

Anne-Marie Kelterer

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1522552/publications.pdf>

Version: 2024-02-01

64
papers

1,088
citations

394421

19
h-index

454955

30
g-index

68
all docs

68
docs citations

68
times ranked

1133
citing authors

#	ARTICLE	IF	CITATIONS
1	Wavelength-Dependent Photochemistry of Oxime Ester Photoinitiators. <i>Macromolecules</i> , 2017, 50, 1815-1823.	4.8	140
2	HF/6-31G* energy surfaces for disaccharide analogs. <i>Journal of Computational Chemistry</i> , 2001, 22, 65-78.	3.3	78
3	Constructing and evaluating energy surfaces of crystalline disaccharides. <i>Journal of Molecular Graphics and Modelling</i> , 2000, 18, 95-107.	2.4	63
4	A QM/MM analysis of the conformations of crystalline sucrose moieties. <i>Carbohydrate Research</i> , 2000, 326, 305-322.	2.3	48
5	Intramolecular hydrogen bonding in 2-aminoethanol, 3-aminopropanol and 4-aminobutanol. <i>Computational and Theoretical Chemistry</i> , 1991, 232, 189-201.	1.5	44
6	Ab initio and molecular mechanics conformational analysis of neutral L-proline. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 1033-1045.	2.0	43
7	Quantum Mechanics Studies of the Intrinsic Conformation of Trehalose. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4988-4997.	2.5	39
8	Weinhold's QCE model – A modified parameter fit. Model study of liquid methanol based on MP2 cluster geometries. <i>Computational and Theoretical Chemistry</i> , 2010, 956, 103-109.	1.5	33
9	Application of the Quantum Cluster Equilibrium (QCE) Model for the Liquid Phase of Primary Alcohols Using B3LYP and B3LYP-D DFT Methods. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3936-3941.	2.6	30
10	Coordination of Methanol Clusters to Benzene: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10556-10564.	2.5	29
11	Intramolecular interactions in L-alanine, 3-aminopropanol and 3-aminopropanol. <i>Computational and Theoretical Chemistry</i> , 1992, 276, 61-81.	1.5	27
12	Understanding Reactivity Patterns in Light-Induced Nitrile Imine Mediated Tetrazole-ene Cycloadditions. <i>ChemPhotoChem</i> , 2017, 1, 159-163.	3.0	27
13	Theoretical structure investigations of N-acetyl-L-proline amide. <i>Journal of Molecular Structure</i> , 1995, 352-353, 59-70.	3.6	25
14	Conductometric and computational study of cationic polymer membranes in H ⁺ and Na ⁺ -forms at various hydration levels. <i>Journal of Membrane Science</i> , 2013, 444, 127-138.	8.2	24
15	QM/MM distortion energies in di- and oligosaccharides complexed with proteins. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 416-425.	2.0	23
16	ESR and ENDOR Investigations on Various Wurster's Radical Cations in Solution. Experimental Results, Theoretical Ab Initio, and DFT Calculations. <i>Monatshefte für Chemie</i> , 2005, 136, 519-536.	1.8	23
17	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 577-586.	1.8	21
18	When anomeric effects collide. <i>Journal of Computational Chemistry</i> , 2001, 22, 1194-1204.	3.3	20

#	ARTICLE	IF	CITATIONS
19	The Effect of Protonation on the Optical Properties of Conjugated Fluorene-Pyridine Copolymers. <i>Macromolecular Chemistry and Physics</i> , 2008, 209, 2122-2134.	2.2	20
20	Infrared absorption of methanol-water clusters (CH ₃ OH) _n (H ₂ O), $n = 1-4$, recorded with the VUV-ionization/IR-depletion technique. <i>Journal of Chemical Physics</i> , 2017, 146, 144308.	3.0	18
21	Wavelength-Dependent Photochemical Stability of Photoinitiator-Derived Macromolecular Chain Termini. <i>ACS Macro Letters</i> , 2017, 6, 952-958.	4.8	18
22	The Chemistry of Acylgermanes: Triacylgermenolates Represent Valuable Building Blocks for the Synthesis of a Variety of Germanium-Based Photoinitiators. <i>Inorganic Chemistry</i> , 2020, 59, 15204-15217.	4.0	18
23	Bis(mesityl)phosphinic acid: photo-triggered release of metaphosphorous acid in solution. <i>Chemical Communications</i> , 2016, 52, 9917-9920.	4.1	17
24	Effect of the polar-nonpolar liquid mixtures on pervaporative behavior of perfluorinated sulfonic membranes in lithium form. <i>Journal of Membrane Science</i> , 2016, 518, 313-327.	8.2	15
25	Theoretical Study of Structure, Electronic Properties, and Photophysics of Cyano-Substituted Thiophenes and Terthiophenes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10931-10938.	2.5	14
26	Noncovalent Interaction between Aniline and Carbon Nanotubes: Effect of Nanotube Diameter and the Hydrogen-Bonded Solvent Methanol on the Adsorption Energy and the Photophysics. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5898-5905.	3.1	14
27	Theoretical study of structure and electronic properties of cyano-substituted pyrroles. <i>Chemical Physics</i> , 2008, 353, 177-184.	1.9	13
28	On Complex Formation between 5-Fluorouracil and β -Cyclodextrin in Solution and in the Solid State: IR Markers and Detection of Short-Lived Complexes by Diffusion NMR. <i>Molecules</i> , 2020, 25, 5706.	3.8	13
29	Ab initio SCF investigation of 3-aminopropanol and 3-aminopropanal. <i>Computational and Theoretical Chemistry</i> , 1992, 276, 35-59.	1.5	12
30	Basis set influence in ab initio calculations: the case of 2-aminoethanol and N-formylproline amide. <i>Computational and Theoretical Chemistry</i> , 1994, 310, 45-53.	1.5	12
31	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. <i>Journal of Molecular Structure</i> , 2011, 994, 61-69.	3.6	12
32	Systematic Assessment of the Photochemical Stability of Photoinitiator-Derived Macromolecular Chain Termini. <i>Macromolecules</i> , 2015, 48, 8451-8460.	4.8	12
33	Bisquinolones as chiral fluorophores - A combined experimental and computational study of absorption and emission characteristics. <i>Journal of Molecular Structure</i> , 2009, 929, 85-96.	3.6	11
34	Ab initio study of cationic polymeric membranes in water and methanol. <i>Ionics</i> , 2016, 22, 357-367.	2.4	11
35	Photoinduced processes of 3-substituted 6-fluoro-1,4-dihydro-4-oxoquinoline derivatives: A theoretical and spectroscopic study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010, 211, 47-58.	3.9	9
36	Computational and experimental studies on the triplet states of various N-substituted 4,5,6,7-tetrachlorophthalimides. <i>Journal of Molecular Modeling</i> , 2014, 20, 2344.	1.8	9

#	ARTICLE	IF	CITATIONS
37	Exciton Coupling and Conformational Changes Impacting the Excited State Properties of Metal Organic Frameworks. <i>Molecules</i> , 2020, 25, 4230.	3.8	9
38	Interaction of 5-Fluorouracil with β -Cyclodextrin: A density functional theory study with dispersion correction. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26487.	2.0	9
39	A Theoretical Study on Trivalent Europium: From the Free Ion to the Water Complex. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11499-11511.	2.5	7
40	Interplay of Intermolecular and Intramolecular Hydrogen Bonds on Complex Formation: The 3-Aminopropanol-Water van der Waals Complex. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6646-6651.	2.5	7
41	Isolable Geminal Bisgermenolates: A New Synthons in Organometallic Chemistry. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 23646-23650.	13.8	7
42	Long wavelength absorbing carbostyrils as test cases for different TDDFT procedures and solvent models. <i>Journal of Molecular Modeling</i> , 2014, 20, 2217.	1.8	6
43	Ab initio SCF investigation of the potential energy surface of 4-aminobutanol. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 479-490.	2.0	5
44	Unprecedented Bifunctional Chemistry of Bis(acyl)phosphane Oxides in Aqueous and Alcoholic Media. <i>Chemistry - A European Journal</i> , 2019, 25, 8982-8986.	3.3	5
45	Anharmonicity of Vibrational Modes in Hydrogen Chloride-Water Mixtures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2535-2547.	5.3	5
46	Isolable Stannenolates Enable the Synthesis of Visible-Light Photoinitiators. <i>ChemPhotoChem</i> , 0, , .	3.0	5
47	Spectroscopic behavior of loratadine and desloratadine in different aqueous media conditions studied by means of TD-DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 250-258.	3.9	4
48	Rational design of long-wavelength absorbing and emitting carbostyrils aided by time-dependent density functional calculations. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 25-32.	2.5	4
49	Synthesis and characterization of diacylgermanes: persistent derivatives with superior photoreactivity. <i>Dalton Transactions</i> , 2021, 50, 11965-11974.	3.3	4
50	Theoretical studies on the dimerization of substituted paraphenylenediamine radical cations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 368-378.	3.9	3
51	Installing lactone chain termini during photoinduced polymerization. <i>Polymer Chemistry</i> , 2018, 9, 3336-3341.	3.9	3
52	Quantum chemical computation-based strategy for alternating least squares initialization in multivariate curve resolution analysis of spectral-pH data. <i>Microchemical Journal</i> , 2018, 140, 183-188.	4.5	3
53	Conformational Analyses of Physiological Binary and Ternary Copper(II) Complexes with Asparagine and Histidine; Study of Tridentate Binding of Copper(II) in Aqueous Solution. <i>ChemistryOpen</i> , 2019, 8, 852-868.	1.9	3
54	The "Dark Side" of Germanium-Based Photoinitiators: Connecting Redox Properties and Optical Absorption. <i>Organometallics</i> , 2020, 39, 2257-2268.	2.3	3

#	ARTICLE	IF	CITATIONS
55	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
56	Competing Intramolecular Hydrogen Bond Strengths and Intermolecular Interactions in the 4-Aminobutanol-Water Complex. Journal of Physical Chemistry A, 2018, 122, 8505-8510.	2.5	2
57	An NHC-Mediated Metal-Free Approach towards an NHC-Coordinated Endocyclic Disilene. ChemistryOpen, 2022, , e202100240.	1.9	2
58	The Road to Bisacyldigermanes - A New Compound Class Suitable as Visible Light Photoinitiators. ChemPhotoChem, 0, , .	3.0	2
59	Charge-Transfer Salts of 6,6-Dicyanopentafulvenes: From Topology to Charge Separation in Solution. Chemistry - A European Journal, 2018, 24, 13616-13623.	3.3	1
60	Anharmonicity modeling in hydrogen bonded solvent dimers. Journal of Molecular Liquids, 2021, 339, 116735.	4.9	1
61	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
62	Insights into the Hydrogen-Atom Transfer of the Blue Aroxyl. ChemPhysChem, 2017, 18, 2932-2938.	2.1	0
63	Isolable Geminal Bisgermenolates: A New Synthon in Organometallic Chemistry. Angewandte Chemie, 2021, 133, 23838.	2.0	0
64	Methionine-Based Radicals: Time Scales and Species. Applied Magnetic Resonance, 0, , .	1.2	0