Willem Klopper

List of Publications by Year in Descending Order

306 papers	20,483 citations	66 h-index	135 g-index
334 ext. papers	21,912 ext. citations	4.3 avg, IF	6.84 L-index

#	Paper	IF	Citations
306	Investigation of the Coordination Chemistry of a Bisamidinate Ferrocene Ligand with Cu, Ag, and Au.. *ACS Omega*, **2022**, 7, 4683-4693	3.9	
305	Molecular point groups and symmetry in external magnetic fields. *Journal of Chemical Physics*, **2021**, 155, 201101	3.9	1
304	The GW/BSE Method in Magnetic Fields.. *Frontiers in Chemistry*, **2021**, 9, 746162	5	2
303	Structures of Small Tantalum Cluster Anions: Experiment and Theory. *Journal of Physical Chemistry A*, **2021**, 125, 3135-3145	2.8	4
302	Investigation of Luminescent Triplet States in Tetranuclear Cu Complexes: Thermochromism and Structural Characterization. *Chemistry - A European Journal*, **2021**, 27, 5439-5452	4.8	12
301	Effects of rotational conformation on electronic properties of 4,4?-bis(carbazol-9-yl)biphenyl (CBP): the single-molecule picture and beyond. *Molecular Physics*, **2021**, 119, e1876936	1.7	0
300	18-Crown-6 Coordinated Metal Halides with Bright Luminescence and Nonlinear Optical Effects. *Journal of the American Chemical Society*, **2021**, 143, 798-804	16.4	17
299	Chiral Resolution of Spin-Crossover Active Iron(II) [2x2] Grid Complexes. *Chemistry - A European Journal*, **2021**, 27, 15171-15179	4.8	2
298	Versatile Heteroleptic Cu(I) Complexes Based on Quino(xa)-line-Triazole Ligands: from Visible-Light Absorption and Cooperativity to Luminescence and Photoredox Catalysis. *European Journal of Inorganic Chemistry*, **2021**, 2021, 4074	2.3	0
297	Time-Resolved Spectroscopy and Electronic Structure of Mono-and Dinuclear Pyridyl-Triazole/DPEPhos-Based Cu(I) Complexes. *Chemistry - A European Journal*, **2021**, 27, 15251-15270	4.8	1
296	Bright Luminescence in Three Phases-A Combined Synthetic, Spectroscopic and Theoretical Approach. *Angewandte Chemie - International Edition*, **2021**, 60, 23365-23372	16.4	5
295	Bright Luminescence in Three PhasesÅ Combined Synthetic, Spectroscopic and Theoretical Approach. *Angewandte Chemie*, **2021**, 133, 23553	3.6	0
294	Bi- and trinuclear coinage metal complexes of a PNNP ligand featuring metallophilic interactions and an unusual charge separation. *Dalton Transactions*, **2021**, 50, 13412-13420	4.3	4
293	The first microsolvation step for furans: New experiments and benchmarking strategies. *Journal of Chemical Physics*, **2020**, 152, 164303	3.9	14
292	Structural Characterization and Lifetimes of Triple-Stranded Helical Coinage Metal Complexes: Synthesis, Spectroscopy and Quantum Chemical Calculations. *Chemistry - A European Journal*, **2020**, 26, 10743-10751	4.8	3
291	Structural Phase Transition of Ruthenium Cluster Hydrides. *Journal of Physical Chemistry C*, **2020**, 124, 14306-14315	3.8	3
290	Computation of Electromagnetic Properties of Molecular Ensembles. *ChemPhysChem*, **2020**, 21, 878-887	3.2	13

289	Quasirelativistic two-component core excitations and polarisabilities from a damped-response formulation of the Bethe–Salpeter equation. *Molecular Physics*, **2020**, 118, e1755064	1.7	17
288	Synthesis of New Donor-Substituted Biphenyls: Pre-ligands for Highly Luminescent (C^C^D) Gold(III) Pincer Complexes. *Chemistry - A European Journal*, **2020**, 26, 17156-17164	4.8	8
287	[BMIm][Mn(CO)(GeI)]: Carbonyl Compound with an {MnGe} Cluster Unit. *Inorganic Chemistry*, **2020**, 59, 12895-12902	5.1	1
286	Efficient evaluation of three-centre two-electron integrals over London orbitals. *Molecular Physics*, **2020**, 118, e1736675	1.7	15
285	Werner Kutzelnigg – Full of ideas. *Molecular Physics*, **2020**, 118, e1749954	1.7	
284	Discovery of a size-record breaking green-emissive fluorophore: small, smaller, HINA. *Chemical Science*, **2020**, 12, 1392-1397	9.4	3
283	Photoinitiated Charge Transfer in a Triangular Silver(I) Hydride Complex and Its Oxophilicity. *Chemistry - A European Journal*, **2019**, 25, 11176	4.8	2
282	Highly soluble fluorine containing Cu(i) AlkylPyrPhos TADF complexes. *Dalton Transactions*, **2019**, 48, 15687-15698	4.3	20
281	Explicitly Correlated Dispersion and Exchange Dispersion Energies in Symmetry-Adapted Perturbation Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 5965-5986	6.4	5
280	The extended explicitly-correlated second-order approximate coupled-cluster singles and doubles ansatz suitable for response theory. *Journal of Chemical Physics*, **2019**, 150, 184110	3.9	2
279	Ionized, electron-attached, and excited states of molecular systems with spin-orbit coupling: Two-component GW and Bethe-Salpeter implementations. *Journal of Chemical Physics*, **2019**, 150, 204116	3.9	30
278	GW quasiparticle energies of atoms in strong magnetic fields. *Journal of Chemical Physics*, **2019**, 150, 214112	3.9	10
277	Photoinitiated Charge Transfer in a Triangular Silver(I) Hydride Complex and Its Oxophilicity. *Chemistry - A European Journal*, **2019**, 25, 11269-11284	4.8	3
276	[Pb{Mn(CO)}][AlCl]: a lead-manganese carbonyl with AlCl-linked PbMn clusters. *Dalton Transactions*, **2019**, 48, 4696-4701	4.3	10
275	Excited state vibrational coherence in a binuclear metal adduct: wave packet phase dependant molecular fragmentation under variation of ligand size. *EPJ Web of Conferences*, **2019**, 205, 09019	0.3	
274	Accuracy Assessment of GW Starting Points for Calculating Molecular Excitation Energies Using the Bethe-Salpeter Formalism. *Journal of Chemical Theory and Computation*, **2018**, 14, 2127-2136	6.4	49
273	Vibronic Coupling Analysis of the Ligand-Centered Phosphorescence of Gas-Phase Gd(III) and Lu(III) 9-Oxophenalen-1-one Complexes. *Journal of Physical Chemistry A*, **2018**, 122, 2461-2467	2.8	4
272	Vibrational Coherence Controls Molecular Fragmentation: Ultrafast Photodynamics of the [AgCl] Scaffold. *Journal of Physical Chemistry Letters*, **2018**, 9, 804-810	6.4	10

271	Ge{Fe(CO)}(μ): a germanium-iron cluster with Ge, Ge and Ge units. *Chemical Communications*, **2018**, 54, 1217-1220	5.8	10
270	The furan microsolvation blind challenge for quantum chemical methods: First steps. *Journal of Chemical Physics*, **2018**, 148, 014301	3.9	34
269	Bethe-Salpeter correlation energies of atoms and molecules. *Journal of Chemical Physics*, **2018**, 149, 144106	3.9	16
268	Communication: A hybrid Bethe-Salpeter/time-dependent density-functional-theory approach for excitation energies. *Journal of Chemical Physics*, **2018**, 149, 101101	3.9	17
267	Correlation of the structural information obtained for europium-chelate ensembles from gas-phase photoluminescence and ion-mobility spectroscopy with density-functional computations and ligand-field theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 6105-6112	3.6	6
266	Quasi-relativistic two-component computations of intermolecular dispersion energies. *Molecular Physics*, **2017**, 115, 2775-2781	1.7	9
265	Natural transition orbitals for the calculation of correlation and excitation energies. *Chemical Physics Letters*, **2017**, 679, 52-59	2.5	20
264	The Structure of Diphenyl Ether-Methanol in the Electronically Excited and Ionic Ground States: A Combined IR/UV Spectroscopic and Theoretical Study. *ChemPhysChem*, **2017**, 18, 3634-3641	3.2	6
263	Computational Study of the Molecular Structure and Hydrogen Bonding in the Hamilton Wedge/Cyanuric Acid Binding Motif. *ChemPhysChem*, **2017**, 18, 3352-3359	3.2	1
262	Ultrafast excited-state relaxation of a binuclear Ag(i) phosphine complex in gas phase and solution. *Physical Chemistry Chemical Physics*, **2017**, 19, 22785-22800	3.6	12
261	Communication: Symmetry-adapted perturbation theory with intermolecular induction and dispersion energies from the Bethe-Salpeter equation. *Journal of Chemical Physics*, **2017**, 147, 181101	3.9	21
260	A Dinuclear Gold(I) Bis(Carbene) Complex Based on a Ditopic Cyclic (Aryl)(Amino)Carbene Framework. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2016**, 642, 1320-1328	1.3	10
259	A Boron-Fluorinated Tris(pyrazolyl)borate Ligand ((F) Tp*) and Its Mono- and Dinuclear Copper Complexes [Cu((F) Tp*)2] and [Cu2 ((F) Tp*)2]: Synthesis, Structures, and DFT Calculations. *Chemistry - A European Journal*, **2016**, 22, 7935-43	4.8	11
258	Gas-Phase Photoluminescence Characterization of Stoichiometrically Pure Nonanuclear Lanthanoid Hydroxo Complexes Comprising Europium or Gadolinium. *Inorganic Chemistry*, **2016**, 55, 3316-23	5.1	9
257	UV fragmentation and ultrafast dynamics of trinuclear silver/1-methylthymine and silver/1-methyluracil metal-base pairs in an ion trap. *Chemical Physics Letters*, **2016**, 659, 55-60	2.5	3
256	Accurate dissociation energies of two isomers of the 1-naphthol?cyclopropane complex. *Journal of Chemical Physics*, **2016**, 145, 164304	3.9	14
255	Communication: A simplified coupled-cluster Lagrangian for polarizable embedding. *Journal of Chemical Physics*, **2016**, 144, 041101	3.9	6
254	Differential Many-Body Cooperativity in Electronic Spectra of Oligonuclear Transition-Metal Complexes. *ChemPhysChem*, **2016**, 17, 37-45	3.2	14

253	Experimental and Theoretical Determination of Dissociation Energies of Dispersion-Dominated Aromatic Molecular Complexes. *Chemical Reviews*, **2016**, 116, 5614-41	68.1	50
252	Approaching Phosphorescence Lifetimes in Solution: The Two-Component Polarizable-Embedding Approximate Coupled-Cluster Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 2853-60	6.4	9
251	Photophysical Properties of Benzoylgermane and para-Substituted Derivatives: Substituent Effects on Electronic Transitions. *ChemPhysChem*, **2016**, 17, 3460-3469	3.2	15
250	Explicitly-correlated ring-coupled-cluster-doubles theory: Including exchange for computations on closed-shell systems. *Chemical Physics*, **2016**, 479, 160-169	2.3	3
249	Unprecedented pseudo-ortho and ortho metallation of [2.2]paracyclophanes--a methyl group matters. *Chemical Communications*, **2015**, 51, 4793-5	5.8	14
248	Ab Initio Study of the Adsorption of Small Molecules on Metal-Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. *Inorganic Chemistry*, **2015**, 54, 8251-63	5.1	43
247	Modeling the Histidine-Phenylalanine Interaction: The NH□□□Hydrogen Bond of Imidazole□Benzene. *Journal of Physical Chemistry B*, **2015**, 119, 7778-90	3.4	22
246	Coupled-cluster reference values for the GW27 and GW100 test sets for the assessment of GW methods. *Molecular Physics*, **2015**, 113, 1952-1960	1.7	57
245	Time-resolved IR spectroscopy of a trinuclear palladium complex in solution. *Physical Chemistry Chemical Physics*, **2015**, 17, 14138-44	3.6	22
244	Non-covalent Interactions of CO□with Functional Groups of Metal-Organic Frameworks from a CCSD(T) Scheme Applicable to Large Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 1574-84	6.4	24
243	[(Pb6I8){Mn(CO)5}6](2-): an octahedral (M6X8)-like cluster with inverted bonding. *Inorganic Chemistry*, **2015**, 54, 3989-94	5.1	13
242	Explicitly correlated ring-coupled-cluster-doubles theory. *Journal of Chemical Physics*, **2015**, 142, 194106	3.9	8
241	Description of spin-orbit coupling in excited states with two-component methods based on approximate coupled-cluster theory. *Journal of Chemical Physics*, **2015**, 142, 104109	3.9	17
240	Tris(3,5-dimethylpyrazolyl)methane-based heterobimetallic complexes that contain Zn - and Cd - transition-metal bonds: synthesis, structures, and quantum chemical calculations. *Chemistry - A European Journal*, **2015**, 21, 2905-14	4.8	14
239	Activation enthalpies and entropies of the atropisomerization of substituted butyl-bridged biphenyls. *Physical Chemistry Chemical Physics*, **2015**, 17, 11165-73	3.6	9
238	Accurate atomization energies from combining coupled-cluster computations with interference-corrected explicitly correlated second-order perturbation theory. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	26
237	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
236	Substitutional photoluminescence modulation in adducts of a europium chelate with a range of alkali metal cations: a gas-phase study. *Journal of Physical Chemistry A*, **2014**, 118, 94-102	2.8	12

235	Coinage Metal Complexes of Tris(pyrazolyl)methanide-Based Redox-Active Metalloligands. *Organometallics*, **2014**, 33, 941-951	3.8	25
234	In-depth exploration of the photophysics of a trinuclear palladium complex. *Physical Chemistry Chemical Physics*, **2014**, 16, 8332-8	3.6	9
233	Characterization of Nonanuclear Europium and Gadolinium Complexes by Gas-Phase Luminescence Spectroscopy. *Journal of Physical Chemistry Letters*, **2014**, 5, 1727-31	6.4	12
232	Mechanochemistry: the effect of dynamics. *Journal of Physical Chemistry A*, **2014**, 118, 7683-94	2.8	19
231	Effect of Proton Substitution by Alkali Ions on the Fluorescence Emission of Rhodamine B Cations in the Gas Phase. *Journal of Physical Chemistry A*, **2014**, 118, 3787-3794	2.8	19
230	Oriented circular dichroism analysis of chiral surface-anchored metal-organic frameworks grown by liquid-phase epitaxy and upon loading with chiral guest compounds. *Chemistry - A European Journal*, **2014**, 20, 9879-82	4.8	51
229	Accurate computations of the structures and binding energies of the imidazole. *Chemical Physics*, **2014**, 441, 17-22	2.3	19
228	Turbomole. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 91-100	7.9	710
227	ortho-Perfluoroalkylation and ethoxycarbonyldifluoromethylation of aromatic triazenes. *Journal of Organic Chemistry*, **2013**, 78, 7938-48	4.2	54
226	Systematic construction of complementary auxiliary basis sets from and for atomic natural orbitals. *Molecular Physics*, **2013**, 111, 2585-2593	1.7	
225	Accurate non-covalent interactions with basis-set corrections from interference-corrected perturbation theory: comparison with the S22B database. *Molecular Physics*, **2013**, 111, 2299-2305	1.7	14
224	Robust fitting techniques in the chain of spheres approximation to the Fock exchange: The role of the complementary space. *Journal of Chemical Physics*, **2013**, 139, 094111	3.9	59
223	Electron tunneling from electronically excited states of isolated bisdisulizole-derived trianion chromophores following UV absorption. *Physical Chemistry Chemical Physics*, **2013**, 15, 6726-36	3.6	15
222	Quantification of intramolecular cooperativity in polynuclear spin crossover Fe(II) complexes by density functional theory calculations. *Physical Chemistry Chemical Physics*, **2013**, 15, 15450-8	3.6	14
221	Intrinsic fluorescence properties of rhodamine cations in gas-phase: triplet lifetimes and dispersed fluorescence spectra. *Physical Chemistry Chemical Physics*, **2013**, 15, 8162-70	3.6	29
220	Single and Multiple Additions of Dibenzoylmethane onto Buckminsterfullerene. *European Journal of Organic Chemistry*, **2013**, 2013, 7907-7913	3.2	9
219	Synthesis, structure, and characterization of dinuclear copper(I) halide complexes with P^N ligands featuring exciting photoluminescence properties. *Inorganic Chemistry*, **2013**, 52, 2292-305	5.1	282
218	Atropisomerization of di-para-substituted propyl-bridged biphenyl cyclophanes. *Organic and Biomolecular Chemistry*, **2013**, 11, 110-8	3.9	20

217	Communication: explicitly-correlated second-order correction to the correlation energy in the random-phase approximation. *Journal of Chemical Physics*, **2013**, 138, 181104	3.9	8
216	Communication: Extension of a universal explicit electron correlation correction to general complete active spaces. *Journal of Chemical Physics*, **2013**, 138, 211101	3.9	7
215	Communication: two-component ring-coupled-cluster computation of the correlation energy in the random-phase approximation. *Journal of Chemical Physics*, **2013**, 139, 191102	3.9	6
214	Tethering for selective synthesis of 2,2'-biphenols: the acetal method. *Chemistry - A European Journal*, **2013**, 19, 17827-35	4.8	16
213	A composite density fitting + numerical integration approximation for electron-repulsion integrals. *Molecular Physics*, **2013**, 111, 1129-1142	1.7	5
212	Benchmarking the lithium-thiophene complex. *ChemPhysChem*, **2013**, 14, 708-15	3.2	14
211	A universal explicit electron correlation correction applied to Mukherjee's multi-reference perturbation theory. *Chemical Physics Letters*, **2012**, 531, 247-251	2.5	20
210	Theoretical reference values for the AE6 and BH6 test sets from explicitly correlated coupled-cluster theory. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	29
209	New accurate reference energies for the G2/97 test set. *Journal of Chemical Physics*, **2012**, 136, 164102	3.9	40
208	Structure revision of plakotenin based on computational investigation of transition states and spectroscopic properties. *Journal of the American Chemical Society*, **2012**, 134, 2154-60	16.4	8
207	The plakotenins: biomimetic Diels-Alder reactions, total synthesis, structural investigations, and chemical biology. *Chemistry - A European Journal*, **2012**, 18, 15004-20	4.8	4
206	[XIm][FeI(CO)3(SnI3)2] (XIm: EMIm, EHIm, PMIm) containing a barbell-shaped FeSn2-carbonyl complex. *Dalton Transactions*, **2012**, 41, 10605-11	4.3	9
205	[{Fe(CO)3}4{SnI}6I4]2-: the first bimetallic adamantane-like cluster. *Chemistry - A European Journal*, **2012**, 18, 13600-4	4.8	14
204	[2.2]Paracyclophanediyldiphosphane Complexes of Gold. *European Journal of Inorganic Chemistry*, **2012**, 2012, 5033-5042	2.3	30
203	Explicitly correlated electrons in molecules. *Chemical Reviews*, **2012**, 112, 4-74	68.1	419
202	Calculation of the two-electron Darwin term using explicitly correlated wave functions. *Chemical Physics*, **2012**, 401, 146-151	2.3	2
201	The MP2 binding energy of the ethene dimer and its dependence on the auxiliary basis sets: a benchmark study using a newly developed infrastructure for the processing of quantum chemical data. *Molecular Physics*, **2012**, 110, 2523-2534	1.7	7
200	Tuning the Gap: Electronic Properties and Radical-Type Reactivities of Heteronuclear [1.1.1]Propellanes of Heavier Group 14 Elements. *Organometallics*, **2011**, 30, 1419-1428	3.8	25

199	Experimental and Theoretical Study of Novel Luminescent Di-, Tri-, and Tetranuclear Copper Triazole Complexes. *Organometallics*, **2011**, 30, 3275-3283	3.8	65
198	Ab Initio Theory for Accurate Spectroscopic Constants and Molecular Properties **2011**,		2
197	The phenyl + phenyl reaction as pathway to benzynes: An experimental and theoretical study. *Chemical Physics Letters*, **2011**, 513, 20-26	2.5	17
196	Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of ammonia, water, and hydrogen fluoride. *Physical Chemistry Chemical Physics*, **2011**, 13, 1230-8	3.6	30
195	Interference-corrected explicitly-correlated second-order perturbation theory. *Chemical Physics Letters*, **2011**, 503, 157-161	2.5	23
194	Magnetic properties of paddlewheels and trinuclear clusters with exposed metal sites. *ChemPhysChem*, **2011**, 12, 3307-19	3.2	27
193	The MP2-F12 method in the Turbomole program package. *Journal of Computational Chemistry*, **2011**, 32, 2492-513	3.5	92
192	Acceleration of self-consistent-field convergence by combining conventional diagonalization and a diagonalization-free procedure. *Journal of Computational Chemistry*, **2011**, 32, 3129-34	3.5	6
191	Heating a bowl of single-molecule-soup: structure and desorption energetics of water-encapsulated open-cage [60] fullerenoid anions in the gas-phase. *Physical Chemistry Chemical Physics*, **2011**, 13, 9818-23	3.6	29
190	The formal combination of three singlet biradicaloid entities to a singlet hexaradicaloid metalloid Ge14[Si(SiMe3)3]5[Li(THF)2]3 cluster. *Journal of the American Chemical Society*, **2011**, 133, 2518-24	16.4	39
189	Genetic algorithm density functional theory study of crown ether□dibenzylammonium [2]pseudorotaxanes. *Computational and Theoretical Chemistry*, **2011**, 966, 186-193	2	5
188	Spin flipping in ring-coupled-cluster-doubles theory. *Chemical Physics Letters*, **2011**, 510, 147-153	2.5	41
187	Scalar relativistic explicitly correlated R12 methods. *Journal of Chemical Physics*, **2010**, 132, 214104	3.9	17
186	Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne. *Physical Review A*, **2010**, 81,	2.6	32
185	Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order M□ller-Plesset Level. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 695-708	3.1	11
184	Second-order electron-correlation and self-consistent spin-orbit treatment of heavy molecules at the basis-set limit. *Journal of Chemical Physics*, **2010**, 132, 094108	3.9	28
183	Large-amplitude vibrations of an N-H...pi hydrogen bonded cis-amide-benzene complex. *Physical Chemistry Chemical Physics*, **2010**, 12, 8208-18	3.6	14
182	Synthesis of a pentasilapropellane. Exploring the nature of a stretched silicon-silicon bond in a nonclassical molecule. *Journal of the American Chemical Society*, **2010**, 132, 10264-5	16.4	88

181	Open-shell explicitly correlated F12 methods. *Molecular Physics*, **2010**, 108, 315-325	1.7	38
180	Analytical nuclear gradients of the explicitly correlated M□ller□Plesset second-order energy. *Molecular Physics*, **2010**, 108, 1783-1796	1.7	15
179	Ridge-tile-like chiral topology: synthesis, resolution, and complete chiroptical characterization of enantiomers of edge-sharing binuclear square planar complexes of Ni(II) bearing achiral ligands. *Journal of the American Chemical Society*, **2010**, 132, 10477-83	16.4	39
178	Automated incremental scheme for explicitly correlated methods. *Journal of Chemical Physics*, **2010**, 132, 164114	3.9	34
177	Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. *Theoretical Chemistry Accounts*, **2010**, 126, 289-304	1.9	54
176	Switchable Open-Cage Fullerene for Water Encapsulation. *Angewandte Chemie*, **2010**, 122, 10131-10134	3.6	24
175	Switchable open-cage fullerene for water encapsulation. *Angewandte Chemie - International Edition*, **2010**, 49, 9935-8	16.4	67
174	Hydrogen abstraction from biphenyl, acenaphthylene, naphthalene and phenanthrene by atomic hydrogen and methyl radical: DFT and G3(MP2)-RAD data. *Computational and Theoretical Chemistry*, **2010**, 940, 115-118		25
173	Interaction of the alcohol molecules methanol and ethanol with single-walled carbon nanotubes □ A computational study. *Chemical Physics Letters*, **2010**, 498, 345-348	2.5	7
172	Explicitly Correlated Coupled-Cluster Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 535-572	0.7	39
171	Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order Mller-Plesset Level **2010**, 405-418		
170	Non-IPR C60 solids. *Journal of Chemical Physics*, **2009**, 130, 164705	3.9	17
169	Magnetically induced current densities in aromatic, antiaromatic, homoaromatic, and nonaromatic hydrocarbons. *Journal of Physical Chemistry A*, **2009**, 113, 8668-76	2.8	138
168	Pentagerma[1.1.1]propellane: A Combined Experimental and Quantum Chemical Study on the Nature of the Interactions between the Bridgehead Atoms. *Angewandte Chemie*, **2009**, 121, 1439-1444	3.6	25
167	Ab initio study of the interactions between CO(2) and N-containing organic heterocycles. *ChemPhysChem*, **2009**, 10, 374-83	3.2	164
166	Momentaufnahmen bei der Bildung einer Al-Al-□Bindung aus {AlR2}-Einheiten □experimentelle und quantenchemische Befunde. *Angewandte Chemie*, **2009**, 121, 8285-8290	3.6	37
165	Pentagerma[1.1.1]propellane: a combined experimental and quantum chemical study on the nature of the interactions between the bridgehead atoms. *Angewandte Chemie - International Edition*, **2009**, 48, 1411-6	16.4	38
164	Snapshots of the Al-Al sigma-bond formation starting from {AlR2} units: experimental and computational observations. *Angewandte Chemie - International Edition*, **2009**, 48, 8141-5	16.4	71

163	The geminal basis in explicitly correlated wave functions. *Chemical Physics*, **2009**, 356, 25-30	2.3	24
162	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. *Chemical Physics*, **2009**, 356, 14-24	2.3	84
161	Thermochemistry of the HOSO2+O2 association reaction and enthalpy of formation of HOSO4: A quantum chemical study. *Chemical Physics Letters*, **2009**, 470, 59-62	2.5	8
160	Unexpected Trimerization of Pyrazine in the Coordination Sphere of Low-Valent Titanocene Fragments. *Journal of Chemical Theory and Computation*, **2009**, 5, 2044-9	6.4	12
159	Expanding the coordination cage: a ruthenium(II)-polypyridine complex exhibiting high quantum yields under ambient conditions. *Inorganic Chemistry*, **2009**, 48, 5677-84	5.1	67
158	Origin of the Argon Nanocoating Shift in the OH Stretching Fundamental of n-Propanol: A Combined Experimental and Quantum Chemical Study. *Journal of Physical Chemistry C*, **2009**, 113, 10929-10938	3.8	22
157	Strong N-H...pi hydrogen bonding in amide-benzene interactions. *Journal of Physical Chemistry B*, **2009**, 113, 2937-43	3.4	94
156	Accurate coupled cluster calculations of the reaction barrier heights of two CH3* + CH4 reactions. *Journal of Physical Chemistry A*, **2009**, 113, 11679-84	2.8	9
155	Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods. *Journal of Chemical Physics*, **2009**, 131, 224315	3.9	30
154	Assessment of basis sets for F12 explicitly-correlated molecular electronic-structure methods. *Molecular Physics*, **2009**, 107, 963-975	1.7	65
153	Ab initio study of the magnetic exchange coupling constants of a structural model [CaMn(3)(III)Mn(II)] of the oxygen evolving center in photosystem II. *Physical Chemistry Chemical Physics*, **2009**, 11, 3900-9	3.6	20
152	An in-depth study on hydrogen-bonded 3-D frameworks possessing hydrophobic layers and hydrophilic pillars. *CrystEngComm*, **2009**, 11, 2480	3.3	6
151	One-dimensional Cu(II) coordination polymers: tuning the structure by modulating the carboxylate arm lengths of polycarboxylate ligands. *CrystEngComm*, **2009**, 11, 1089	3.3	20
150	Hydrides and dimers of C(58) fullerenes: structures and stabilities. *Physical Chemistry Chemical Physics*, **2009**, 11, 1050-9	3.6	5
149	Scope and limitations of the SCS-MP2 method for stacking and hydrogen bonding interactions. *Physical Chemistry Chemical Physics*, **2008**, 10, 2758-66	3.6	78
148	Accurate benchmark calculation of the reaction barrier height for hydrogen abstraction by the hydroperoxyl radical from methane. Implications for C(n)H(2n+2) where n = 2 --> 4. *Journal of Physical Chemistry A*, **2008**, 112, 7047-54	2.8	87
147	Self-consistent treatment of spin-orbit interactions with efficient Hartree-Fock and density functional methods. *Physical Chemistry Chemical Physics*, **2008**, 10, 1748-56	3.6	125
146	Quantitative quantum chemistry. *Molecular Physics*, **2008**, 106, 2107-2143	1.7	179

145	Calculation of magnetically induced currents in hydrocarbon nanorings. *Journal of Physical Chemistry A*, **2008**, 112, 13584-92	2.8	32
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