Theis I SÃ, lling

List of Publications by Year in descending order

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201674 182427 3,100 126 27 51 citations h-index g-index papers 131 131 131 3716 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Enhanced Mobility of Poly(3-hexylthiophene) Transistors by Spin-Coating from High-Boiling-Point Solvents. Chemistry of Materials, 2004, 16, 4772-4776.	6.7	878
2	Induced Alignment of a Solution-Cast Discotic Hexabenzocoronene Derivative for Electronic Devices Investigated by Surface X-ray Diffraction. Journal of the American Chemical Society, 2003, 125, 2252-2258.	13.7	109
3	Femtochemistry of Norrish Type-I Reactions: III. Highly Excited Ketones—Theoretical. ChemPhysChem, 2002, 3, 57-78.	2.1	80
4	Are Conical Intersections Responsible for the Ultrafast Processes of Adenine, Protonated Adenine, and the Corresponding Nucleosides?. ChemPhysChem, 2005, 6, 1276-1281.	2.1	80
5	Femtochemistry of Norrish Type″ Reactions: IV. Highly Excited Ketones—Experimental. ChemPhysChem, 2002, 3, 79-97.	2.1	72
6	Structure of Zone-Cast HBCâ^'C12H25Films. Journal of the American Chemical Society, 2005, 127, 11288-11293.	13.7	63
7	Interpretation of the Ultrafast Photoinduced Processes in Pentacene Thin Films. Journal of the American Chemical Society, 2010, 132, 3431-3439.	13.7	59
8	Energy Flow and Fragmentation Dynamics of N,N-Dimethylisopropylamine. Journal of Physical Chemistry A, 2006, 110, 4251-4255.	2.5	51
9	Heavy-Atom-Substituted Nucleobases in Photodynamic Applications: Substitution of Sulfur with Selenium in 6-Thioguanine Induces a Remarkable Increase in the Rate of Triplet Decay in 6-Selenoguanine. Journal of the American Chemical Society, 2018, 140, 11214-11218.	13.7	48
10	Foamstability: The interplay between salt-, surfactant- and critical micelle concentration. Journal of Petroleum Science and Engineering, 2020, 187, 106871.	4.2	48
11	Macroscopic Alignment of Graphene Stacks by Langmuirâ-'Blodgett Deposition of Amphiphilic Hexabenzocoronenes. Langmuir, 2004, 20, 4139-4146.	3 . 5	46
12	Control of Local Ionization and Charge Transfer in the Bifunctional Molecule 2-Phenylethyl-N,N-dimethylamine Using Rydberg Fingerprint Spectroscopy. Journal of Physical Chemistry A, 2005, 109, 1920-1925.	2.5	46
13	The Influence of Push–Pull States on the Ultrafast Intersystem Crossing in Nitroaromatics. Journal of Physical Chemistry B, 2013, 117, 9947-9955.	2.6	42
14	On the Condensed Phase Ring-Closure of Vinylheptafulvalene and Ring-Opening of Gaseous Dihydroazulene. Journal of Physical Chemistry A, 2013, 117, 3340-3347.	2.5	42
15	The Proton Affinities of Imines and the Heats of Formation of Immonium Ions Investigated with Composite ab Initio Methods. Journal of the American Chemical Society, 1999, 121, 6002-6009.	13.7	39
16	Determining Orientations of Optical Transition Dipole Moments Using Ultrafast X-ray Scattering. Journal of Physical Chemistry Letters, 2018, 9, 6556-6562.	4.6	36
17	New insights on the photodynamics of acetone excited with 253â^288nm femtosecond pulses. Chemical Physics Letters, 2008, 461, 193-197.	2.6	34
18	The role of novel Rydberg-valence behaviour in the non-adiabatic dynamics of tertiary aliphatic amines. Chemical Science, 2016, 7, 1826-1839.	7.4	34

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19	Structural Surprises in Friction-Deposited Films of Poly(tetrafluoroethylene). Macromolecules, 2005, 38, 2383-2390.	4.8	33
20	The Nonâ€Ergodic Nature of Internal Conversion. ChemPhysChem, 2014, 15, 249-259.	2.1	33
21	Characterization of petrophysical properties using pore-network and lattice-Boltzmann modelling: Choice of method and image sub-volume size. Journal of Petroleum Science and Engineering, 2016, 145, 256-265.	4.2	31
22	The effects of symmetry and rigidity on non-adiabatic dynamics in tertiary amines: a time-resolved photoelectron velocity-map imaging study of the cage-amine ABCO. Physical Chemistry Chemical Physics, 2016, 18, 9715-9723.	2.8	31
23	Novel Piâ^'Ligand Exchange and Insertion Reactions Involving Three-Membered Phosphorus Heterocycles:Â An ab Initio Investigation. Journal of the American Chemical Society, 1998, 120, 7063-7068.	13.7	30
24	The effect of organic acids and salinity on the interfacial tension of n-decane/ water systems. Journal of Petroleum Science and Engineering, 2019, 173, 1047-1052.	4.2	30
25	Optoelectronic Properties of Quasi-Linear, Self-Assembled Platinum Complexes: Pt–Pt Distance Dependence. Advanced Functional Materials, 2004, 14, 323-328.	14.9	29
26	Ultrafast relaxation dynamics of electronically excited piperidine: ionization signatures of Rydberg/valence evolution. Physical Chemistry Chemical Physics, 2016, 18, 25070-25079.	2.8	29
27	Coherent Motion Reveals Nonâ€Ergodic Nature of Internal Conversion between Excited States. ChemPhysChem, 2012, 13, 820-827.	2.1	28
28	Are Pi-Ligand Exchange Reactions of Thiirenium and Thiiranium Ions Feasible? An Ab Initio Investigation. Chemistry - A European Journal, 1999, 5, 509-514.	3.3	27
29	A high-level ab initio investigation of identity and nonidentity gas-phase SN2 reactions of halide ions with halophosphines. International Journal of Mass Spectrometry, 2001, 210-211, 1-11.	1.5	26
30	Electrophilic organic selenium reagentsâ€"protonated seleninic acids as precursors for unsymmetrical aromatic selenides. Tetrahedron, 2011, 67, 2633-2643.	1.9	26
31	Dynamics of Molecules near Ionization. Journal of Physical Chemistry A, 2003, 107, 10872-10887.	2.5	24
32	Computational investigation of photo induced processes in alkyl nitrites and the product alkoxy radicals. Chemical Physics Letters, 2010, 484, 113-118.	2.6	24
33	Source identification of beached oil at Al Zubarah, Northwestern Qatar. Journal of Petroleum Science and Engineering, 2017, 149, 107-113.	4.2	24
34	Inverting the Selectivity of the Newman–Kwart Rearrangement via One Electron Oxidation at Room Temperature. Journal of Organic Chemistry, 2018, 83, 12000-12006.	3.2	24
35	A G2 Ab Initio Investigation of Ligand-Exchange Reactions Involving Mono- and Bis-Adducts of the Phosphenium Ion. Inorganic Chemistry, 1999, 38, 6049-6054.	4.0	23
36	Croconamides: a new dual hydrogen bond donating motif for anion recognition and organocatalysis. Organic and Biomolecular Chemistry, 2017, 15, 2784-2790.	2.8	23

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37	Conversion of Phenols into Selenophenols: Seleno Newman–Kwart Rearrangement. Angewandte Chemie - International Edition, 2013, 52, 12346-12349.	13.8	22
38	Improving long-term hydraulic fracture conductivity by alteration of rock minerals. Journal of Petroleum Science and Engineering, 2021, 196, 108046.	4.2	22
39	Atmospheric photochemical loss of H and H2from formaldehyde: the relevance of ultrafast processes. Physical Chemistry Chemical Physics, 2008, 10, 674-680.	2.8	21
40	Coherent Dynamics in Complex Elimination Reactions:  Experimental and Theoretical Femtochemistry of 1,3-Dibromopropane and Related Systems,. Journal of Physical Chemistry A, 2002, 106, 7530-7546.	2.5	20
41	Probing the Lifetimes of Internally Excited Amyl Nitrite Cations. Journal of Physical Chemistry A, 2010, 114, 7021-7025.	2.5	20
42	Surprising Intrinsic Photostability of the Disulfide Bridge Common in Proteins. Journal of the American Chemical Society, 2012, 134, 20279-20281.	13.7	20
43	Transient IR Spectroscopic Observation of Singlet and Triplet States of 2-Nitrofluorene: Revisiting the Photophysics of Nitroaromatics. Journal of Physical Chemistry A, 2016, 120, 28-35.	2.5	20
44	Atmospheric chemistry of Z- and E-CF ₃ CHî€CHCF ₃ . Physical Chemistry Chemical Physics, 2017, 19, 735-750.	2.8	20
45	A MALDI-TOF study of bio-remediation in highly weathered oil contaminated soils. Journal of Petroleum Science and Engineering, 2018, 168, 569-576.	4.2	20
46	Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation. Angewandte Chemie - International Edition, 2013, 52, 2247-2250.	13.8	19
47	Initial Dynamics of The Norrish Type I Reaction in Acetone: Probing Wave Packet Motion. Journal of Physical Chemistry A, 2011, 115, 556-561.	2.5	18
48	Pseudoâ€Bimolecular [2+2] Cycloaddition Studied by Timeâ€Resolved Photoelectron Spectroscopy. Chemistry - A European Journal, 2011, 17, 3922-3931.	3.3	18
49	Conserving Coherence and Storing Energy during Internal Conversion: Photoinduced Dynamics of <i>ci>cis</i> and <i>trans-</i> Azobenzene Radical Cations. Journal of Physical Chemistry A, 2017, 121, 8642-8651.	2.5	18
50	Competing Simple Cleavage Reactions:Â The Elimination of Alkyl Radicals from Amine Radical Cations. Journal of the American Chemical Society, 2005, 127, 6466-6475.	13.7	17
51	On the absorption of the phenolatechromophore in the green fluorescent protein—role of individual interactions. Chemical Communications, 2010, 46, 734-736.	4.1	17
52	Symmetry, vibrational energy redistribution and vibronic coupling: The internal conversion processes of cycloketones. Journal of Chemical Physics, 2012, 137, 22A522.	3.0	17
53	Revisiting the photophysics of 9-fluorenone: Ultrafast time-resolved fluorescence and theoretical studies. Chemical Physics Letters, 2017, 686, 218-222.	2.6	17
54	Substituent effects on the stability of extended benzylic carbocations: a computational study of conjugation. Organic and Biomolecular Chemistry, 2005, 3, 2441.	2.8	16

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55	Real-Time Probing of Structural Dynamics by Interaction between Chromophores. Journal of Physical Chemistry A, 2011, 115, 12120-12125.	2.5	16
56	A G2 Study of SH+ Exchange Reactions Involving Lone-Pair Donors and Unsaturated Hydrocarbons. Chemistry - A European Journal, 2001, 7, 1516-1524.	3.3	15
57	Distortion dependent intersystem crossing: A femtosecond time-resolved photoelectron spectroscopy study of benzene, toluene, and p-xylene. Structural Dynamics, 2017, 4, 044008.	2.3	15
58	The Paternò–Büchi reaction: importance of triplet states in the excited-state reaction pathway. Physical Chemistry Chemical Physics, 2012, 14, 8572.	2.8	14
59	Vacuum ultraviolet excited state dynamics of the smallest ring, cyclopropane. II. Time-resolved photoelectron spectroscopy and <i>ab initio</i> dynamics. Journal of Chemical Physics, 2018, 149, 144311.	3.0	14
60	Improving carbonate rock hardness by consolidating additives to sustain long term fracture conductivity. Journal of Petroleum Science and Engineering, 2020, 195, 107897.	4.2	14
61	Symmetry controlled excited state dynamics. Physical Chemistry Chemical Physics, 2019, 21, 2283-2294.	2.8	13
62	Exchange and insertion reactions involving borane adducts of phosphirane and phosphirene: a G2(MP2) ab initio investigation. Journal of Organometallic Chemistry, 1999, 580, 320-327.	1.8	12
63	On the photostability of the disulfide bond: An electronic or a structural property?. Chemical Physics, 2014, 442, 77-80.	1.9	12
64	Charge-resonance excitations in symmetric molecules $\hat{a}\in$ "Comparison of linear response DFT with CC3 for the excited states of a model dimer. Chemical Physics Letters, 2009, 478, 127-131.	2.6	11
65	Solvent-dependent dual fluorescence of the push–pull system 2-diethylamino-7-nitrofluorene. Physical Chemistry Chemical Physics, 2018, 20, 5942-5951.	2.8	11
66	Carbonate Rock Chemical Consolidation Methods: Advancement and Applications. Energy & Energy	5.1	11
67	Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation. International Journal of Mass Spectrometry, 1999, 185-187, 263-270.	1.5	10
68	Synthesis, Structure, and Properties of 4,7-Dimethoxybenzo[c]tellurophene: A Molecular Pyroelectric Material. Angewandte Chemie - International Edition, 2006, 45, 5666-5670.	13.8	10
69	Excited-State Ions in Femtosecond Time-Resolved Mass Spectrometry: An Investigation of Highly Excited Chloroamines. Journal of Physical Chemistry A, 2009, 113, 40-43.	2.5	10
70	Comment on "Theoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffraction― Journal of Physical Chemistry A, 2009, 113, 6849-6850.	2.5	10
71	Internal conversion mediated by specific nuclear motions: The nitrogen inversion in amines. Chemical Physics, 2014, 442, 62-67.	1.9	10
72	Excited $\hat{a} \in S$ tate Topology Modifications of the Dihydroazulene Photoswitch Through Aromaticity. ChemPhotoChem, 2019, 3, 619-629.	3.0	10

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73	Prevention of Hematite Settling in Water-Based Mud at High Pressure and High Temperature. ACS Omega, 2021, 6, 23607-23613.	3.5	10
74	Are the Approach Directions of Ïf and Ï€ Nucleophiles to the Sulfur Atom of Thiiranium and Thiirenium lons Different?. Chemistry - A European Journal, 2000, 6, 590-591.	3.3	9
75	Wave Packet Simulation of Nonadiabatic Dynamics in Highly Excited 1,3-Dibromopropane. Journal of Physical Chemistry A, 2008, 112, 10481-10486.	2.5	9
76	Sparing the orthoâ€position in nucleophilic aromatic substitutionâ€specific displacement of the 4‧ePh group in 2,4â€bis(phenylseleno)nitrobenzene. Heteroatom Chemistry, 2009, 20, 101-108.	0.7	9
77	Benzylic Thio and Seleno Newman–Kwart Rearrangements. Journal of Organic Chemistry, 2018, 83, 10786-10797.	3.2	9
78	Real-time monitoring of oil-induced micellar transitions in viscoelastic surfactants by small-angle X-ray scattering. Journal of Colloid and Interface Science, 2020, 580, 399-406.	9.4	9
79	Exchange of Cl+ between Lone-Pair Donors and π-Donors: A Computational Study. European Journal of Mass Spectrometry, 2000, 6, 153-160.	1.0	8
80	Isomerization of the protonated acetone dimer in the gas phase. Journal of Mass Spectrometry, 2005, 40, 1076-1087.	1.6	8
81	Hydrocarbon Binding by Proteins: Structures of Protein Binding Sites for ≥C ₁₀ Linear Alkanes or Long-Chain Alkyl and Alkenyl Groups. Journal of Organic Chemistry, 2015, 80, 997-1005.	3.2	8
82	The involvement of triplet receiver states in the ultrafast excited state processes of small esters. Physical Chemistry Chemical Physics, 2016, 18, 24484-24497.	2.8	8
83	Chemical Composition and Structure of Adsorbed Material on Pore Surfaces in Middle East Reservoir Rocks. Energy & Energy	5.1	8
84	The retro-ene reaction of gaseous immonium ions revisitedElectronic supplementary information (ESI) available: Table s1 [G2(MP2) total energies of the involved species] and Table s2 [archive entries for MP2(full)/6-31G(d) optimised geometries]. See http://www.rsc.org/suppdata/p2/b1/b105386h. Perkin Transactions II RSC, 2001, , 2324-2328.	1.1	7
85	How a range of metal ions influence the interfacial tension of n-decane/carboxylic acid/water systems: The impact of concentration, molecular- and electronic structure. Journal of Petroleum Science and Engineering, 2019, 182, 106307.	4.2	7
86	Vacuum ultraviolet excited state dynamics of small amides. Journal of Chemical Physics, 2019, 150, 054301.	3.0	7
87	Quantification of Extracellular Dopamine Release in Schizophrenia and Cocaine Use by Means of TREMBLE 1 1Transcripts of the BRAINPET97 discussion of this chapter can be found in Section VIII, 1998, , 463-468.		7
88	Hardness Enhancement of Carbonate Rocks by Formation of Smithsonite and Fluorite. Rock Mechanics and Rock Engineering, 2022, 55, 1001-1012.	5.4	7
89	Computational predictions regarding ultrafast bond breakage and conformational changes in aliphatic chloro-amines. Computational and Theoretical Chemistry, 2007, 811, 117-124.	1.5	6
90	The influence of fragment size and intermediate barriers on competing near-identical simple cleavage reactions: A variational RRKM study. International Journal of Mass Spectrometry, 2011, 306, 175-181.	1.5	6

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91	The expulsion of alkyl radicals from the methyliumylaminomethyl radical cation, ˙CH2NH2CH3+, and related distonic ions. Journal of the Chemical Society Perkin Transactions II, 1997, , 391-396.	0.9	5
92	The competition between H $_2$ O and CO $_2$ adhesion at reservoir conditions: A DFT study of simple mineral models and the entropy, ZPE, dispersion and T , P variations. Computational and Theoretical Chemistry, 2015, 1073, 55-60.	2.5	5
93	Crystalizing the interface – The first X-Ray structure of an oil/surfactant/brine transition layer. Journal of Petroleum Science and Engineering, 2020, 188, 106953.	4.2	5
94	Formation of three-membered phosphorus heterocycles via ligand-exchange reactions in mono-adducts of the phosphenium ion: an ab initio investigation. International Journal of Mass Spectrometry, 2000, 201, 205-213.	1.5	4
95	Atmospheric chemistry of (Z)-CF3CHHCl: products and mechanisms of the Cl atom, OH radical and O3 reactions, and role of (E)–(Z) isomerization. Physical Chemistry Chemical Physics, 2018, 20, 27949-27958.	2.8	4
96	Symmetry-induced kinetic isotope effects in the dissociation dynamics of CHCl3+ and CHCl4â^'. Chemical Physics, 2018, 515, 375-380.	1.9	4
97	Tuning and Tracking of Coherent Shear Waves in Molecular Films. ACS Omega, 2018, 3, 9929-9933.	3.5	4
98	Conformational Impact on Energy Storage Efficiency of Subphthalocyanine–Fullerene Hybrids. Journal of Physical Chemistry A, 2018, 122, 6683-6692.	2.5	4
99	Comprehensive Geophysical Study at Wabar Crater, Rub Alâ€Khali Desert, Saudi Arabia. Earth and Space Science, 2021, 8, e2020EA001432.	2.6	4
100	Transient Symmetry Controls Photo Dynamics near Conical Intersections. Journal of Physical Chemistry Letters, 2021, 12, 9220-9225.	4.6	4
101	Nonstatistical Photoinduced Processes in Gaseous Organic Molecules. ACS Omega, 2021, 6, 29325-29344.	3.5	4
102	Improving Long-Term Hydraulic Fracture Conductivity in Carbonate Formations by Substitution of Harder Minerals., 2021,,.		4
103	Far-UV Photochemical Bond Cleavage of <i>n</i> -Amyl Nitrite: Bypassing a Repulsive Surface. Journal of Physical Chemistry A, 2012, 116, 810-819.	2.5	3
104	Synthetic and mechanistic insight into nosylation of glycine residues. Organic and Biomolecular Chemistry, 2013, 11, 2288.	2.8	3
105	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	3.2	3
106	Coherent motion of excited state cyclic ketones: The have and the have-nots. Chemical Physics Letters, 2017, 683, 495-499.	2.6	3
107	Conformationally controlled ultrafast intersystem crossing in bithiophene systems. Physical Chemistry Chemical Physics, 2018, 20, 13412-13418.	2.8	3
108	Perspective: Preservation of coherence in photophysical processes. Structural Dynamics, 2018, 5, 060901.	2.3	3

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109	Putting the Disulfide Bridge at Risk: How UVâ€C Radiation Leads to Ultrafast Rupture of the Sâ€S Bond. ChemPhysChem, 2018, 19, 2829-2834.	2.1	3
110	Metaquat, a Paraquat Isomer Isolated from an Arrow Poison Acta Chemica Scandinavica, 1998, 52, 372-373.	0.7	3
111	Electronic Predissociation in the Dichloromethane Cation CH ₂ Cl ₂ _{+ Electronic State ²A₁. Journal of Physical Chemistry A, 2019, 123, 4048-4056.}	2.5	2
112	Design of Greenâ€Emitting Salts from Substituted Pyridines: Understanding the Solidâ€State Photodimerization of <i>trans</i> à€1,2â€bis(4â€pyridyl)ethylene. ChemPhysChem, 2021, 22, 1088-1093.	2.1	2
113	Molecular Transport across Oil–Brine Interfaces Impacts Interfacial Tension: Time-Effects in Buoyant and Pendant Drop Measurements. Langmuir, 2021, 37, 585-595.	3.5	2
114	Using Manganese Tetroxide for Hematite Settling Prevention in Water-Based Mud. Arabian Journal for Science and Engineering, 0 , 1 .	3.0	2
115	Methyl loss from conventional and distonic isomers of C3H7N·+. International Journal of Mass Spectrometry, 2000, 195-196, 459-466.	1.5	1
116	Vibrational and condensed phase dynamics: general discussion. Faraday Discussions, 2016, 194, 747-775.	3.2	1
117	Time-Resolved Photoelectron Studies of Thiophene and 2,5-Dimethylthiophene. Journal of Physical Chemistry A, 2018, 122, 8809-8818.	2.5	1
118	Tracing Production with Analytical Chemistry: Can Oil Finger Printing Provide New Answers., 2019,,.		1
119	Theoretical study of hydroxyl radical (OHË™) induced decomposition of <i>tert</i> -butyl methyl ether (MTBE). Environmental Sciences: Processes and Impacts, 2020, 22, 1037-1044.	3.5	1
120	The Sulfolene Protecting Group: Observation of a Direct Photoinitiated Cheletropic Ring Opening. ChemPhotoChem, 2021, 5, 863-870.	3.0	1
121	Femtochemistry of Norrish Type-I Reactions: III. Highly Excited Ketones—Theoretical. , 2002, 3, 57.		1
122	Atmospheric chemistry of CF3CN: kinetics and products of reaction with OH radicals, Cl atoms and O3. Physical Chemistry Chemical Physics, 2022, 24, 2638-2645.	2.8	1
123	Atmospheric chemistry of ($\langle i \rangle Z \langle i \rangle$)- and ($\langle i \rangle E \langle i \rangle$)-1,2-dichloroethene: kinetics and mechanisms of the reactions with Cl atoms, OH radicals, and O $\langle sub \rangle 3 \langle sub \rangle$. Physical Chemistry Chemical Physics, 2022, 24, 7356-7373.	2.8	1
124	Rýcktitelbild: Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation (Angew. Chem. 8/2013). Angewandte Chemie, 2013, 125, 2432-2432.	2.0	0
125	Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone. EPJ Web of Conferences, 2013, 41, 02033.	0.3	0
126	The consequences of two distinct reaction coordinates in the decomposition of the ethylamine cation conformers. Chemical Physics Letters, 2018, 701, 165-170.	2.6	0