Ulrike Salzner

List of Publications by Year
in descending order

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59	3,455	218381	143772
papers	citations	26 h-index	57 g-index

60	60	60	3762
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optoelectronic properties of diketopyrrolopyrrole homopolymers compared to donorâ€“acceptor copolymers. Journal of Chemical Physics, 2021, 154, 054309.	1.2	2
2	Fermi Level Pinning Induced by Doping in Air Stable n-Type Organic Semiconductor. ACS Applied Electronic Materials, 2020, 2, 66-73.	2.0	9
3	Electrochemical Stability and Ambipolar Charge Transport in Diketopyrrolopyrrole-Based Organic Materials. ACS Applied Electronic Materials, 2019, 1, 2037-2046.	2.0	5
4	Electrochemical polymerization of ambipolar carbonyl-functionalized indenofluorene with memristive properties. Optical Materials, 2019, 94, 187-195.	1.7	19
5	Spin density encodes intramolecular singlet exciton fission in pentacene dimers. Nature Communications, 2019, 10, 33.	5.8	34
6	Trends in molecular design strategies for ambient stable n-channel organic field effect transistors. Journal of Materials Chemistry C, 2017, 5, 7404-7430.	2.7	56
7	XPS-evidence for in-situ electrochemically-generated carbene formation. Electrochimica Acta, 2017, 234, 37-42.	2.6	28
8	Synthesis and Characterization of Quinoidal Diketopyrrolopyrrole Derivatives with Exceptionally High Electron Affinities. Journal of Physical Chemistry C, 2017, 121, 16088-16097.	1.5	19
9	Air-Stable n-channel Diketopyrrolopyrroleâ^'Diketopyrrolopyrrole Oligomers for High Performance Ambipolar Organic Transistors. ACS Applied Materials & Interfaces, 2016, 8, 25415-25427.	4.0	36
10	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
11	Selenium in Diketopyrrolopyrroleâ€based Polymers: Influence on Electronic Properties and Charge Carrier Mobilities. Israel Journal of Chemistry, 2014, 54, 817-827.	1.0	6
12	Electronic structure of conducting organic polymers: insights from timeâ€dependent density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 601-622.	6.2	79
13	Effect of Donorâ€“Acceptor Substitution on Optoelectronic Properties of Conducting Organic Polymers. Journal of Chemical Theory and Computation, 2014, 10, 4921-4937.	2.3	26
14	Use of side-chain for rational design of n-type diketopyrrolopyrrole-based conjugated polymers: what did we find out?. Physical Chemistry Chemical Physics, 2014, 16, 17253-17265.	1.3	54
15	Quantitatively Correct UV-vis Spectrum of Ferrocene with TDB3LYP. Journal of Chemical Theory and Computation, 2013, 9, 4064-4073.	2.3	48
16	Density functional theory orbital energies for predicting ionization energies. , 2012, , .		1
17	Improved Prediction of Properties of Ï€-Conjugated Oligomers with Range-Separated Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 2568-2583.	2.3	202
18	Modeling Photoelectron Spectra of Conjugated Oligomers with Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2010, 114, 10997-11007.	1.1	16

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19	Effects of Perfluorination on Thiophene and Pyrrole Oligomers. Journal of Physical Chemistry A, 2010, 114, 5397-5405.	1.1	23
20	Tuned Range-Separated Hybrids in Density Functional Theory. Annual Review of Physical Chemistry, 2010, 61, 85-109.	4.8	661
21	Koopmansâ€™ springs to life. Journal of Chemical Physics, 2009, 131, 231101.	1.2	184
22	Theoretical Investigation of Excited States of Oligothiophene Anions. Journal of Physical Chemistry A, 2008, 112, 6053-6058.	1.1	23
23	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
24	Investigation of Charge Carriers in Doped Thiophene Oligomers through Theoretical Modeling of their UV/Vis Spectra. Journal of Physical Chemistry A, 2008, 112, 5458-5466.	1.1	55
25	Nature of Charge Carriers in Long Doped Oligothiophenes: The Effect of Counterions. Journal of Physical Chemistry C, 2008, 112, 8408-8418.	1.5	57
26	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
27	Theoretical Investigation of Excited States of Oligothiophenes and of Their Monocations. Journal of Chemical Theory and Computation, 2007, 3, 1143-1157.	2.3	60
28	Does the donorâ€“acceptor concept work for designing synthetic metals?. Journal of Molecular Modeling, 2006, 12, 687-701.	0.8	52
29	Does the donor-acceptor concept work for designing synthetic metals?. , 2006, , 687-701.		0
30	Theoretical Design of Conjugated Organic Polymers. Current Organic Chemistry, 2004, 8, 569-590.	0.9	43
31	Theoretical Analysis of Poly(difluoroacetylene). Journal of Physical Chemistry B, 2003, 107, 1129-1134.	1.2	15
32	Theoretical Analysis of Poly(difluoroacetylene) PDFA. Synthetic Metals, 2003, 135-136, 311-312.	2.1	4
33	Does the Donorâ”Acceptor Concept Work for Designing Synthetic Metals? 1. Theoretical Investigation of Poly(3-cyano-3â€˜-hydroxybithiophene). Journal of Physical Chemistry B, 2002, 106, 9214-9220.	1.2	62
34	Does the Donorâ”Acceptor Concept Work for Designing Synthetic Metals? 2. Theoretical Investigation of Copolymers of 4-(Dicyanomethylene)-4H-cyclopenta[2,1-b:3,4-bâ€˜]dithiophene and 3,4-(Ethylenedioxy)thiophene. Journal of Physical Chemistry B, 2002, 106, 9221-9226.	1.2	68
35	Investigation of the effect of donor-acceptor substitution on band gap, band width, and conductivity. Synthetic Metals, 2001, 119, 215-216.	2.1	17
36	Schade, daÃŸ Deutschland seine jungen Akademiker nicht brauchen kann. Nachrichten Aus Der Chemie, 2001, 49, 515-516.	0.0	0

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37	Electronic Structure Analysis of a New Quinoid Conjugated Polymer. Journal of Molecular Modeling, 2000, 6, 195-204.	0.8	9
38	Theoretical Analysis of Effects of Ï€-Conjugating Substituents on Building Blocks for Conducting Polymers. Journal of Organic Chemistry, 1999, 64, 7419-7425.	1.7	17
39	Density Functional Theory Investigation of Substituent Effects on Building Blocks of Conducting Polymers. Synthetic Metals, 1999, 101, 482-483.	2.1	21
40	Theoretical Analysis of Substituent Effects on Building Blocks of Conducting Polymers:Â 3,4â€˜-Substituted Bithiophenes. Journal of Organic Chemistry, 1999, 64, 764-769.	1.7	18
41	Pyramidalized Double Bonds Containing Endoperoxide Linkages:Â Photooxygenation of Dimethylcis-3,8-Dihydroheptalene-3,8-dicarboxylate. Journal of Organic Chemistry, 1999, 64, 6670-6676.	1.7	13
42	Comparison of geometries and electronic structures of polyacetylene, polyborole, polycyclopentadiene, polypyrrole, polyfuran, polysilole, polyphosphole, polythiophene, polyselenophene and polytellurophene. Synthetic Metals, 1998, 96, 177-189.	2.1	331
43	Accurate Method for Obtaining Band Gaps in Conducting Polymers Using a DFT/Hybrid Approach. Journal of Physical Chemistry A, 1998, 102, 2572-2578.	1.1	153
44	Cycloaddition reactions between 2 H-phosphole and phosphaketene: Ab initio examination of [2 + 2] and [4 + 2] pathways. Journal of Organometallic Chemistry, 1997, 529, 15-22.	0.8	13
45	Ab initio investigation of the diels-alder reaction between 2H-phosphole and phosphaethene: A model for phosphole dimerization. Journal of Computational Chemistry, 1997, 18, 198-210.	1.5	9
46	Design of low band gap polymers employing density functional theory?hybrid functionals ameliorate band gap problem. Journal of Computational Chemistry, 1997, 18, 1943-1953.	1.5	144
47	Conducting Copolymers of Pyridine with Thiophene, N-Methylpyrrole, and Selenophene. Chemistry of Materials, 1996, 8, 2444-2450.	3.2	60
48	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
49	Topological electron density analysis of organosulfur compounds. Computational and Theoretical Chemistry, 1995, 337, 201-207.	1.5	10
50	1,6-Diphospha-1,5-hexadiene and the Phospha-Cope Rearrangement: An ab Initio Investigation. Journal of Organic Chemistry, 1995, 60, 7101-7109.	1.7	7
51	Origin of the Anomeric Effect Revisited. Theoretical Conformation Analysis of 2-Hydroxypiperidine and 2-Hydroxyhexahydropyrimidine. Journal of Organic Chemistry, 1995, 60, 986-995.	1.7	54
52	Ab Initio Examination of Anomeric Effects in Tetrahydropyrans, 1,3-Dioxanes, and Glucose. Journal of Organic Chemistry, 1994, 59, 2138-2155.	1.7	224
53	Ab Initio Studies of the Dimerization of Ketene and Phosphaketene. Journal of the American Chemical Society, 1994, 116, 6850-6855.	6.6	31
54	Generalized anomeric effects and hyperconjugation in CH2(OH)2, CH2(SH)2, CH2(SeH)2, and CH2(TeH)2. Journal of the American Chemical Society, 1993, 115, 10231-10236.	6.6	180

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55	A successful ab initio study of the adiabatic electron affinity of the methyl radical. Chemical Physics Letters, 1992, 199, 267-274.	1.2	18
56	CH4â^'nXn: a comparison between the stabilized X î—» F series and the destabilized X î—» CN series. Chemical Physics Letters, 1992, 190, 401-406.	1.2	22
57	Ab initio studies of the geometries and electronic structures of CaF2 and CaCl2. Chemical Physics Letters, 1990, 172, 461-470.	1.2	26
58	Numerical solution of a partial differential equation system describing chemical kinetics and diffusion in a cell with the aid of compartmentalization. Journal of Computational Chemistry, 1990, 11, 194-204.	1.5	9
59	Are there anomeric effects involving selenium?. Journal of the Chemical Society Chemical Communications, 1990, , 190-192.	2.0	13