Hans Lischka

List of Publications by Year in Descending Order

318 papers	14,286 citations	61 h-index	107 g-index
323 ext. papers	15,438 ext. citations	4.4 avg, IF	6.51 L-index

#	Paper	IF	Citations
318	A General New Method for Calculating the Molecular Nonpolar Surface for Analysis of LC-MS Data. *International Journal of Mass Spectrometry*, **2021**, 461, 116495-116495	1.9	2
317	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. *Applied Materials Today*, **2021**, 22, 100924	6.6	23
316	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. *Journal of Chemical Physics*, **2021**, 154, 104308	3.9	2
315	Molecular Dynamics Simulation of the Excited-State Proton Transfer Mechanism in 3-Hydroxyflavone Using Explicit Hydration Models. *Journal of Physical Chemistry A*, **2021**, 125, 5765-5778	2.8	4
314	Ab initio calculation of the excited states of nitropyrenes. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	1
313	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. *Journal of Chemical Physics*, **2021**, 154, 044306	3.9	6
312	Triple-Columned and Multiple-Layered 3D Polymers: Design, Synthesis, Aggregation-Induced Emission (AIE), and Computational Study. *Research*, **2021**, 2021, 3565791	7.8	7
311	Unexpected Charge Effects Strengthen Stacking Pancake Bonding. *Jacs Au*, **2021**, 1, 1647-1655		6
310	Exploration of Graphene Defect Reactivity toward a Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. *Journal of Physical Chemistry A*, **2021**, 125, 1152-1165	2.8	4
309	Energy transfer mechanism in luminescence Eu(III) and Tb(III) complexes of coumarin-3-carboxylic acid: A theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 240, 118591	4.4	5
308	Effects on the aromaticity and on the biradicaloid nature of acenes by the inclusion of a cyclobutadiene linkage. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	2
307	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. *Journal of Physical Chemistry C*, **2020**, 124, 14327-14337	3.8	13
306	A computational study of the ground and excited state acidities of synthetic analogs of red wine pyranoanthocyanins. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	5
305	Diradical Organic One-Dimensional Polymers Synthesized on a Metallic Surface. *Angewandte Chemie*, **2020**, 132, 17747-17752	3.6	5
304	Memorial Viewpoint for William L. Hase. *Journal of Physical Chemistry A*, **2020**, 124, 4183-4184	2.8	
303	Diradical Organic One-Dimensional Polymers Synthesized on a Metallic Surface. *Angewandte Chemie - International Edition*, **2020**, 59, 17594-17599	16.4	7
302	Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for -/-Diindenoacenes and Related Benzothiophene-Capped Oligomers as Revealed by Extended Multireference Calculations. *Journal of Organic Chemistry*, **2020**, 85, 3664-3675	4.2	10

301	Benchmark ab initio calculations on intermolecular structures and the exciton character of poly(p-phenylenevinylene) dimers. *Journal of Chemical Physics*, **2020**, 152, 044306	3.9	3
300	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
299	Multi-layer 3D chirality: new synthesis, AIE and computational studies. *Science China Chemistry*, **2020**, 63, 692-698	7.9	14
298	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. *Journal of Materials Chemistry C*, **2020**, 8, 7793-7804	7.1	12
297	Multi-Reference Configuration Interaction **2020**, 277-297		1
296	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. *Journal of Physical Chemistry A*, **2020**, 124, 8907-8917	2.8	7
295	Cycloaddition of Strained Cyclic Alkenes and -Quinones: A Distortion/Interaction Analysis. *Journal of Organic Chemistry*, **2020**, 85, 13557-13566	4.2	3
294	Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorization valence bond theory and high-level computational approaches. *Physical Chemistry Chemical Physics*, **2020**, 22, 22003-22015	3.6	3
293	Doping Capabilities of Fluorine on the UV Absorption and Emission Spectra of Pyrene-Based Graphene Quantum Dots. *Journal of Physical Chemistry A*, **2020**, 124, 10954-10966	2.8	4
292	Nonadiabatic Dynamics of Charge-Transfer States Using the Anthracene-Tetracyanoethylene Complex as a Prototype. *Journal of Physical Chemistry A*, **2020**, 124, 3347-3357	2.8	8
291	Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. *Journal of Physical Chemistry Letters*, **2019**, 10, 5592-5597	6.4	7
290	The electronic transitions of analogs of red wine pyranoanthocyanin pigments. *Photochemical and Photobiological Sciences*, **2019**, 18, 45-53	4.2	7
289	The characterization of electronic defect states of single and double carbon vacancies in graphene sheets using molecular density functional theory. *Molecular Physics*, **2019**, 117, 1519-1531	1.7	7
288	Solvent effect on Al(III) hydrolysis constants from density functional theory. *Molecular Physics*, **2019**, 117, 1507-1518	1.7	
287	Dynamics of benzene excimer formation from the parallel-displaced dimer. *Physical Chemistry Chemical Physics*, **2019**, 21, 13916-13924	3.6	16
286	Conical intersections and the weak fluorescence of betalains. *Photochemical and Photobiological Sciences*, **2019**, 18, 1972-1981	4.2	3
285	Introduction of polar or nonpolar groups at the hydroquinone units can lead to the destruction of the columnar structure of Pillar[5]arenes. *Computational and Theoretical Chemistry*, **2019**, 1161, 1-9	2	7
284	Characterization of Charge Transfer in Excited States of Extended Clusters of Stacked Donor and Acceptor Complexes in Lock-Arm Supramolecular Ordering. *Journal of Physical Chemistry A*, **2019**, 123, 4532-4542	2.8	5

283	Quantum chemical evidence for the origin of the red/blue colors of Hydrangea macrophylla sepals. *New Journal of Chemistry*, **2019**, 43, 7532-7540	3.6	4
282	Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. *Physical Chemistry Chemical Physics*, **2019**, 21, 9077-9088	3.6	23
281	High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. *Journal of Chemical Physics*, **2019**, 150, 124302	3.9	19
280	Theoretical analysis of the stabilization of graphene nanosheets by means of strongly polarized pyrene derivatives. *Chemical Physics*, **2019**, 527, 110468	2.3	2
279	Adsorption process of polar and nonpolar compounds in a nanopore model of humic substances. *European Journal of Soil Science*, **2019**, 71, 845	3.4	3
278	Characterization of glycan isomers using magnetic carbon nanoparticles as a MALDI co-matrix. *RSC Advances*, **2019**, 9, 20137-20148	3.7	8
277	Microhydration of Polymer Electrolyte Membranes: A Comparison of Hydrogen-Bonding Networks and Spectral Properties of Nafion and Bis[(perfluoroalkyl)sulfonyl] Imide. *Journal of Physical Chemistry B*, **2019**, 123, 9899-9911	3.4	2
276	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. *Journal of Physical Chemistry A*, **2019**, 123, 2049-2057	2.8	7
275	Kinetics of the Strain-Promoted Oxidation-Controlled Cycloalkyne-1,2-quinone Cycloaddition: Experimental and Theoretical Studies. *Journal of Organic Chemistry*, **2018**, 83, 244-252	4.2	16
274	The effect of hydrogen bonding on the nonadiabatic dynamics of a thymine-water cluster. *Chemical Physics*, **2018**, 515, 472-479	2.3	7
273	Multireference Approaches for Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7293-7361	68.1	181
272	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. *ChemPhysChem*, **2018**, 19, 2492-2499	3.2	10
271	Analysis of charge transfer transitions in stacked π-electron donor-acceptor complexes. *Physical Chemistry Chemical Physics*, **2018**, 20, 26957-26967	3.6	9
270	Electronic structure theory gives insights into the higher efficiency of the PTB electron-donor polymers for organic photovoltaics in comparison with prototypical P3HT. *Journal of Chemical Physics*, **2018**, 149, 184905	3.9	
269	Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. *Journal of Physical Chemistry A*, **2018**, 122, 9464-9473	2.8	3
268	Model Systems for Dynamics of π-Conjugated Biomolecules in Excited States **2017**, 1697-1739		1
267	Cation-π interactions in competition with cation microhydration: a theoretical study of alkali metal cation-pyrene complexes. *Journal of Molecular Modeling*, **2017**, 23, 131	2	8
266	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor-Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. *Journal of Chemical Theory and Computation*, **2017**, 13, 2612-2622	6.4	10

265	High-level Ab Initio Absorption Spectra Simulations of Neutral, Anionic and Neutral+ Chromophore of Green Fluorescence Protein Chromophore Models in Gas Phase and Solution. *Photochemistry and Photobiology*, **2017**, 93, 1356-1367	3.6	4
264	Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. *Journal of Chemical Physics*, **2017**, 146, 064106	3.9	15
263	Lagrange function method for energy optimization directly in the space of natural orbitals. *International Journal of Quantum Chemistry*, **2017**, 117, e25376	2.1	3
262	Investigation of the ozone formation reaction pathway: Comparisons of full configuration interaction quantum Monte Carlo and fixed-node diffusion Monte Carlo with contracted and uncontracted MRCI. *Journal of Chemical Physics*, **2017**, 147, 094306	3.9	9
261	Singlet L and L Bands for N-Acenes (N = 2-7): A CASSCF/CASPT2 Study. *Journal of Chemical Theory and Computation*, **2017**, 13, 4297-4306	6.4	22
260	Structure and electronic states of a graphene double vacancy with an embedded Si dopant. *Journal of Chemical Physics*, **2017**, 147, 194702	3.9	6
259	How to efficiently tune the biradicaloid nature of acenes by chemical doping with boron and nitrogen. *Physical Chemistry Chemical Physics*, **2017**, 19, 19225-19233	3.6	18
258	Single and double carbon vacancies in pyrene as first models for graphene defects: A survey of the chemical reactivity toward hydrogen. *Chemical Physics*, **2017**, 482, 346-354	2.3	8
257	The crucial role of a spacer material on the efficiency of charge transfer processes in organic donor-acceptor junction solar cells. *Nanoscale*, **2017**, 10, 451-459	7.7	5
256	□-stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 22300-10	3.6	44
255	Polyradical Character of Triangular Non-Kekulé Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. *Journal of Physical Chemistry A*, **2016**, 120, 1625-36	2.8	70
254	Model Systems for Dynamics of □-Conjugated Biomolecules in Excited States **2016**, 1-43		
253	New Insights into the State Trapping of UV-Excited Thymine. *Molecules*, **2016**, 21,	4.8	23
252	The Antiferromagnetic Spin Coupling in Non-Kekulé Acenes-Impressive Polyradical Character Revealed by High-Level Multireference Methods. *ChemPhysChem*, **2016**, 17, 2013-21	3.2	3
251	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
250	Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno[3,4-b]thiophene benzodithiophene) by Means of ab Initio and Density Functional Theory. *Journal of Physical Chemistry C*, **2016**, 120, 21818-21826	3.8	19
249	Organic and Contaminant Geochemistry **2016**, 177-243		3
248	The electronic states of a double carbon vacancy defect in pyrene: a model study for graphene. *Physical Chemistry Chemical Physics*, **2015**, 17, 12778-85	3.6	14

247	A comparison of neutral and charged species of one- and two-dimensional models of graphene nanoribbons using multireference theory. *Journal of Chemical Physics*, **2015**, 142, 054302	3.9	14
246	Concave or convex π-dimers: the role of the pancake bond in substituted phenalenyl radical dimers. *Physical Chemistry Chemical Physics*, **2015**, 17, 23963-9	3.6	33
245	Hydrogen abstraction from the hydrazine molecule by an oxygen atom. *Journal of Physical Chemistry A*, **2015**, 119, 1628-35	2.8	9
244	Electronic excitation processes in single-strand and double-strand DNA: a computational approach. *Topics in Current Chemistry*, **2015**, 356, 1-37		17
243	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the π State. *Journal of Physical Chemistry A*, **2015**, 119, 6232-43	2.8	46
242	Why water makes 2-aminopurine fluorescent?. *Physical Chemistry Chemical Physics*, **2015**, 17, 15452-9	3.6	24
241	Absorption and fluorescence spectra of poly(p-phenylenevinylene) (PPV) oligomers: an ab initio simulation. *Journal of Physical Chemistry A*, **2015**, 119, 1787-95	2.8	17
240	Thermochemical and Kinetics of Hydrazine Dehydrogenation by an Oxygen Atom in Hydrazine-Rich Systems: A Dimer Model. *Journal of Physical Chemistry A*, **2015**, 119, 12607-14	2.8	5
239	Radical sites in humic acids: A theoretical study on protocatechuic and gallic acids. *Computational and Theoretical Chemistry*, **2014**, 1032, 42-49	2	18
238	Comparison of multireference configuration interaction potential energy surfaces for H + O2 -ĸHO2: the effect of internal contraction. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	20
237	Proton transfer processes in polar regions of humic substances initiated by aqueous aluminum cation bridges: A computational study. *Geoderma*, **2014**, 213, 115-123	6.7	9
236	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbon-tetracyanoethylene complexes. *Physical Chemistry Chemical Physics*, **2014**, 16, 20586-97	3.6	37
235	Double pancake bonds: pushing the limits of strong π-stacking interactions. *Journal of the American Chemical Society*, **2014**, 136, 12958-65	16.4	63
234	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405	6.4	139
233	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	51
232	Rotational barrier in phenalenyl neutral radical dimer: separating pancake and van der Waals interactions. *Journal of the American Chemical Society*, **2014**, 136, 5539-42	16.4	101
231	Direct dynamics simulation of the activation and dissociation of 1,5-dinitrobiuret (HDNB). *Journal of Physical Chemistry A*, **2014**, 118, 2228-36	2.8	10
230	Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. *Journal of Chemical Theory and Computation*, **2014**, 10, 3280-9	6.4	42

229	Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 26-33	7.9	280
228	A multireference configuration interaction study of the photodynamics of nitroethylene. *Journal of Physical Chemistry A*, **2014**, 118, 12011-20	2.8	7
227	Study of the diradicaloid character in a prototypical pancake-bonded dimer: the stacked tetracyanoethylene (TCNE) anion dimer and the neutral K(2)TCNE(2) complex. *ChemPhysChem*, **2014**, 15, 165-76	3.2	39
226	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. *Journal of Chemical Physics*, **2014**, 141, 074105	3.9	24
225	The diverse manifold of electronic states generated by a single carbon defect in a graphene sheet: multireference calculations using a pyrene defect model. *ChemPhysChem*, **2014**, 15, 3334-41	3.2	9
224	Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 158-166	2	6
223	Molecular Models of Cation and Water Molecule Bridges in Humic Substances **2014**, 107-115		3
222	Ab initio modeling of excitonic and charge-transfer states in organic semiconductors: the PTB1/PCBM low band gap system. *Journal of the American Chemical Society*, **2013**, 135, 18252-5	16.4	52
221	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO2(110) Intermolecular Interaction. *Journal of Physical Chemistry C*, **2013**, 117, 17613-17622	3.8	16
220	Multiscale simulation of the ground and photo-induced charge-separated states of a molecular triad in polar organic solvent: exploring the conformations, fluctuations, and free energy landscapes. *Journal of Physical Chemistry B*, **2013**, 117, 12065-75	3.4	20
219	The effect of dimerization on the excited state behavior of methylated xanthine derivatives: a computational study. *Photochemical and Photobiological Sciences*, **2013**, 12, 1496-508	4.2	5
218	Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. *Photochemical and Photobiological Sciences*, **2013**, 12, 1440-52	4.2	43
217	The multiradical character of one- and two-dimensional graphene nanoribbons. *Angewandte Chemie - International Edition*, **2013**, 52, 2581-4	16.4	168
216	Synthesis, spectroscopy, and computational analysis of photoluminescent bis(aminophenyl)-substituted thiophene derivatives. *ChemPhysChem*, **2013**, 14, 1016-24	3.2	15
215	Nonadiabatic photodynamics of a retinal model in polar and nonpolar environment. *Journal of Physical Chemistry A*, **2013**, 117, 2790-9	2.8	50
214	Electronically excited states in poly(p-phenylenevinylene): vertical excitations and torsional potentials from high-level ab initio calculations. *Journal of Physical Chemistry A*, **2013**, 117, 2181-9	2.8	59
213	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. *Molecular Physics*, **2013**, 111, 2439-2450	1.7	37
212	Der Multiradikalcharakter ein- und zweidimensionaler Graphen-Nanobänder. *Angewandte Chemie*, **2013**, 125, 2641-2644	3.6	21

211	Electronically excited states and photodynamics: a continuing challenge. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	69
210	Multiconfiguration self-consistent field and multireference configuration interaction methods and applications. *Chemical Reviews*, **2012**, 112, 108-81	68.1	462
209	The stability of the acetic acid dimer in microhydrated environments and in aqueous solution. *Physical Chemistry Chemical Physics*, **2012**, 14, 4162-70	3.6	14
208	Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine. *Journal of Chemical Physics*, **2012**, 137, 22A503	3.9	90
207	Laser pulse trains for controlling excited state dynamics of adenine in water. *Physical Chemistry Chemical Physics*, **2012**, 14, 4687-94	3.6	22
206	Strikingly different effects of hydrogen bonding on the photodynamics of individual nucleobases in DNA: comparison of guanine and cytosine. *Journal of the American Chemical Society*, **2012**, 134, 13662-9	16.4	29
205	Direct dynamics simulation of dioxetane formation and decomposition via the singlet □O-O-CH2-CH2□biradical: non-RRKM dynamics. *Journal of Chemical Physics*, **2012**, 137, 044305	3.9	21
204	QM/MM non-adiabatic decay dynamics of formamide in polar and non-polar solvents. *Physical Chemistry Chemical Physics*, **2012**, 14, 13262-72	3.6	7
203	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 2777-89	6.4	284
202	Non-adiabatic excited state dynamics of riboflavin after photoexcitation. *Physical Chemistry Chemical Physics*, **2012**, 14, 8693-702	3.6	19
201	UV absorption spectrum of alternating DNA duplexes. Analysis of excitonic and charge transfer interactions. *Journal of Physical Chemistry A*, **2012**, 116, 11151-60	2.8	61
200	Electronic spectra of nitroethylene. *International Journal of Quantum Chemistry*, **2012**, 112, 1225-1232	2.1	9
199	Model Systems for Dynamics of □Conjugated Biomolecules in Excited States **2012**, 1175-1213		1
198	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2Phydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 9016-25	3.6	60
197	O + C2H4 potential energy surface: excited states and biradicals at the multireference level. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	7
196	Proton exchange reactions of C2□4 alkanes sorbed in ZSM-5 zeolite. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	10
195	Cis-transphotoisomerization of azobenzene upon excitation to the S1state: an ab initio molecular dynamics and QM/MM study **2012**,		1
194	O + C2H4 potential energy surface: lowest-lying singlet at the multireference level. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	4

193	Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. *Journal of Chemical Physics*, **2012**, 137, 22A514	3.9	139
192	Electronically excited states and photodynamics: a continuing challenge **2012**, 147-160		1
191	Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules. *Advanced Series in Physical Chemistry*, **2011**, 415-462		16
190	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. *Physical Chemistry Chemical Physics*, **2011**, 13, 6145-55	3.6	79
189	Nonadiabatic dynamics of uracil: population split among different decay mechanisms. *Journal of Physical Chemistry A*, **2011**, 115, 5247-55	2.8	77
188	The decay mechanism of photoexcited guanine - a nonadiabatic dynamics study. *Journal of Chemical Physics*, **2011**, 134, 014304	3.9	66
187	Semiclassical dynamics simulations of charge transport in stacked □systems. *Journal of Chemical Physics*, **2011**, 134, 034309	3.9	27
186	Nonadiabatic molecular dynamics study of the cis-trans photoisomerization of azobenzene excited to the S1 state. *Journal of Physical Chemistry A*, **2011**, 115, 11136-43	2.8	97
185	Study of solvent effect on the stability of water bridge-linked carboxyl groups in humic acid models. *Geoderma*, **2011**, 169, 20-26	6.7	25
184	Wettability of kaolinite (001) surfaces □Molecular dynamic study. *Geoderma*, **2011**, 169, 47-54	6.7	128
183	Absorption and fluorescence of PRODAN in phospholipid bilayers: a combined quantum mechanics and classical molecular dynamics study. *Journal of Physical Chemistry A*, **2011**, 115, 11428-37	2.8	41
182	Columbus□ program system for advanced multireference theory calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 191-199	7.9	147
181	Sorption of Selected Aromatic Substances□Application of Kinetic Concepts and Quantum Mechanical Modeling. *Water, Air, and Soil Pollution*, **2011**, 215, 449-464	2.6	4
180	Theoretical study of the excitation spectrum of azomethane. *Chemical Physics*, **2011**, 380, 9-16	2.3	13
179	The functionality of cation bridges for binding polar groups in soil aggregates. *International Journal of Quantum Chemistry*, **2011**, 111, 1531-1542	2.1	45
178	Influence of the active space on CASSCF nonadiabatic dynamics simulations. *International Journal of Quantum Chemistry*, **2011**, 111, 3307-3315	2.1	17
177	The charge-transfer states in a stacked nucleobase dimer complex: a benchmark study. *Journal of Computational Chemistry*, **2011**, 32, 1217-27	3.5	67
176	Methyl and pentyl chloride in a microhydrated environment and at the liquid water-vapor interface: a theoretical study. *Journal of Physical Chemistry B*, **2011**, 115, 1807-16	3.4	7

175	Molecular dynamics simulations of water molecule-bridges in polar domains of humic acids. *Environmental Science & Technology*, **2011**, 45, 8411-9	10.3	47
174	Excited-state intermolecular proton transfer reactions of 7-azaindole(MeOH)(n) (n = 1-3) clusters in the gas phase: on-the-fly dynamics simulation. *Journal of Physical Chemistry A*, **2011**, 115, 14129-36	2.8	39
173	Photodynamics of the adenine model 4-aminopyrimidine embedded within double strand of DNA. *Collection of Czechoslovak Chemical Communications*, **2011**, 76, 631-643		10
172	TORSIONAL POTENTIALS AND FULL-DIMENSIONAL SIMULATION OF ELECTRONIC ABSORPTION SPECTRA OF para-PHENYLENEVINYLENE OLIGOMERS USING SEMIEMPIRICAL HAMILTONIANS. *Journal of Theoretical and Computational Chemistry*, **2010**, 09, 249-263	1.8	13
171	Does stacking restrain the photodynamics of individual nucleobases?. *Journal of the American Chemical Society*, **2010**, 132, 8261-3	16.4	64
170	Photodynamics of azomethane: a nonadiabatic surface-hopping study. *Journal of Physical Chemistry A*, **2010**, 114, 8778-85	2.8	29
169	Azomethane: nonadiabatic photodynamical simulations in solution. *Journal of Physical Chemistry A*, **2010**, 114, 12585-90	2.8	39
168	Nonadiabatic excited-state dynamics with hybrid ab initio quantum-mechanical/molecular-mechanical methods: solvation of the pentadieniminium cation in apolar media. *Journal of Physical Chemistry A*, **2010**, 114, 6757-65	2.8	67
167	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21453-8	11.5	323
166	The UV absorption of nucleobases: semi-classical ab initio spectra simulations. *Physical Chemistry Chemical Physics*, **2010**, 12, 4959-67	3.6	179
165	Solvatochromic and ionochromic effects of Iron(II)bis(1,10-phenanthroline)dicyano: a theoretical study. *Inorganic Chemistry*, **2010**, 49, 1634-46	5.1	23
164	Supporting Molecular Modeling Workflows within a Grid Services Cloud. *Lecture Notes in Computer Science*, **2010**, 13-28	0.9	4
163	The effect of C5 substitution on the photochemistry of uracil. *Physical Chemistry Chemical Physics*, **2010**, 12, 4924-33	3.6	19
162	Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine. *Physical Chemistry Chemical Physics*, **2010**, 12, 5375-88	3.6	25
161	Photostability and solvation: photodynamics of microsolvated zwitterionic glycine. *Physical Chemistry Chemical Physics*, **2010**, 12, 4906-14	3.6	10
160	Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. *Physical Chemistry Chemical Physics*, **2010**, 12, 12719-26	3.6	26
159	A grid services cloud for molecular modelling workflows. *International Journal of Web and Grid Services*, **2010**, 6, 176	1.4	8
158	Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 77-106	0.7	6

157	Singlet and triplet potential surfaces for the O2+C2H4 reaction. *Journal of Chemical Physics*, **2010**, 133, 184306	3.9	16
156	The photodynamics of 2,4-diaminopyrimidine in comparison with 4-aminopyrimidine: The effect of amino-substitution. *Chemical Physics Letters*, **2010**, 497, 129-134	2.5	14
155	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. *Chemical Physics*, **2010**, 375, 26-34	2.3	115
154	The effect of hydration on the photo-deactivation pathways of 4-aminopyrimidine. *Chemical Physics* , **2010**, 375, 110-117	2.3	14
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