Theis I SÃ¸lling

List of Publications by Year
in descending order

126 papers	3,100 citations	230014 27 h-index	206121 51 g-index
131 all docs	131 docs citations	131 times ranked	4238 citing authors

#	Article	IF	Citations
1	Hardness Enhancement of Carbonate Rocks by Formation of Smithsonite and Fluorite. Rock Mechanics and Rock Engineering, 2022, 55, 1001-1012.	2.6	7
2	Atmospheric chemistry of CF3CN: kinetics and products of reaction with OH radicals, Cl atoms and O3. Physical Chemistry Chemical Physics, 2022, 24, 2638-2645.	1.3	1
3	Atmospheric chemistry of (Z)- and (E)-1,2-dichloroethene: kinetics and mechanisms of the reactions with Cl atoms, OH radicals, and O₃. Physical Chemistry Chemical Physics, 2022, 24, 7356-7373.	1.3	1
4	Carbonate Rock Chemical Consolidation Methods: Advancement and Applications. Energy & Fuels, 2022, 36, 4186-4197.	2.5	11
5	Improving long-term hydraulic fracture conductivity by alteration of rock minerals. Journal of Petroleum Science and Engineering, 2021, 196, 108046.	2.1	22
6	Design of Greenâ€Emitting Salts from Substituted Pyridines: Understanding the Solidâ€State Photodimerization of transâ€1,2â€bis(4â€pyridyl)ethylene. ChemPhysChem, 2021, 22, 1088-1093.	1.0	2
7	The Sulfolene Protecting Group: Observation of a Direct Photoinitiated Cheletropic Ring Opening. ChemPhotoChem, 2021, 5, 863-870.	1.5	1
8	Prevention of Hematite Settling in Water-Based Mud at High Pressure and High Temperature. ACS Omega, 2021, 6, 23607-23613.	1.6	10
9	Comprehensive Geophysical Study at Wabar Crater, Rub Alâ€Khali Desert, Saudi Arabia. Earth and Space Science, 2021, 8, e2020EA001432.	1.1	4
10	Transient Symmetry Controls Photo Dynamics near Conical Intersections. Journal of Physical Chemistry Letters, 2021, 12, 9220-9225.	2.1	4
11	Nonstatistical Photoinduced Processes in Gaseous Organic Molecules. ACS Omega, 2021, 6, 29325-29344.	1.6	4
12	Molecular Transport across Oilâ€“Brine Interfaces Impacts Interfacial Tension: Time-Effects in Buoyant and Pendant Drop Measurements. Langmuir, 2021, 37, 585-595.	1.6	2
13	Improving Long-Term Hydraulic Fracture Conductivity in Carbonate Formations by Substitution of Harder Minerals. , 2021, , .		4
14	Foamstability: The interplay between salt-, surfactant- and critical micelle concentration. Journal of Petroleum Science and Engineering, 2020, 187, 106871.	2.1	48
15	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.	5.0	9
16	Improving carbonate rock hardness by consolidating additives to sustain long term fracture conductivity. Journal of Petroleum Science and Engineering, 2020, 195, 107897.	2.1	14
17	Theoretical study of hydroxyl radical (OHË™) induced decomposition of tert-butyl methyl ether (MTBE). Environmental Sciences: Processes and Impacts, 2020, 22, 1037-1044.	1.7	1
18	Crystalizing the interface â€“ The first X-Ray structure of an oil/surfactant/brine transition layer. Journal of Petroleum Science and Engineering, 2020, 188, 106953.	2.1	5

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19	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.	2.1	7
20	Symmetry controlled excited state dynamics. Physical Chemistry Chemical Physics, 2019, 21, 2283-2294.	1.3	13
21	Excitedâ€State Topology Modifications of the Dihydroazulene Photoswitch Through Aromaticity. ChemPhotoChem, 2019, 3, 619-629.	1.5	10
22	Electronic Predissociation in the Dichloromethane Cation CH₂Cl₂⁺ Electronic State ²A₁. Journal of Physical Chemistry A, 2019, 123, 4048-4056.	1.1	2
23	Tracing Production with Analytical Chemistry: Can Oil Finger Printing Provide New Answers. , 2019, , .		1
24	Vacuum ultraviolet excited state dynamics of small amides. Journal of Chemical Physics, 2019, 150, 054301.	1.2	7
25	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.	2.1	30
26	Solvent-dependent dual fluorescence of the pushâ€“pull system 2-diethylamino-7-nitrofluorene. Physical Chemistry Chemical Physics, 2018, 20, 5942-5951.	1.3	11
27	The consequences of two distinct reaction coordinates in the decomposition of the ethylamine cation conformers. Chemical Physics Letters, 2018, 701, 165-170.	1.2	0
28	Conformationally controlled ultrafast intersystem crossing in bithiophene systems. Physical Chemistry Chemical Physics, 2018, 20, 13412-13418.	1.3	3
29	Perspective: Preservation of coherence in photophysical processes. Structural Dynamics, 2018, 5, 060901.	0.9	3
30	Atmospheric chemistry of (Z)-CF3CHî€CHCl: products and mechanisms of the Cl atom, OH radical and O3 reactions, and role of (E)â€“(Z) isomerization. Physical Chemistry Chemical Physics, 2018, 20, 27949-27958.	1.3	4
31	Determining Orientations of Optical Transition Dipole Moments Using Ultrafast X-ray Scattering. Journal of Physical Chemistry Letters, 2018, 9, 6556-6562.	2.1	36
32	Chemical Composition and Structure of Adsorbed Material on Pore Surfaces in Middle East Reservoir Rocks. Energy & Fuels, 2018, 32, 11234-11242.	2.5	8
33	Vacuum ultraviolet excited state dynamics of the smallest ring, cyclopropane. II. Time-resolved photoelectron spectroscopy and ab initio dynamics. Journal of Chemical Physics, 2018, 149, 144311.	1.2	14
34	Time-Resolved Photoelectron Studies of Thiophene and 2,5-Dimethylthiophene. Journal of Physical Chemistry A, 2018, 122, 8809-8818.	1.1	1
35	Inverting the Selectivity of the Newmanâ€“Kwart Rearrangement via One Electron Oxidation at Room Temperature. Journal of Organic Chemistry, 2018, 83, 12000-12006.	1.7	24
36	Symmetry-induced kinetic isotope effects in the dissociation dynamics of CHCl3+ and CHCl4â^'. Chemical Physics, 2018, 515, 375-380.	0.9	4

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37	Putting the Disulfide Bridge at Risk: How UVâ€€ Radiation Leads to Ultrafast Rupture of the Sâ€€ Bond. ChemPhysChem, 2018, 19, 2829-2834.	1.0	3
38	A MALDI-TOF study of bio-remediation in highly weathered oil contaminated soils. Journal of Petroleum Science and Engineering, 2018, 168, 569-576.	2.1	20
39	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.	6.6	48
40	Tuning and Tracking of Coherent Shear Waves in Molecular Films. ACS Omega, 2018, 3, 9929-9933.	1.6	4
41	Benzylic Thio and Seleno Newmanâ€“Kwart Rearrangements. Journal of Organic Chemistry, 2018, 83, 10786-10797.	1.7	9
42	Conformational Impact on Energy Storage Efficiency of Subphthalocyanineâ€“Fullerene Hybrids. Journal of Physical Chemistry A, 2018, 122, 6683-6692.	1.1	4
43	Croconamides: a new dual hydrogen bond donating motif for anion recognition and organocatalysis. Organic and Biomolecular Chemistry, 2017, 15, 2784-2790.	1.5	23
44	Distortion dependent intersystem crossing: A femtosecond time-resolved photoelectron spectroscopy study of benzene, toluene, and p-xylene. Structural Dynamics, 2017, 4, 044008.	0.9	15
45	Coherent motion of excited state cyclic ketones: The have and the have-nots. Chemical Physics Letters, 2017, 683, 495-499.	1.2	3
46	Atmospheric chemistry of Z- and E-CF₃CHî€CHCF₃. Physical Chemistry Chemical Physics, 2017, 19, 735-750.	1.3	20
47	Revisiting the photophysics of 9-fluorenone: Ultrafast time-resolved fluorescence and theoretical studies. Chemical Physics Letters, 2017, 686, 218-222.	1.2	17
48	Conserving Coherence and Storing Energy during Internal Conversion: Photoinduced Dynamics of cis- and trans-Azobenzene Radical Cations. Journal of Physical Chemistry A, 2017, 121, 8642-8651.	1.1	18
49	Source identification of beached oil at Al Zubarah, Northwestern Qatar. Journal of Petroleum Science and Engineering, 2017, 149, 107-113.	2.1	24
50	Vibrational and condensed phase dynamics: general discussion. Faraday Discussions, 2016, 194, 747-775.	1.6	1
51	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	1.6	3
52	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.	2.1	31
53	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.	1.3	31
54	The involvement of triplet receiver states in the ultrafast excited state processes of small esters. Physical Chemistry Chemical Physics, 2016, 18, 24484-24497.	1.3	8

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55	Ultrafast relaxation dynamics of electronically excited piperidine: ionization signatures of Rydberg/valence evolution. Physical Chemistry Chemical Physics, 2016, 18, 25070-25079.	1.3	29
56	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.	1.1	20
57	The role of novel Rydberg-valence behaviour in the non-adiabatic dynamics of tertiary aliphatic amines. Chemical Science, 2016, 7, 1826-1839.	3.7	34
58	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.	1.1	5
59	Hydrocarbon Binding by Proteins: Structures of Protein Binding Sites for â‰¥C₁₀ Linear Alkanes or Long-Chain Alkyl and Alkenyl Groups. Journal of Organic Chemistry, 2015, 80, 997-1005.	1.7	8
60	Internal conversion mediated by specific nuclear motions: The nitrogen inversion in amines. Chemical Physics, 2014, 442, 62-67.	0.9	10
61	The Nonâ€Ergodic Nature of Internal Conversion. ChemPhysChem, 2014, 15, 249-259.	1.0	33
62	On the photostability of the disulfide bond: An electronic or a structural property?. Chemical Physics, 2014, 442, 77-80.	0.9	12
63	The Influence of Pushâ€“Pull States on the Ultrafast Intersystem Crossing in Nitroaromatics. Journal of Physical Chemistry B, 2013, 117, 9947-9955.	1.2	42
64	Conversion of Phenols into Selenophenols: Seleno Newmanâ€“Kwart Rearrangement. Angewandte Chemie - International Edition, 2013, 52, 12346-12349.	7.2	22
65	Synthetic and mechanistic insight into nosylation of glycine residues. Organic and Biomolecular Chemistry, 2013, 11, 2288.	1.5	3
66	On the Condensed Phase Ring-Closure of Vinylheptafulvalene and Ring-Opening of Gaseous Dihydroazulene. Journal of Physical Chemistry A, 2013, 117, 3340-3347.	1.1	42
67	Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation. Angewandte Chemie - International Edition, 2013, 52, 2247-2250.	7.2	19
68	RÃ¼cktitelbild: Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation (Angew. Chem. 8/2013). Angewandte Chemie, 2013, 125, 2432-2432.	1.6	0
69	Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone. EPJ Web of Conferences, 2013, 41, 02033.	0.1	0
70	Symmetry, vibrational energy redistribution and vibronic coupling: The internal conversion processes of cycloketones. Journal of Chemical Physics, 2012, 137, 22A522.	1.2	17
71	Surprising Intrinsic Photostability of the Disulfide Bridge Common in Proteins. Journal of the American Chemical Society, 2012, 134, 20279-20281.	6.6	20
72	Far-UV Photochemical Bond Cleavage of n-Amyl Nitrite: Bypassing a Repulsive Surface. Journal of Physical Chemistry A, 2012, 116, 810-819.	1.1	3

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73	The PaternÃ²â€“BÃ¼chi reaction: importance of triplet states in the excited-state reaction pathway. Physical Chemistry Chemical Physics, 2012, 14, 8572.	1.3	14
74	Coherent Motion Reveals Nonâ€Ergodic Nature of Internal Conversion between Excited States. ChemPhysChem, 2012, 13, 820-827.	1.0	28
75	Initial Dynamics of The Norrish Type I Reaction in Acetone: Probing Wave Packet Motion. Journal of Physical Chemistry A, 2011, 115, 556-561.	1.1	18
76	Real-Time Probing of Structural Dynamics by Interaction between Chromophores. Journal of Physical Chemistry A, 2011, 115, 12120-12125.	1.1	16
77	Electrophilic organic selenium reagentsâ€”protonated seleninic acids as precursors for unsymmetrical aromatic selenides. Tetrahedron, 2011, 67, 2633-2643.	1.0	26
78	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.	0.7	6
79	Pseudoâ€Bimolecular [2+2] Cycloaddition Studied by Timeâ€Resolved Photoelectron Spectroscopy. Chemistry - A European Journal, 2011, 17, 3922-3931.	1.7	18
80	Computational investigation of photo induced processes in alkyl nitrites and the product alkoxy radicals. Chemical Physics Letters, 2010, 484, 113-118.	1.2	24
81	On the absorption of the phenolatechromophore in the green fluorescent proteinâ€”role of individual interactions. Chemical Communications, 2010, 46, 734-736.	2.2	17
82	Probing the Lifetimes of Internally Excited Amyl Nitrite Cations. Journal of Physical Chemistry A, 2010, 114, 7021-7025.	1.1	20
83	Interpretation of the Ultrafast Photoinduced Processes in Pentacene Thin Films. Journal of the American Chemical Society, 2010, 132, 3431-3439.	6.6	59
84	Sparing the orthoâ€position in nucleophilic aromatic substitutionâ€specific displacement of the 4â€SePh group in 2,4â€bis(phenylseleno)nitrobenzene. Heteroatom Chemistry, 2009, 20, 101-108.	0.4	9
85	Charge-resonance excitations in symmetric molecules â€“ Comparison of linear response DFT with CC3 for the excited states of a model dimer. Chemical Physics Letters, 2009, 478, 127-131.	1.2	11
86	Excited-State Ions in Femtosecond Time-Resolved Mass Spectrometry: An Investigation of Highly Excited Chloroamines. Journal of Physical Chemistry A, 2009, 113, 40-43.	1.1	10
87	Comment on â€œTheoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffractionâ€. Journal of Physical Chemistry A, 2009, 113, 6849-6850.	1.1	10
88	New insights on the photodynamics of acetone excited with 253â¯288nm femtosecond pulses. Chemical Physics Letters, 2008, 461, 193-197.	1.2	34
89	Atmospheric photochemical loss of H and H2from formaldehyde: the relevance of ultrafast processes. Physical Chemistry Chemical Physics, 2008, 10, 674-680.	1.3	21
90	Wave Packet Simulation of Nonadiabatic Dynamics in Highly Excited 1,3-Dibromopropane. Journal of Physical Chemistry A, 2008, 112, 10481-10486.	1.1	9

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91	Computational predictions regarding ultrafast bond breakage and conformational changes in aliphatic chloro-amines. Computational and Theoretical Chemistry, 2007, 811, 117-124.	1.5	6
92	Energy Flow and Fragmentation Dynamics ofN,N-Dimethylisopropylamine. Journal of Physical Chemistry A, 2006, 110, 4251-4255.	1.1	51
93	Synthesis, Structure, and Properties of 4,7-Dimethoxybenzo[c]tellurophene: A Molecular Pyroelectric Material. Angewandte Chemie - International Edition, 2006, 45, 5666-5670.	7.2	10
94	Are Conical Intersections Responsible for the Ultrafast Processes of Adenine, Protonated Adenine, and the Corresponding Nucleosides?. ChemPhysChem, 2005, 6, 1276-1281.	1.0	80
95	Isomerization of the protonated acetone dimer in the gas phase. Journal of Mass Spectrometry, 2005, 40, 1076-1087.	0.7	8
96	Structure of Zone-Cast HBCâˆ’C12H25Films. Journal of the American Chemical Society, 2005, 127, 11288-11293.	6.6	63
97	Competing Simple Cleavage Reactions:Â The Elimination of Alkyl Radicals from Amine Radical Cations. Journal of the American Chemical Society, 2005, 127, 6466-6475.	6.6	17
98	Structural Surprises in Friction-Deposited Films of Poly(tetrafluoroethylene). Macromolecules, 2005, 38, 2383-2390.	2.2	33
99	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.	1.1	46
100	Substituent effects on the stability of extended benzylic carbocations: a computational study of conjugation. Organic and Biomolecular Chemistry, 2005, 3, 2441.	1.5	16
101	Enhanced Mobility of Poly(3-hexylthiophene) Transistors by Spin-Coating from High-Boiling-Point Solvents. Chemistry of Materials, 2004, 16, 4772-4776.	3.2	878
102	Optoelectronic Properties of Quasi-Linear, Self-Assembled Platinum Complexes: Ptâ€“Pt Distance Dependence. Advanced Functional Materials, 2004, 14, 323-328.	7.8	29
103	Macroscopic Alignment of Graphene Stacks by Langmuirâˆ’Blodgett Deposition of Amphiphilic Hexabenzocoronenes. Langmuir, 2004, 20, 4139-4146.	1.6	46
104	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.	6.6	109
105	Dynamics of Molecules near Ionization. Journal of Physical Chemistry A, 2003, 107, 10872-10887.	1.1	24
106	Coherent Dynamics in Complex Elimination Reactions:â€‰ Experimental and Theoretical Femtochemistry of 1,3-Dibromopropane and Related Systems,. Journal of Physical Chemistry A, 2002, 106, 7530-7546.	1.1	20
107	Femtochemistry of Norrish Type-I Reactions: III. Highly Excited Ketonesâ€”Theoretical. ChemPhysChem, 2002, 3, 57-78.	1.0	80
108	Femtochemistry of Norrish Type-I Reactions: IV. Highly Excited Ketonesâ€”Experimental. ChemPhysChem, 2002, 3, 79-97.	1.0	72

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109	Femtochemistry of Norrish Type-I Reactions: III. Highly Excited Ketonesâ€"Theoretical. , 2002, 3, 57.		1
110	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
111	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.	0.7	26
112	A G2 Study of SH+ Exchange Reactions Involving Lone-Pair Donors and Unsaturated Hydrocarbons. Chemistry - A European Journal, 2001, 7, 1516-1524.	1.7	15
113	Exchange of Cl+ between Lone-Pair Donors and Ï€-Donors: A Computational Study. European Journal of Mass Spectrometry, 2000, 6, 153-160.	0.5	8
114	Are the Approach Directions of Ïƒ and Ï€ Nucleophiles to the Sulfur Atom of Thiiranium and Thiirenium Ions Different?. Chemistry - A European Journal, 2000, 6, 590-591.	1.7	9
115	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.	0.7	4
116	Methyl loss from conventional and distonic isomers of C3H7NÂ·+. International Journal of Mass Spectrometry, 2000, 195-196, 459-466.	0.7	1
117	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.	0.8	12
118	Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation. International Journal of Mass Spectrometry, 1999, 185-187, 263-270.	0.7	10
119	Are Pi-Ligand Exchange Reactions of Thiirenium and Thiiranium Ions Feasible? An Ab Initio Investigation. Chemistry - A European Journal, 1999, 5, 509-514.	1.7	27
120	A G2 Ab Initio Investigation of Ligand-Exchange Reactions Involving Mono- and Bis-Adducts of the Phosphenium Ion. Inorganic Chemistry, 1999, 38, 6049-6054.	1.9	23
121	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.	6.6	39
122	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.	6.6	30
123	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
124	Metaquat, a Paraquat Isomer Isolated from an Arrow Poison.. Acta Chemica Scandinavica, 1998, 52, 372-373.	0.7	3
125	The expulsion of alkyl radicals from the methyliumylaminomethyl radical cation, Ë™CH2NH2CH3+, and related distonic ions. Journal of the Chemical Society Perkin Transactions II, 1997, , 391-396.	0.9	5
126	Using Manganese Tetroxide for Hematite Settling Prevention in Water-Based Mud. Arabian Journal for Science and Engineering, 0, , 1.	1.7	2