, 429-437		46
218	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
217	The hyperfine coupling constants of the X 3Σstates of NH. *Molecular Physics*, **1989**, 67, 583-600	1.7	45
216	Ab initio study of the energy difference between the cyclic and linear forms of the C6 molecule. *Journal of Chemical Physics*, **1994**, 101, 4042-4048	3.9	43
215	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
214	A multireference configuration interaction study of the hyperfine structure of the molecules CCO, CNN, and NCN in their triplet ground states. *Journal of Chemical Physics*, **1994**, 101, 7686-7691	3.9	42
213	Ab initio investigation of the vibronic structure of the C2H spectrum: Computation of the vibronically averaged values for the hyperfine coupling constants. *Journal of Molecular Spectroscopy*, **1991**, 150, 70-85	1.3	42
212	Study of the hyperfine coupling constants of the molecules NH2, NHD and ND2. *Chemical Physics Letters*, **1990**, 172, 180-186	2.5	42
211	Isolation of diborenes and their 90°-twisted diradical congeners. *Nature Communications*, **2018**, 9, 1197	17.4	41
210	Atomistic insights into the inhibition of cysteine proteases: first QM/MM calculations clarifying the stereoselectivity of epoxide-based inhibitors. *Journal of Physical Chemistry B*, **2008**, 112, 11798-808	3.4	41
209	Atomistic insights into the inhibition of cysteine proteases: first QM/MM calculations clarifying the regiospecificity and the inhibition potency of epoxide- and aziridine-based inhibitors. *Journal of Physical Chemistry B*, **2008**, 112, 5458-69	3.4	41
208	A detailed study of the configuration selected multireference configuration interaction method combined with perturbation theory to correct the wave function. *Journal of Chemical Physics*, **1994**, 100, 1380-1386	3.9	40
207	Theoretical study of electron spin resonance parameters: H2CN and H2CO+. *Journal of Chemical Physics*, **1994**, 100, 2936-2942	3.9	39

206	Difficulties in the calculation of electron spin resonance parameters using density functional methods. *Chemical Physics Letters*, **1994**, 230, 398-404	2.5	39
205	Estimation of the influence of the configurations neglected within truncated multi-reference CI wavefunctions on molecular properties. *Chemical Physics Letters*, **1991**, 179, 398-404	2.5	39
204	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
203	The importance of the active site histidine for the activity of epoxide- or aziridine-based inhibitors of cysteine proteases. *ChemMedChem*, **2007**, 2, 120-8	3.7	37
202	Ab initio configuration interaction description of excitation energy transfer between closely packed molecules. *Chemical Physics*, **2008**, 343, 353-361	2.3	37
201	An MRD-CI study of low-lying electronic states in CaF. *Chemical Physics Letters*, **1991**, 176, 407-412	2.5	37
200	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
199	New dyes based on amino-substituted acridizinium salts--synthesis and exceptional photochemical properties. *Chemistry - A European Journal*, **2000**, 6, 2854-64	4.8	36
198	An experimental and computational study on the reactivity and regioselectivity for the nitrosoarene ene reaction: comparison with triazolinedione and singlet oxygen. *Journal of the American Chemical Society*, **2001**, 123, 5542-8	16.4	36
197	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
196	A combined computational and experimental study of the hydrogen-bonded dimers of xanthine and hypoxanthine. *Journal of Physical Chemistry A*, **2005**, 109, 1703-12	2.8	35
195	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
194	Cation-□interactions: accurate intermolecular potential from symmetry-adapted perturbation theory. *Journal of Physical Chemistry B*, **2013**, 117, 10093-102	3.4	34
193	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
192	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
191	Anisotropy of singlet exciton diffusion in organic semiconductor crystals from ab initio approaches. *Journal of Chemical Physics*, **2014**, 140, 024503	3.9	33
190	Ab initio investigation of the vibronic structure of the C2H spectrum: Calculation of the hyperfine coupling constants for the three lowest-lying electronic states. *Journal of Molecular Spectroscopy*, **1991**, 150, 56-69	1.3	33
189	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

188	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
187	Ring size effects in the C2C6 biradical cyclisation of enyne allenes and the relevance for neocarzinostatin. *Perkin Transactions II RSC*, **2001**, 1331-1339		32
186	Geometry and cooperativity effects in adenosine-carboxylic acid complexes. *Journal of the American Chemical Society*, **2005**, 127, 16151-8	16.4	31
185	Dipeptidyl Nitroalkenes as Potent Reversible Inhibitors of Cysteine Proteases Rhodesain and Cruzain. *ACS Medicinal Chemistry Letters*, **2016**, 7, 1073-1076	4.3	31
184	Oligo(borolyl)benzenes--synthesis and properties. *Chemistry - A European Journal*, **2012**, 18, 14292-304	4.8	30
183	Conformational analysis of arginine in gas phase--a strategy for scanning the potential energy surface effectively. *Journal of Computational Chemistry*, **2008**, 29, 407-15	3.5	30
182	Theoretical study of FC2H4. *The Journal of Physical Chemistry*, **1989**, 93, 4462-4470		30
181	Structural and chemical insights into the covalent-allosteric inhibition of the protein kinase Akt. *Chemical Science*, **2019**, 10, 3573-3585	9.4	30
180	Theoretical study of weak CC double bond coordination in a gold (I) catalyst precursor. *Computational and Theoretical Chemistry*, **2010**, 957, 21-25		29
179	Theoretical study of the reaction of alkynes with furan catalyzed by AuCl3 and AuCl. *International Journal of Quantum Chemistry*, **2007**, 107, 359-365	2.1	29
178	On a theoretical model for the Renner Teller effect in tetra-atomic molecules. *Journal of Chemical Physics*, **1996**, 105, 8569-8585	3.9	29
177	Theoretical study of the potential energy surface governing the stereochemistry in chloroethyl radical reactions. *The Journal of Physical Chemistry*, **1990**, 94, 1267-1275		29
176	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
175	On the regioselectivity of the cyclization of enyne-ketenes: a computational investigation and comparison with the Myers-Saito and Schmittel reaction. *Journal of the American Chemical Society*, **2002**, 124, 1823-8	16.4	28
174	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
173	Origin of the reactivity differences of substituted aziridines: CN vs CC bond breakages. *Journal of Organic Chemistry*, **2009**, 74, 5244-9	4.2	27
172	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
171	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

170	Advantages and limitations of Kohn–Sham orbitals as single electron basis for multireference configuration interaction and multireference perturbation theory. *Journal of Chemical Physics*, **2003**, 119, 11591-11601	3.9	25
169	Study of the hyperfine coupling constants (14N and 1H) of the NH2 molecules in the X 2B1 ground state and the A 2A1 excited state. *Journal of Chemical Physics*, **1992**, 96, 4526-4535	3.9	25
168	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
167	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
166	The Stereochemical Course of the Generation and Interception of aSix-Membered Cyclic Allene: 3,4-1H-Naphthalene (2,3-Didehydro-1,2-dihydronaphthalene). *European Journal of Organic Chemistry*, **2006**, 2006, 5045-5058	3.2	24
165	cAAC-Stabilized 9,10-diboraanthracenes-Acenes with Open-Shell Singlet Biradical Ground States. *Angewandte Chemie - International Edition*, **2020**, 59, 19338-19343	16.4	24
164	A general ansatz for constructing quasi-diabatic states in electronically excited aggregated systems. *Journal of Chemical Physics*, **2015**, 143, 084106	3.9	23
163	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
162	Femtosecond dynamics of the tert-butyl radical, t-C4H9. *Journal of Physical Chemistry A*, **2007**, 111, 1771-78	2.8	23
161	Reexchange Controlled Diffusion in Surfactant-Mediated Epitaxial Growth: Si on As-Terminated Si(111). *Physical Review Letters*, **1998**, 80, 2873-2876	7.4	23
160	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
159	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
158	Efficiency of tabu-search-based conformational search algorithms. *Journal of Computational Chemistry*, **2011**, 32, 2245-53	3.5	22
157	Ab initio treatment of the Renner-Teller effect in tetra-atomic molecules undergoing large amplitude bending vibrations. *Chemical Physics*, **1997**, 225, 63-76	2.3	22
156	Individually selecting multi-reference CI and its application to biradicalic cyclizations. *Computers & Chemistry*, **2001**, 25, 15-38		22
155	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
154	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
153	How important is molecular rigidity for the complex stability of artificial host-guest systems? A theoretical study on self-assembly of gas-phase arginine. *Chemistry - A European Journal*, **2007**, 13, 6644-53	4.8	20

152	Ab Initio Study of the Renner-Teller Effect in the X2 Electronic State of B2H+2. *Journal of Molecular Spectroscopy*, **1995**, 171, 494-503	1.3	20
151	Theoretical study of the bridging in halo ethyl. *Computational and Theoretical Chemistry*, **1986**, 138, 59-68		20
150	Nonthermally activated exciton transport in crystalline organic semiconductor thin films. *Physical Review B*, **2014**, 89,	3.3	19
149	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
148	Rational design of improved aziridine-based inhibitors of cysteine proteases. *Journal of Physical Chemistry B*, **2009**, 113, 5282-9	3.4	19
147	Analysis and Deperturbation of the C2 and D2 + States of CaF. *Journal of Molecular Spectroscopy*, **1993**, 161, 303-311	1.3	19
146	A theoretical description of charge reorganization energies in molecular organic P-type semiconductors. *Journal of Computational Chemistry*, **2016**, 37, 1335-44	3.5	19
145	Solvent Controlled Energy Transfer Processes in Triarylamine-Triazole Based Dendrimers. *Journal of Physical Chemistry C*, **2013**, 117, 19816-19831	3.8	18
144	Tabu search based strategies for conformational search. *Journal of Physical Chemistry A*, **2009**, 113, 11692-8705	2.8	18
143	Gradient tabu search. *Journal of Computational Chemistry*, **2007**, 28, 601-11	3.5	18
142	Orbitals from a self-interaction free KohnSham potential as a single electron basis for ab initio methods. *Chemical Physics Letters*, **2002**, 360, 175-181	2.5	18
141	Specific Purine-Purine Base Pairing in Linear Alanyl-Peptide Nucleic Acids. *Helvetica Chimica Acta*, **2000**, 83, 2580-2593	2	18
140	Ab initio investigation of the vibronic spectrum involving the two lowest-lying electronic states of HCCO. *Journal of Chemical Physics*, **1999**, 110, 7802-7810	3.9	18
139	Ab Initio Investigation of the Vibronic and Magnetic Hyperfine Effects in theX2State of[formula]. *Journal of Molecular Spectroscopy*, **1995**, 174, 334-352	1.3	18
138	Methylbismuth: an organometallic bismuthinidene biradical. *Chemical Science*, **2020**, 11, 7562-7568	9.4	17
137	The electronic structure of pyracene: a spectroscopic and computational study. *Physical Chemistry Chemical Physics*, **2013**, 15, 8151-61	3.6	17
136	Structure and dynamics of the silacyclobutane radical cation, studied by ab initio and density functional theory and electron spin resonance spectroscopy. *Journal of Chemical Physics*, **1997**, 107, 297-306	3.9	17
135	New Tabu Search based global optimization methods outline of algorithms and study of efficiency. *Journal of Computational Chemistry*, **2008**, 29, 768-80	3.5	17

134	The hyperfine coupling constants of the five lowest states of CH: An ab initio MRDCI study. *Chemical Physics Letters*, **1988**, 152, 397-401	2.5	17
133	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
132	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
131	Protocol for rational design of covalently interacting inhibitors. *ChemPhysChem*, **2014**, 15, 3226-35	3.2	16
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	Ab Initio Study of the Electronic Spectrum of B2H2. *Journal of Molecular Spectroscopy*, **1997**, 182, 280-94	1.3	16
128	Theoretical study of the ethylene radical cation: geometry and hyperfine structure. *Chemical Physics*, **1998**, 236, 53-61	2.3	16
127	Computational assessment of the electronic structure of 1-azacyclohexa-2,3,5-triene (3 delta 2-1H-pyridine) and its benzo derivative (3 delta 2-1H-quinoline) as well as generation and interception of 1-methyl-3 delta 2-1H-quinoline. *Chemistry - A European Journal*, **2003**, 9, 4641-9	4.8	16
126	Measurement and theoretical simulation of the HCCO□anion photoelectron spectrum. *Journal of Chemical Physics*, **2001**, 115, 1777-1788	3.9	16
125	The hyperfine coupling constants of 19F: An ab initio MRD-CI basis set study. *International Journal of Quantum Chemistry*, **1989**, 36, 255-263	2.1	16
124	Study of the 1s and 2s shell contributions to the isotropic hyperfine coupling constant in nitrogen. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1988**, 21, 3459-3471	1.3	16
123	Inhibitor-Induced Dimerization of an Essential Oxidoreductase from African Trypanosomes. *Angewandte Chemie - International Edition*, **2019**, 58, 3640-3644	16.4	16
122	Photoisomerization among ring-open merocyanines. II. A computational study. *Journal of Chemical Physics*, **2014**, 140, 224311	3.9	15
121	1-Phenyl-1,2-cyclohexadiene: astoundingly high enantioselectivities on generation in a Doering-Moore-Skatteb□reaction and interception by activated olefins. *Chemistry - A European Journal*, **2009**, 15, 11266-72	4.8	15
120	The structure of C6Si. *Chemical Physics Letters*, **1999**, 302, 288-294	2.5	15
119	Ab initio calculations of the vibronically averaged hyperfine coupling constants in the 12□u (X2B1, A2A1) state of the water cation. *Molecular Physics*, **1993**, 80, 1485-1497	1.7	15
118	Experimental and theoretical investigations into the stability of cyclic aminals. *Beilstein Journal of Organic Chemistry*, **2016**, 12, 2280-2292	2.5	15
117	Vinyl sulfone building blocks in covalently reversible reactions with thiols. *New Journal of Chemistry* , **2015**, 39, 5841-5853	3.6	14

116	Challenging Problems in Charge Density Determination: Polar Bonds and Influence of the Environment. *Structure and Bonding*, **2011**, 47-97	0.9	14
115	Comprehensive Model for the Electronic Structures of 1,2,4-Cyclohexatriene and Related Compounds. *Journal of Physical Chemistry A*, **2003**, 107, 11223-11230	2.8	14
114	Ab initio calculation of the vibronically averaged values for the hyperfine coupling constants in NH2, NHD, and ND2. *Journal of Chemical Physics*, **1992**, 97, 4996-5006	3.9	14
113	Naphthoquinones as Covalent Reversible Inhibitors of Cysteine Proteases-Studies on Inhibition Mechanism and Kinetics. *Molecules*, **2020**, 25,	4.8	14
112	Product-oriented chemical surface modification of a levansucrase (SacB) an ene-type reaction. *Chemical Science*, **2018**, 9, 5312-5321	9.4	14
111	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
110	Photoinduced Electron Transfer Dynamics in Triarylamine□Naphthalene Diimide Cascades. *Journal of Physical Chemistry C*, **2014**, 118, 27698-27714	3.8	12
109	Paracyclophanes as model compounds for strongly interacting □-systems, part 3: influence of the substitution pattern on photoabsorption properties. *Journal of Physical Chemistry A*, **2011**, 115, 3583-91	2.8	12
108	Ab initio study of the electronic spectrum of C2H2+.. *Chemical Physics*, **1998**, 238, 33-46	2.3	12
107	Ab initio study of the electronic spectrum of C2H2+: Investigation of structure of spectra involving low-lying doublet electronic states. *Journal of Chemical Physics*, **1998**, 109, 3086-3095	3.9	12
106	Conformation and Hydrogen Bonding Properties of an Aziridinyl Peptide: X-ray Structure Analysis, Raman Spectroscopy and Theoretical Investigations. *Journal of Physical Chemistry A*, **2004**, 108, 11398-11408	2.8	12
105	4- and 4,5-Substituted N-Methoxythiazole-2(3H)-thiones □Preparation,UV/Vis Spectra, and Assignment of Electronic Transitions in Comparison to N-Methoxypyridine-2(1H)-thione Using Time-Dependent Density Functional Theory Calculations. *European Journal of Organic Chemistry*, **2005**, 2005, 869-881	3.2	12
104	Ab Initio Investigation of the Structure of the X2A?, A2A? (12)□Spectral System of HCO: Investigation of the Magnetic Hyperfine Effects. *Journal of Molecular Spectroscopy*, **1994**, 166, 423-440	1.3	12
103	The Influence of Charge Distribution on Bond Lengths in the P4O6 Framework in Compounds of the Type P4O6X. *Angewandte Chemie International Edition in English*, **1994**, 33, 563-565		12
102	Ab initio calculations of the vibronically averaged hyperfine coupling constants for the 1 2□ electronic state of CH2+. *Journal of Chemical Physics*, **1992**, 97, 7629-7636	3.9	12
101	The ortho-benzyne cation is not planar. *Physical Chemistry Chemical Physics*, **2018**, 20, 3988-3996	3.6	11
100	A New Tabu-Search-Based Algorithm for Solvation of Proteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 814-21	6.4	11
99	On the homolytic cleavage of the N,O bond in N-(methoxy)pyridine-2(1H)-thione and N-(methoxy)thiazole-2(3H)-thione in thermally and photochemically induced reactions: a theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 5943-50	2.8	11

98	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
97	Reduction and Rearrangement of a Boron(I) Carbonyl Complex. *Angewandte Chemie - International Edition*, **2021**, 60, 2963-2968	16.4	11
96	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
95	Isolation and Reactivity of an Antiaromatic s-Block Metal Compound. *Angewandte Chemie - International Edition*, **2021**, 60, 3812-3819	16.4	11
94	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
93	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
92	Effects of characteristic length scales on the exciton dynamics in rubrene single crystals. *Physical Review B*, **2014**, 90,	3.3	10
91	Tautomeric equilibria of 3-formylacetylacetone: low-temperature NMR spectroscopy and ab initio calculations. *Journal of Organic Chemistry*, **2009**, 74, 4878-81	4.2	10
90	Ab initio study of the electronic spectrum of C2H2+.. *Chemical Physics*, **1998**, 238, 47-57	2.3	10
89	Unsubstituted bicyclo[1.1.0]but-2-ylcarbinyl cations. *Journal of Organic Chemistry*, **2006**, 71, 1018-26	4.2	10
88	Theoretical investigation of the photochemical C2-C6 cyclisation of enyne-heteroallenes. *Chemistry - A European Journal*, **2003**, 9, 4670-7	4.8	10
87	Ab Initio Investigation of the Hyperfine Structure in the 12Π(X2A1, A2B1) System of BH2. *Journal of Molecular Spectroscopy*, **1994**, 163, 221-237	1.3	10
86	New Cysteine Protease Inhibitors: Electrophilic (Het)arenes and Unexpected Prodrug Identification for the Protease Rhodesain. *Molecules*, **2020**, 25,	4.8	9
85	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
84	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
83	Theoretical and spectroscopic studies on the conformational equilibrium of 9-oxabispidines in solution. *Journal of Molecular Structure*, **2011**, 1005, 178-185	3.4	9
82	A Comparative Study of the Bonding Character in the P4On (n = 6−10) Series by Means of a Vibrational Analysis. *Journal of Physical Chemistry A*, **1998**, 102, 3690-3696	2.8	9
81	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

80	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
79	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
78	Mechanistical Insights into the Bioconjugation Reaction of Triazolinediones with Tyrosine. *Journal of Organic Chemistry*, **2018**, 83, 10248-10260	4.2	8
77	Studies on the stereochemistry of 1,2,6-trimethyl-4-piperidone. *Tetrahedron*, **2005**, 61, 6993-7001	2.4	8
76	An ab initio study of the hyperfine structure in the X2 Pi electronic state of CCCH. *Journal of Chemical Physics*, **2004**, 121, 2636-45	3.9	8
75	Ab initio study of the hyperfine structure of the X2 electronic state of HCCS. *Molecular Physics*, **2004**, 102, 2623-2634	1.7	8
74	Ab initio configuration-interaction studies of the ground state potential energy and hyperfine coupling constants of 35Cl- 2. *Molecular Physics*, **1990**, 69, 549-557	1.7	8
73	cAAC-stabilisierte 9,10-Diboraanthracene offenschalige Singulettbiradikale. *Angewandte Chemie*, **2020**, 132, 19502-19507	3.6	8
72	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
71	Isolation and Characterization of Crystalline, Neutral Diborane(4) Radicals. *Angewandte Chemie - International Edition*, **2018**, 57, 10752-10755	16.4	8
70	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
69	Macrocyclic cis-Indolenine Squaraine Dyes as Efficient Near Infrared Emitters. *Journal of Physical Chemistry C*, **2015**, 119, 6174-6180	3.8	7
68	Similarities and differences in the optical response of perylene-based hetero-bichromophores and their monomeric units. *ChemPhysChem*, **2013**, 14, 1413-22	3.2	7
67	PathOpt--a global transition state search approach: outline of algorithm. *Journal of Computational Chemistry*, **2013**, 34, 1810-8	3.5	7
66	An ab initio study of the vibronic, spin-orbit, and magnetic hyperfine structure in the X2Pi electronic state of NCO. *Journal of Chemical Physics*, **2005**, 122, 144306	3.9	7
65	Charge carrier mobilities in organic semiconductor crystals based on the spectral overlap. *Journal of Computational Chemistry*, **2016**, 37, 2146-56	3.5	7
64	Eine neue Strukturklasse neutraler borhaltiger Diradikale verbrkt ber zwei Kohlenstoffatome. *Angewandte Chemie*, **2019**, 131, 1857-1861	3.6	7
63	Selective one- and two-electron reductions of a haloborane enabled by a withdrawing carbene ligand. *Chemical Communications*, **2018**, 54, 9015-9018	5.8	7

62	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
61	Boranediyl- and Diborane(4)-1,2-diyl-Bridged Platinum A-Frame Complexes. *Chemistry - A European Journal*, **2020**, 26, 8518-8523	4.8	6
60	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
59	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
58	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
57	Study of the P(4)O(7), P(4)O(6)S, and P(4)O(6)Se Vibrational Spectra. *Inorganic Chemistry*, **1997**, 36, 2451-2457	3.1	6
56	Analysis of the Quality of Kohn□Sham Orbitals for Subsequent MRSD-CI Calculations of Excitation Energies. *Zeitschrift Fur Physikalische Chemie*, **2003**, 217, 133-160	3.1	6
55	An ab initio calculation of the anisotropic hyperfine coupling constants in the low-lying vibronic levels of the X 2Pi electronic state of CCCH. *Journal of Chemical Physics*, **2004**, 121, 12361-70	3.9	6
54	An ab initio study of the vibronic, spin□orbit and hyperfine coupling in the X2□electronic state of the CCCD radical. *Chemical Physics Letters*, **2004**, 393, 552-557	2.5	6
53	Theoretical study of the dimethylamino radical (CH3)2N and its protonated cation (CH3)2NH+. *Chemical Physics*, **1994**, 183, 27-36	2.3	6
52	The chemi-ionization reaction O+CH-JHCO++e□Collinear O?CH approach. *Chemical Physics Letters*, **1993**, 204, 333-338	2.5	6
51	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
50	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
49	Theoretical investigation of the interactions between the □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
48	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
47	An ab initio study of the hyperfine structure in the X2 □electronic state of HCCS□alculation of vibronically averaged components of the anizotropic hyperfine tensor. *Molecular Physics*, **2005**, 103, 587-598	1.7	5
46	Isolierung und Reaktivit□eines s-Block-Metall-Antiaromaten. *Angewandte Chemie*, **2021**, 133, 3856-3863	3.6	5
45	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

44	Testing the validity of the conventional resonance model for protonated carbonyl, imine and thiocarbonyl compounds. An Ab initio valence bond study. *Organic Letters*, **2008**, 10, 1951-4	6.2	4
43	DIESEL-MP2: a new program to perform large-scale multireference-MP2 computations. *Journal of Computational Chemistry*, **2006**, 27, 1055-62	3.5	4
42	A quantum chemical investigation of possible intermediates in the reaction of the amidogen and hydroperoxyl radicals. *Journal of Chemical Physics*, **1996**, 105, 8117-8125	3.9	4
41	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
40	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	9.5	4
39	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
38	Reduktion und Umlagerung eines Bor(I)-Carbonylkomplexes. *Angewandte Chemie*, **2021**, 133, 3000-3005	3.6	4
37	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
36	Rational design of substituted N-alkoxypyridine-2(1H)thiones with increased stability against daylight. *Journal of Physical Chemistry A*, **2007**, 111, 3161-5	2.8	3
35	Computer-aided design of promising photochemical alkoxy radical precursors. *Journal of Physical Chemistry A*, **2006**, 110, 12330-7	2.8	3
34	Theoretische Chemie 1998. *Nachrichten Aus Der Chemie*, **1999**, 47, 186-195		3
33	An ab initio determination of the magnetic hyperfine structure of C2 in the four lowest triplet states. *Chemical Physics Letters*, **1996**, 261, 644-650	2.5	3
32	One- and two-electron reduction of triarylborane-based helical donor-acceptor compounds. *Chemical Science*, **2021**, 12, 11864-11872	9.4	3
31	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
30	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
29	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
28	Diborane(4) Azides: Surprisingly Stable Sources of Transient Iminoboranes. *Angewandte Chemie - International Edition*, **2020**, 59, 15480-15486	16.4	2
27	Vibrational Spectroscopy of a Low-Band-Gap Donor–Acceptor Copolymer and Blends. *Journal of Physical Chemistry C*, **2017**, 121, 19543-19547	3.8	2

26	Force field-based conformational searches: efficiency and performance for peptide receptor complexes. *Molecular Physics*, **2013**, 111, 2489-2500	1.7	2
25	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
24	Tuneable reduction of cymantrenylboranes to diborenes or borylene-derived boratafulvenes. *Chemical Communications*, **2020**, 56, 14809-14812	5.8	2
23	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
22	Inhibitor-induzierte Dimerisierung einer essentiellen Oxidoreduktase aus afrikanischen Trypanosomen. *Angewandte Chemie*, **2019**, 131, 3679-3683	3.6	2
21	Unexpected formation of a dodecanuclear {CoII6CuII6} nanowheel under ambient conditions: magneto-structural correlations. *Dalton Transactions*, **2021**, 50, 12430-12434	4.3	2
20	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
19	The Dimethylbismuth Cation: Entry Into Dative Bi-Bi Bonding and Unconventional Methyl Exchange. *Angewandte Chemie - International Edition*, **2021**, 60, 24388-24394	16.4	2
18	Bindungsstärkende Rückbindung in Aminoborylen-stabilisierten Aminoborylenen: an der Grenze zwischen Borylenen und Diborenen. *Angewandte Chemie*, **2019**, 131, 13025-13029	3.6	1
17	Photochemical Reactions of Silylene with Ethene and Silene. *Journal of Physical Chemistry A*, **1997**, 101, 10053-10062	2.8	1
16	Investigations of the Chemical Bonding in the P4O6Sm (m = 0–4) Series by Combination of Experimental and Theoretical Vibrational Analysis. *Journal of Physical Chemistry A*, **1999**, 103, 6214-6219	2.8	1
15	2-Sulfonylpyrimidines as Privileged Warheads for the Development of Sortase A Inhibitors.. *Frontiers in Molecular Biosciences*, **2021**, 8, 804970	5.6	1
14	Fragmentation of isocyanic acid, HNCO, following core excitation and ionization. *Journal of Chemical Physics*, **2021**, 154, 114302	3.9	1
13	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
12	New Algorithms for Global Optimization and Reaction Path Determination. *Methods in Enzymology*, **2016**, 578, 145-67	1.7	1
11	About the Chemistry of Phosphorus Suboxides The authors thank J. Clade, A. Tellenbach, and M. Jansen (Max-Planck-Institut, Stuttgart) for many fruitful discussions. This work was supported by the Deutsche Forschungsgesellschaft (Sonderforschungsbereich 334) and the Fonds der	16.4	1
10	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
9	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

8	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
7	St□prozesse in organischen Solarzellen. *Chemie in Unserer Zeit*, **2013**, 47, 142-142	0.2	
6	Theorie pur: A New Dimension to Quantum Chemistry. Analytic Derivative Methods in Ab Initio Molecular Electronic Structure Theory. Von Y. Yamaguchi, Y. Osamura, J. D. Goddard und H. F. Schaefer III. Oxford University Press, Oxford, 1994. 471 S., geb., 60,- □. ISBN 0-19-507028-3. *Nachrichten Aus Der Chemie*, **1995**, 43, 458-460		
5	Wllenweber: ALBERT Version 1.00 □Experimente ohne Aufbau/Gumm u. Sommer: Einf□rung in die Informatik/Yamagushi, Osamura, Goddard u. Schaefer: A new Dimension to Quantum Chemistry/Gompper: Self-Assembling Amphilic Systems/Chen: Introduction to Scanning Tunneling Microscopy/Herrmann: Ejnar Hertzsprung/Vogel u. Welsch: Lectures on Quantum Optics/Der neue		
4	Excitation localization in a trimeric perylenediimide macrocycle: Synthesis, theory, and single molecule spectroscopy.. *Journal of Chemical Physics*, **2022**, 156, 044304	3.9	
3	Femtosecond dynamics of diphenylpropynylidene in ethanol and dichloromethane. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 254, 119606	4.4	
2	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	
1	Which Structural Elements Are Relevant for the Efficacy of Neocarzinostatin? We thank Prof. Dr. M. Schmittel who brought this problem to our attention. P.W.M. thanks the Stiftung Stipendien-Fonds des Verbandes der Chemischen Industrie for a graduate scholarship.. *Angewandte Chemie - International Edition*, **2001**, 40, 3833-3836	16.4	