Anne-Marie Kelterer

List of Publications by Year
in descending order

64	1,088	394421 19	454955 30
papers	citations	h-index	g-index

68	68	68	1133
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An NHCâ€Mediated Metalâ€Free Approach towards an NHCâ€Coordinated Endocyclic Disilene. ChemistryOpen, 2022, , e202100240.	1.9	2
2	Interaction of 5â€fluorouracil with Î²â€cyclodextrin: A density functional theory study with dispersion correction. International Journal of Quantum Chemistry, 2021, 121, e26487.	2.0	9
3	Isolable Geminal Bisgermenolates: A New Synthon in Organometallic Chemistry. Angewandte Chemie - International Edition, 2021, 60, 23646-23650.	13.8	7
4	Isolable Geminal Bisgermenolates: A New Synthon in Organometallic Chemistry. Angewandte Chemie, 2021, 133, 23838.	2.0	0
5	Anharmonicity modeling in hydrogen bonded solvent dimers. Journal of Molecular Liquids, 2021, 339, 116735.	4.9	1
6	Synthesis and characterization of diacylgermanes: persistent derivatives with superior photoreactivity. Dalton Transactions, 2021, 50, 11965-11974.	3.3	4
7	Exciton Coupling and Conformational Changes Impacting the Excited State Properties of Metal Organic Frameworks. Molecules, 2020, 25, 4230.	3.8	9
8	The Chemistry of Acylgermanes: Triacylgermenolates Represent Valuable Building Blocks for the Synthesis of a Variety of Germanium-Based Photoinitiators. Inorganic Chemistry, 2020, 59, 15204-15217.	4.0	18
9	On Complex Formation between 5-Fluorouracil and Î²-Cyclodextrin in Solution and in the Solid State: IR Markers and Detection of Short-Lived Complexes by Diffusion NMR. Molecules, 2020, 25, 5706.	3.8	13
10	The â€œDark Sideâ€•of Germanium-Based Photoinitiatorsâ€”Connecting Redox Properties and Optical Absorption. Organometallics, 2020, 39, 2257-2268.	2.3	3
11	Conformational Analyses of Physiological Binary and Ternary Copper(II) Complexes with <scp>l</scp>â€Asparagine and <scp>l</scp>â€Histidine; Study of Tridentate Binding of Copper(II) in Aqueous Solution. ChemistryOpen, 2019, 8, 852-868.	1.9	3
12	Unprecedented Bifunctional Chemistry of Bis(acyl)phosphane Oxides in Aqueous and Alcoholic Media. Chemistry - A European Journal, 2019, 25, 8982-8986.	3.3	5
13	Anharmonicity of Vibrational Modes in Hydrogen Chlorideâ€“Water Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 2535-2547.	5.3	5
14	Installing lactone chain termini during photoinduced polymerization. Polymer Chemistry, 2018, 9, 3336-3341.	3.9	3
15	Competing Intramolecular Hydrogen Bond Strengths and Intermolecular Interactions in the 4-Aminobutanolâ€“Water Complex. Journal of Physical Chemistry A, 2018, 122, 8505-8510.	2.5	2
16	Quantum chemical computation-based strategy for alternating least squares initialization in multivariate curve resolution analysis of spectral-pH data. Microchemical Journal, 2018, 140, 183-188.	4.5	3
17	Chargeâ€Transfer Salts of 6,6â€Dicyanopentafulvenes: From Topology to Charge Separation in Solution. Chemistry - A European Journal, 2018, 24, 13616-13623.	3.3	1
18	Understanding Reactivity Patterns in Lightâ€Induced Nitrile Imine Mediated Tetrazoleâ€“Ene Cycloadditions. ChemPhotoChem, 2017, 1, 159-163.	3.0	27

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19	Wavelength-Dependent Photochemistry of Oxime Ester Photoinitiators. Macromolecules, 2017, 50, 1815-1823.	4.8	140
20	Infrared absorption of methanol-water clusters (CH3OH)n(H2O), n = 1â€“4, recorded with the VUV-ionization/IR-depletion technique. Journal of Chemical Physics, 2017, 146, 144308.	3.0	18
21	Insights into the Hydrogenâ€Atom Transfer of the Blue Aroxyl. ChemPhysChem, 2017, 18, 2932-2938.	2.1	0
22	Wavelength-Dependent Photochemical Stability of Photoinitiator-Derived Macromolecular Chain Termini. ACS Macro Letters, 2017, 6, 952-958.	4.8	18
23	Interplay of Intermolecular and Intramolecular Hydrogen Bonds on Complex Formation: The 3-Aminopropanolâ€“Water van der Waals Complex. Journal of Physical Chemistry A, 2017, 121, 6646-6651.	2.5	7
24	Bis(mesitoyl)phosphinic acid: photo-triggered release of metaphosphorous acid in solution. Chemical Communications, 2016, 52, 9917-9920.	4.1	17
25	Effect of the polarâ€“nonpolar liquid mixtures on pervaporative behavior of perfluorinated sulfonic membranes in lithium form. Journal of Membrane Science, 2016, 518, 313-327.	8.2	15
26	Ab initio study of cationic polymeric membranes in water and methanol. Ionics, 2016, 22, 357-367.	2.4	11
27	Rational design of long-wavelength absorbing and emitting carbostyrils aided by time-dependent density functional calculations. Computational and Theoretical Chemistry, 2015, 1055, 25-32.	2.5	4
28	Systematic Assessment of the Photochemical Stability of Photoinitiator-Derived Macromolecular Chain Termini. Macromolecules, 2015, 48, 8451-8460.	4.8	12
29	A Theoretical Study on Trivalent Europium: From the Free Ion to the Water Complex. Journal of Physical Chemistry A, 2014, 118, 11499-11511.	2.5	7
30	Computational and experimental studies on the triplet states of various N-substituted 4,5,6,7-tetrachlorophthalimides. Journal of Molecular Modeling, 2014, 20, 2344.	1.8	9
31	Long wavelength absorbing carbostyrils as test cases for different TDDFT procedures and solvent models. Journal of Molecular Modeling, 2014, 20, 2217.	1.8	6
32	Conductometric and computational study of cationic polymer membranes in H+ and Na+-forms at various hydration levels. Journal of Membrane Science, 2013, 444, 127-138.	8.2	24
33	Spectroscopic behavior of loratadine and desloratadine in different aqueous media conditions studied by means of TD-DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 250-258.	3.9	4
34	On the applicability of the molecular dynamics SCC-DFTB treatment on optical spectra simulations for thiophene and phenyl containing oligomers. Computational and Theoretical Chemistry, 2012, 999, 55-65.	2.5	2
35	Application of the Quantum Cluster Equilibrium (QCE) Model for the Liquid Phase of Primary Alcohols Using B3LYP and B3LYP-D DFT Methods. Journal of Physical Chemistry B, 2011, 115, 3936-3941.	2.6	30
36	Theoretical studies on the dimerization of substituted paraphenylenediamine radical cations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 368-378.	3.9	3

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37	Coordination of Methanol Clusters to Benzene: A Computational Study. Journal of Physical Chemistry A, 2011, 115, 10556-10564.	2.5	29
38	Theoretical and spectroscopic study of ethyl 1,4-dihydro-4-oxoquinoline-3-carboxylate and its 6-fluoro and 8-nitro derivatives in neutral and radical anion forms. Journal of Molecular Structure, 2011, 994, 61-69.	3.6	12
39	Photoinduced processes of 3-substituted 6-fluoro-1,4-dihydro-4-oxoquinoline derivatives: A theoretical and spectroscopic study. Journal of Photochemistry and Photobiology A: Chemistry, 2010, 211, 47-58.	3.9	9
40	Weinholdâ€™s QCE model â€“ A modified parameter fit. Model study of liquid methanol based on MP2 cluster geometries. Computational and Theoretical Chemistry, 2010, 956, 103-109.	1.5	33
41	Noncovalent Interaction between Aniline and Carbon Nanotubes: Effect of Nanotube Diameter and the Hydrogen-Bonded Solvent Methanol on the Adsorption Energy and the Photophysics. Journal of Physical Chemistry C, 2010, 114, 5898-5905.	3.1	14
42	Bisquinolones as chiral fluorophores â€“ A combined experimental and computational study of absorption and emission characteristics. Journal of Molecular Structure, 2009, 929, 85-96.	3.6	11
43	The Effect of Protonation on the Optical Properties of Conjugated Fluoreneâ€“Pyridine Copolymers. Macromolecular Chemistry and Physics, 2008, 209, 2122-2134.	2.2	20
44	Theoretical study of structure and electronic properties of cyano-substituted pyrroles. Chemical Physics, 2008, 353, 177-184.	1.9	13
45	Theoretical Study of Structure, Electronic Properties, and Photophysics of Cyano-Substituted Thiophenes and Terthiophenes. Journal of Physical Chemistry A, 2008, 112, 10931-10938.	2.5	14
46	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. Tetrahedron: Asymmetry, 2005, 16, 577-586.	1.8	21
47	ESR and ENDOR Investigations on Various Wurster?s Radical Cations in Solution. Experimental Results, Theoretical Ab Initio, and DFT Calculations. Monatshefte FÃ¼r Chemie, 2005, 136, 519-536.	1.8	23
48	Quantum Mechanics Studies of the Intrinsic Conformation of Trehalose. Journal of Physical Chemistry A, 2002, 106, 4988-4997.	2.5	39
49	QM/MM distortion energies in di- and oligosaccharides complexed with proteins. International Journal of Quantum Chemistry, 2001, 84, 416-425.	2.0	23
50	HF/6-31G* energy surfaces for disaccharide analogs. Journal of Computational Chemistry, 2001, 22, 65-78.	3.3	78
51	When anomeric effects collide. Journal of Computational Chemistry, 2001, 22, 1194-1204.	3.3	20
52	A QM/MM analysis of the conformations of crystalline sucrose moieties. Carbohydrate Research, 2000, 326, 305-322.	2.3	48
53	Constructing and evaluating energy surfaces of crystalline disaccharides. Journal of Molecular Graphics and Modelling, 2000, 18, 95-107.	2.4	63
54	Ab initio and molecular mechanics conformational analysis of neutralL-proline. International Journal of Quantum Chemistry, 1997, 65, 1033-1045.	2.0	43

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55	Theoretical structure investigations of N-acetyl-l-proline amide. Journal of Molecular Structure, 1995, 352-353, 59-70.	3.6	25
56	Basis set influence in ab initio calculations: The case of 2-aminoethanol and N-formylproline amide. Journal of Molecular Structure, 1994, 310, 45-53.	3.6	0
57	Basis set influence in ab initio calculations: the case of 2-aminoethanol and N-formylproline amide. Computational and Theoretical Chemistry, 1994, 310, 45-53.	1.5	12
58	Ab initio SCF investigation of the potential energy surface of 4-aminobutanol. International Journal of Quantum Chemistry, 1993, 48, 479-490.	2.0	5
59	Ab initio SCF investigation of 3-aminopropanol and 3-aminopropanal. Computational and Theoretical Chemistry, 1992, 276, 35-59.	1.5	12
60	Intramolecular interactions in Î²-alanine, 3-aminopropanal and 3-aminopropanol. Computational and Theoretical Chemistry, 1992, 276, 61-81.	1.5	27
61	Intramolecular hydrogen bonding in 2-aminoethanol, 3-aminopropanol and 4-aminobutanol. Computational and Theoretical Chemistry, 1991, 232, 189-201.	1.5	44
62	Isolable Stannenolates Enable the Synthesis of Visibleâ€Light Photoinitiators. ChemPhotoChem, 0, , .	3.0	5
63	Methionine-Based Radicals: Time Scales and Species. Applied Magnetic Resonance, 0, , .	1.2	0
64	The Road to Bisacyldigermanes â€•A New Compound Class Suitable as Visible Light Photoinitiators. ChemPhotoChem, 0, , .	3.0	2