

Ulrike Salzner

List of Publications by Year in descending order

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59
papers

3,455
citations

218381

26
h-index

143772

57
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60
all docs

60
docs citations

60
times ranked

3762
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuned Range-Separated Hybrids in Density Functional Theory. <i>Annual Review of Physical Chemistry</i> , 2010, 61, 85-109.	4.8	661
2	Comparison of geometries and electronic structures of polyacetylene, polyborole, polycyclopentadiene, polypyrrole, polyfuran, polysilole, polyphosphole, polythiophene, polyselenophene and polytellurophene. <i>Synthetic Metals</i> , 1998, 96, 177-189.	2.1	331
3	Ab Initio Examination of Anomeric Effects in Tetrahydropyrans, 1,3-Dioxanes, and Glucose. <i>Journal of Organic Chemistry</i> , 1994, 59, 2138-2155.	1.7	224
4	Improved Prediction of Properties of π -Conjugated Oligomers with Range-Separated Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2568-2583.	2.3	202
5	Koopmans's ϵ springs to life. <i>Journal of Chemical Physics</i> , 2009, 131, 231101.	1.2	184
6	Generalized anomeric effects and hyperconjugation in $\text{CH}_2(\text{OH})_2$, $\text{CH}_2(\text{SH})_2$, $\text{CH}_2(\text{SeH})_2$, and $\text{CH}_2(\text{TeH})_2$. <i>Journal of the American Chemical Society</i> , 1993, 115, 10231-10236.	6.6	180
7	Accurate Method for Obtaining Band Gaps in Conducting Polymers Using a DFT/Hybrid Approach. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2572-2578.	1.1	153
8	Design of low band gap polymers employing density functional theory/hybrid functionals ameliorate band gap problem. <i>Journal of Computational Chemistry</i> , 1997, 18, 1943-1953.	1.5	144
9	Electronic structure of conducting organic polymers: insights from time-dependent density functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 601-622.	6.2	79
10	Does the Donor-Acceptor Concept Work for Designing Synthetic Metals? 2. Theoretical Investigation of Copolymers of 4-(Dicyanomethylene)-4H-cyclopenta[2,1-b:3,4-b']dithiophene and 3,4-(Ethylenedioxy)thiophene. <i>Journal of Physical Chemistry B</i> , 2002, 106, 9221-9226.	1.2	68
11	Does the Donor-Acceptor Concept Work for Designing Synthetic Metals? 1. Theoretical Investigation of Poly(3-cyano-3'-hydroxybithiophene). <i>Journal of Physical Chemistry B</i> , 2002, 106, 9214-9220.	1.2	62
12	Conducting Copolymers of Pyridine with Thiophene, N-Methylpyrrole, and Selenophene. <i>Chemistry of Materials</i> , 1996, 8, 2444-2450.	3.2	60
13	Theoretical Investigation of Excited States of Oligothiophenes and of Their Monocations. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1143-1157.	2.3	60
14	Nature of Charge Carriers in Long Doped Oligothiophenes: The Effect of Counterions. <i>Journal of Physical Chemistry C</i> , 2008, 112, 8408-8418.	1.5	57
15	Trends in molecular design strategies for ambient stable n-channel organic field effect transistors. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7404-7430.	2.7	56
16	Investigation of Charge Carriers in Doped Thiophene Oligomers through Theoretical Modeling of their UV/Vis Spectra. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5458-5466.	1.1	55
17	Origin of the Anomeric Effect Revisited. Theoretical Conformation Analysis of 2-Hydroxypiperidine and 2-Hydroxyhexahydropyrimidine. <i>Journal of Organic Chemistry</i> , 1995, 60, 986-995.	1.7	54
18	Use of side-chain for rational design of n-type diketopyrrolopyrrole-based conjugated polymers: what did we find out?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17253-17265.	1.3	54

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19	Does the donor-acceptor concept work for designing synthetic metals?. Journal of Molecular Modeling, 2006, 12, 687-701.	0.8	52
20	Quantitatively Correct UV-vis Spectrum of Ferrocene with TDB3LYP. Journal of Chemical Theory and Computation, 2013, 9, 4064-4073.	2.3	48
21	Theoretical Design of Conjugated Organic Polymers. Current Organic Chemistry, 2004, 8, 569-590.	0.9	43
22	Air-Stable <i>n</i> -channel Diketopyrrolopyrrole-Diketopyrrolopyrrole Oligomers for High Performance Ambipolar Organic Transistors. ACS Applied Materials & Interfaces, 2016, 8, 25415-25427.	4.0	36
23	Spin density encodes intramolecular singlet exciton fission in pentacene dimers. Nature Communications, 2019, 10, 33.	5.8	34
24	Theoretical Modeling of the Doping Process in Polypyrrole by Calculating UV/Vis Absorption Spectra of Neutral and Charged Oligomers. Journal of Physical Chemistry A, 2008, 112, 11842-11853.	1.1	33
25	Ab Initio Studies of the Dimerization of Ketene and Phosphaketene. Journal of the American Chemical Society, 1994, 116, 6850-6855.	6.6	31
26	XPS-evidence for in-situ electrochemically-generated carbene formation. Electrochimica Acta, 2017, 234, 37-42.	2.6	28
27	Ab initio studies of the geometries and electronic structures of CaF ₂ and CaCl ₂ . Chemical Physics Letters, 1990, 172, 461-470.	1.2	26
28	Effect of Donor-Acceptor Substitution on Optoelectronic Properties of Conducting Organic Polymers. Journal of Chemical Theory and Computation, 2014, 10, 4921-4937.	2.3	26
29	Cycloaddition Reactions between Cyclopentadiene and Ketene. Ab Initio Examination of [2 + 2] and [4 + 2] Pathways. Journal of Organic Chemistry, 1996, 61, 237-242.	1.7	25
30	Effect of Chalcogens on Electronic and Photophysical Properties of Vinylene-Based Diketopyrrolopyrrole Copolymers. Journal of Physical Chemistry B, 2015, 119, 11307-11316.	1.2	25
31	Theoretical Investigation of Excited States of Oligothiophene Anions. Journal of Physical Chemistry A, 2008, 112, 6053-6058.	1.1	23
32	Effects of Perfluorination on Thiophene and Pyrrole Oligomers. Journal of Physical Chemistry A, 2010, 114, 5397-5405.	1.1	23
33	CH ₄ ⁿ X _n : a comparison between the stabilized X ⁺ → F series and the destabilized X ⁺ → CN series. Chemical Physics Letters, 1992, 190, 401-406.	1.2	22
34	Theoretical Investigation of Excited States of Large Polyene Cations as Model Systems for Lightly Doped Polyacetylene. Journal of Chemical Theory and Computation, 2007, 3, 219-231.	2.3	22
35	Density Functional Theory Investigation of Substituent Effects on Building Blocks of Conducting Polymers. Synthetic Metals, 1999, 101, 482-483.	2.1	21
36	Synthesis and Characterization of Quinoidal Diketopyrrolopyrrole Derivatives with Exceptionally High Electron Affinities. Journal of Physical Chemistry C, 2017, 121, 16088-16097.	1.5	19

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37	Electrochemical polymerization of ambipolar carbonyl-functionalized indenofluorene with memristive properties. <i>Optical Materials</i> , 2019, 94, 187-195.	1.7	19
38	A successful ab initio study of the adiabatic electron affinity of the methyl radical. <i>Chemical Physics Letters</i> , 1992, 199, 267-274.	1.2	18
39	Theoretical Analysis of Substituent Effects on Building Blocks of Conducting Polymers: π -3,4-Substituted Bithiophenes. <i>Journal of Organic Chemistry</i> , 1999, 64, 764-769.	1.7	18
40	Theoretical Analysis of Effects of π -Conjugating Substituents on Building Blocks for Conducting Polymers. <i>Journal of Organic Chemistry</i> , 1999, 64, 7419-7425.	1.7	17
41	Investigation of the effect of donor-acceptor substitution on band gap, band width, and conductivity. <i>Synthetic Metals</i> , 2001, 119, 215-216.	2.1	17
42	Modeling Photoelectron Spectra of Conjugated Oligomers with Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10997-11007.	1.1	16
43	Theoretical Analysis of Poly(difluoroacetylene). <i>Journal of Physical Chemistry B</i> , 2003, 107, 1129-1134.	1.2	15
44	Are there anomeric effects involving selenium?. <i>Journal of the Chemical Society Chemical Communications</i> , 1990, , 190-192.	2.0	13
45	Cycloaddition reactions between 2 H-phosphole and phosphaketene: Ab initio examination of [2 + 2] and [4 + 2] pathways. <i>Journal of Organometallic Chemistry</i> , 1997, 529, 15-22.	0.8	13
46	Pyramidalized Double Bonds Containing Endoperoxide Linkages: Photooxygenation of Dimethylcis-3,8-Dihydroheptalene-3,8-dicarboxylate. <i>Journal of Organic Chemistry</i> , 1999, 64, 6670-6676.	1.7	13
47	Topological electron density analysis of organosulfur compounds. <i>Computational and Theoretical Chemistry</i> , 1995, 337, 201-207.	1.5	10
48	Numerical solution of a partial differential equation system describing chemical kinetics and diffusion in a cell with the aid of compartmentalization. <i>Journal of Computational Chemistry</i> , 1990, 11, 194-204.	1.5	9
49	Ab initio investigation of the diels-alder reaction between 2H-phosphole and phosphoethene: A model for phosphole dimerization. <i>Journal of Computational Chemistry</i> , 1997, 18, 198-210.	1.5	9
50	Electronic Structure Analysis of a New Quinoid Conjugated Polymer. <i>Journal of Molecular Modeling</i> , 2000, 6, 195-204.	0.8	9
51	Fermi Level Pinning Induced by Doping in Air Stable n-Type Organic Semiconductor. <i>ACS Applied Electronic Materials</i> , 2020, 2, 66-73.	2.0	9
52	1,6-Diphospha-1,5-hexadiene and the Phospha-Cope Rearrangement: An ab Initio Investigation. <i>Journal of Organic Chemistry</i> , 1995, 60, 7101-7109.	1.7	7
53	Selenium in Diketopyrrolopyrrole-Based Polymers: Influence on Electronic Properties and Charge Carrier Mobilities. <i>Israel Journal of Chemistry</i> , 2014, 54, 817-827.	1.0	6
54	Electrochemical Stability and Ambipolar Charge Transport in Diketopyrrolopyrrole-Based Organic Materials. <i>ACS Applied Electronic Materials</i> , 2019, 1, 2037-2046.	2.0	5

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55	Theoretical Analysis of Poly(difluoroacetylene) PDFA. Synthetic Metals, 2003, 135-136, 311-312.	2.1	4
56	Optoelectronic properties of diketopyrrolopyrrole homopolymers compared to donor-acceptor copolymers. Journal of Chemical Physics, 2021, 154, 054309.	1.2	2
57	Density functional theory orbital energies for predicting ionization energies. , 2012, , .		1
58	Schade, daŸ Deutschland seine jungen Akademiker nicht brauchen kann. Nachrichten Aus Der Chemie, 2001, 49, 515-516.	0.0	0
59	Does the donor-acceptor concept work for designing synthetic metals?. , 2006, , 687-701.		0