

Egbert Zojer

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5507334/publications.pdf>

Version: 2024-02-01

228
papers

10,134
citations

31949

53
h-index

42364

92
g-index

235
all docs

235
docs citations

235
times ranked

9525
citing authors

#	ARTICLE	IF	CITATIONS
1	Density-Functional Theory with Screened vanÂderÂWaal Interactions for the Modeling of Hybrid Inorganic-Organic Systems. <i>Physical Review Letters</i> , 2012, 108, 146103.	2.9	503
2	The Interface Energetics of Self-Assembled Monolayers on Metals. <i>Accounts of Chemical Research</i> , 2008, 41, 721-729.	7.6	371
3	Title is missing!. <i>Advanced Functional Materials</i> , 2002, 12, 631-641.	7.8	366
4	Interface Energetics and Level Alignment at Covalent Metal-Molecule Junctions: Î€-Conjugated Thiols on Gold. <i>Physical Review Letters</i> , 2006, 96, 196806.	2.9	258
5	Toward Control of the Metalâ”Organic Interfacial Electronic Structure in Molecular Electronics:Â A First-Principles Study on Self-Assembled Monolayers of Î€-Conjugated Molecules on Noble Metals. <i>Nano Letters</i> , 2007, 7, 932-940.	4.5	257
6	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. <i>MRS Bulletin</i> , 2010, 35, 435-442.	1.7	257
7	The Origin of Green Emission in Polyfluorene-Based Conjugated Polymers: On-Chain Defect Fluorescence. <i>Advanced Functional Materials</i> , 2003, 13, 597-601.	7.8	255
8	Metal-Ion Sensing Fluorophores with Large Two-Photon Absorption Cross Sections:Â Aza-Crown Ether Substituted Donorâ”Acceptorâ”Donor Distyrylbenzenes. <i>Journal of the American Chemical Society</i> , 2004, 126, 9291-9306.	6.6	206
9	Impact of Bidirectional Charge Transfer and Molecular Distortions on the Electronic Structure of a Metal-Organic Interface. <i>Physical Review Letters</i> , 2007, 99, 256801.	2.9	206
10	Extended Squaraine Dyes with Large Two-Photon Absorption Cross-Sections. <i>Journal of the American Chemical Society</i> , 2006, 128, 14444-14445.	6.6	205
11	Green emission from poly(fluorene)s: The role of oxidation. <i>Journal of Chemical Physics</i> , 2002, 117, 6794-6802.	1.2	190
12	Theoretical study of PTCDA adsorbed on the coinage metal surfaces, Ag(111), Au(111) and Cu(111). <i>New Journal of Physics</i> , 2009, 11, 053010.	1.2	182
13	Two-Photon Absorption at Telecommunications Wavelengths in a Dipolar Chromophore with a Pyrrole Auxiliary Donor and Thiazole Auxiliary Acceptor. <i>Journal of the American Chemical Society</i> , 2005, 127, 7282-7283.	6.6	150
14	Aromatic Amines:â€” A Comparison of Electron-Donor Strengths. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9346-9352.	1.1	134
15	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. <i>Surface Science</i> , 2006, 600, 4548-4562.	0.8	128
16	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1934-1952.	2.3	128
17	Modeling the Electronic Properties of Î€-Conjugated Self-Assembled Monolayers. <i>Advanced Materials</i> , 2010, 22, 2494-2513.	11.1	126
18	Understanding Chemical versus Electrostatic Shifts in X-ray Photoelectron Spectra of Organic Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3428-3437.	1.5	125

#	ARTICLE	IF	CITATIONS
19	Tuning the two-photon absorption response of quadrupolar organic molecules. <i>Journal of Chemical Physics</i> , 2002, 116, 3646-3658.	1.2	119
20	Breakdown of the mirror image symmetry in the optical absorption/emission spectra of oligo(para-phenylene)s. <i>Journal of Chemical Physics</i> , 2005, 122, 054501.	1.2	117
21	Orders of Magnitude Reduction of the Contact Resistance in Short-Channel Hot Embossed Organic Thin Film Transistors by Oxidative Treatment of Au Electrodes. <i>Advanced Functional Materials</i> , 2007, 17, 2687-2692.	7.8	117
22	F4TCNQ on Cu, Ag, and Au as prototypical example for a strong organic acceptor on coinage metals. <i>Physical Review B</i> , 2009, 79, .	1.1	116
23	Resonant enhancement of two-photon absorption in substituted fluorene molecules. <i>Journal of Chemical Physics</i> , 2004, 121, 3152-3160.	1.2	114
24	Pyrroline Chromophores for Electro-Optics. <i>Chemistry of Materials</i> , 2006, 18, 2982-2988.	3.2	114
25	The Impact of Dipolar Layers on the Electronic Properties of Organic/Inorganic Hybrid Interfaces. <i>Advanced Materials Interfaces</i> , 2019, 6, 1900581.	1.9	112
26	The Dielectric Constant of Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2008, 18, 3999-4006.	7.8	101
27	Threshold Voltage Shifts in Organic Thin-Film Transistors Due to Self-Assembled Monolayers at the Dielectric Surface. <i>Advanced Functional Materials</i> , 2009, 19, 958-967.	7.8	101
28	UV-ozone treated Au for air-stable, low hole injection barrier electrodes in organic electronics. <i>Journal of Applied Physics</i> , 2006, 100, 053701.	1.1	99
29	Efficient Blue-Light-Emitting Polymer Heterostructure Devices: The Fabrication of Multilayer Structures from Orthogonal Solvents. <i>Advanced Materials</i> , 2010, 22, 2087-2091.	11.1	92
30	Bis(dioxaborine) compounds with large two-photon cross sections, and their use in the photodeposition of silver. <i>Chemical Communications</i> , 2003, , 1490-1491.	2.2	90
31	The Effects of Embedded Dipoles in Aromatic Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2015, 25, 3943-3957.	7.8	90
32	Theoretical investigation of the geometric and optical properties of neutral and charged oligophenylenes. <i>Physical Review B</i> , 1999, 59, 7957-7968.	1.1	82
33	Electronic structure of thiol-bonded self-assembled monolayers: Impact of coverage. <i>Physical Review B</i> , 2008, 77, .	1.1	80
34	Structure, morphology, and optical properties of highly ordered films of para-sexiphenyl. <i>Physical Review B</i> , 2000, 61, 16538-16549.	1.1	77
35	Quantitative prediction of optical excitations in conjugated organic oligomers: A density functional theory study. <i>Journal of Chemical Physics</i> , 2002, 117, 5921-5928.	1.2	76
36	Odd-Even Effects in Self-Assembled Monolayers of ω -(Biphenyl-4-yl)alkanethiols: A First-Principles Study. <i>Langmuir</i> , 2008, 24, 474-482.	1.6	75

#	ARTICLE	IF	CITATIONS
37	Gold work function reduction by 2.2eV with an air-stable molecular donor layer. Applied Physics Letters, 2008, 93, .	1.5	75
38	Two-Photon Absorption in Quadrupolar π -Conjugated Molecules: Influence of the Nature of the Conjugated Bridge and the Donor π -Acceptor Separation. Chemistry - A European Journal, 2004, 10, 2668-2680.	1.7	72
39	Influence of molecular conformation on organic/metal interface energetics. Chemical Physics Letters, 2005, 413, 390-395.	1.2	72
40	Organoboron Quinolinolates with Extended Conjugated Chromophores: Synthesis, Structure, and Electronic and Electroluminescent Properties. Chemistry of Materials, 2006, 18, 3539-3547.	3.2	72
41	Work-Function Modification beyond Pinning: When Do Molecular Dipoles Count?. Nano Letters, 2010, 10, 4369-4374.	4.5	70
42	Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy. Molecules, 2014, 19, 2969-2992.	1.7	69
43	Continuously Color-Tunable Rubber Laser. Advanced Materials, 2004, 16, 130-133.	11.1	68
44	Universal exciton size scaling in π conjugated systems. Chemical Physics Letters, 2000, 318, 585-589.	1.2	67
45	Two-Photon Absorption in Quadrupolar Bis(acceptor)-Terminated Chromophores with Electron-Rich Bis(heterocycle)vinylene Bridges. Chemistry of Materials, 2007, 19, 432-442.	3.2	66
46	Embedded Dipole Self-Assembled Monolayers for Contact Resistance Tuning in p π -Type and n π -Type Organic Thin Film Transistors and Flexible Electronic Circuits. Advanced Functional Materials, 2018, 28, 1804462.	7.8	66
47	Limitations of the F \ddot{u} rstner Description of Singlet Exciton Migration: The Illustrative Example of Energy Transfer to Ketonic Defects in Ladder-type Poly(para-phenylenes). Advanced Functional Materials, 2005, 15, 155-160.	7.8	63
48	Chemical Control of Local Doping in Organic Thin π -Film Transistors: From Depletion to Enhancement. Advanced Materials, 2008, 20, 3143-3148.	11.1	62
49	Density-Dependent Reorientation and Rehybridization of Chemisorbed Conjugated Molecules for Controlling Interface Electronic Structure. Physical Review Letters, 2010, 104, 246805.	2.9	55
50	Localized triplet excitations and the effect of photo-oxidation in ladder-type poly(p-phenylene) and oligo(p-phenylene). Physical Review B, 2000, 61, 10807-10814.	1.1	54
51	Excited state localization in organic molecules consisting of conjugated and nonconjugated segments. Journal of Chemical Physics, 2000, 113, 10002-10012.	1.2	54
52	Pressure studies on the intermolecular interactions in biphenyl. Synthetic Metals, 2001, 116, 327-331.	2.1	53
53	Ketonic Defects in Ladder-type Poly(p-phenylene)s. Chemistry of Materials, 2004, 16, 4667-4674.	3.2	53
54	High two-photon cross-sections in bis(diarylamino)styryl chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. Chemical Communications, 2007, , 1372-1374.	2.2	52

#	ARTICLE	IF	CITATIONS
55	Synthesis and Characterization of Novel para- and meta-Phenylenevinylene Derivatives: Fine Tuning of the Electronic and Optical Properties of Conjugated Materials. <i>Journal of Physical Chemistry B</i> , 2002, 106, 6442-6450.	1.2	51
56	Soft-Metallic Contact to Isolated C ₆₀ Molecules. <i>Nano Letters</i> , 2008, 8, 3825-3829.	4.5	50
57	Twisted π -system electro-optic chromophores. A CIS vs. MRD-CI theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 227-235.	1.5	48
58	Understanding the Electronic Structure of Metal/SAM/Organic Semiconductor Heterojunctions. <i>ACS Nano</i> , 2009, 3, 3513-3520.	7.3	48
59	Orientalional Ordering of Nonplanar Phthalocyanines on Cu(111): Strength and Orientation of the Electric Dipole Moment. <i>Physical Review Letters</i> , 2011, 106, 156102.	2.9	48
60	Triptycene Tripods for the Formation of Highly Uniform and Densely Packed Self-Assembled Monolayers with Controlled Molecular Orientation. <i>Journal of the American Chemical Society</i> , 2019, 141, 5995-6005.	6.6	48
61	Suppression of the Keto-Emission in Polyfluorene Light-Emitting Diodes: Experiments and Models. <i>Advanced Functional Materials</i> , 2004, 14, 1097-1104.	7.8	47
62	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. <i>Chemical Science</i> , 2016, 7, 781-787.	3.7	46
63	Impact of Materials versus Geometric Parameters on the Contact Resistance in Organic Thin-Film Transistors. <i>Advanced Functional Materials</i> , 2013, 23, 2941-2952.	7.8	45
64	Effects of Embedded Dipole Layers on Electrostatic Properties of Alkanethiolate Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15815-15830.	1.5	45
65	Stretching and Breaking of a Molecular Junction. <i>Small</i> , 2006, 2, 1468-1475.	5.2	44
66	Tuning the Threshold Voltage in Organic Thin-Film Transistors by Local Channel Doping Using Photoreactive Interfacial Layers. <i>Advanced Materials</i> , 2010, 22, 5361-5365.	11.1	44
67	First-principles study of the geometric and electronic structure of Au_{13} clusters: Importance of the prism motif. <i>Physical Review B</i> , 2008, 77, .	1.1	43
68	Reducing the Metal Work Function beyond Pauli Pushback: A Computational Investigation of Tetrathiafulvalene and Viologen on Coinage Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 20357-20365.	1.5	43
69	The Electronic Structure of Mixed Self-Assembled Monolayers. <i>ACS Nano</i> , 2010, 4, 6735-6746.	7.3	43
70	Theoretical characterization of phenylene-based oligomers, polymers, and dendrimers. <i>Synthetic Metals</i> , 1999, 100, 141-162.	2.1	42
71	Tuning the Electroluminescence Color in Polymer Light-Emitting Devices Using the Thiol-Ene Photoreaction. <i>Advanced Functional Materials</i> , 2005, 15, 403-409.	7.8	42
72	DFT-Assisted Polymorph Identification from Lattice Raman Fingerprinting. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3690-3695.	2.1	42

#	ARTICLE	IF	CITATIONS
73	Bis-aryl substituted dioxaborines as electron-transport materials: a comparative density functional theory investigation with oxadiazoles and siloles. <i>Chemical Physics</i> , 2005, 313, 151-157.	0.9	41
74	Understanding the properties of interfaces between organic self-assembled monolayers and noble metals—a theoretical perspective. <i>Surface and Interface Analysis</i> , 2008, 40, 371-378.	0.8	41
75	Mechanism of mediated alkali peroxide oxidation and triplet versus singlet oxygen formation. <i>Nature Chemistry</i> , 2021, 13, 465-471.	6.6	41
76	Impact of Anchoring Groups on Ballistic Transport: Single Molecule vs Monolayer Junctions. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21198-21208.	1.5	40
77	Electronic Properties of the Interfaces Between the Wide Bandgap Organic Semiconductor Para-Sexiphenyl and Samarium. <i>Advanced Functional Materials</i> , 2001, 11, 51-58.	7.8	39
78	Orientation-Dependent Work-Function Modification Using Substituted Pyrene-Based Acceptors. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24657-24668.	1.5	39
79	Understanding the Properties of Tailor-Made Self-Assembled Monolayers with Embedded Dipole Moments for Interface Engineering. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28757-28774.	1.5	38
80	Efficient acceptor groups for NLO chromophores: competing inductive and resonance contributions in heterocyclic acceptors derived from 2-dicyanomethylidene-3-cyano-4,5,5-trimethyl-2,5-dihydrofuran. <i>Journal of Materials Chemistry</i> , 2007, 17, 2944-2949.	6.7	37
81	Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. <i>Advanced Functional Materials</i> , 2009, 19, 3766-3775.	7.8	37
82	Is there a Au–S bond dipole in self-assembled monolayers on gold?. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4287.	1.3	37
83	Quantum-chemical investigation of second-order nonlinear optical chromophores: Comparison of strong nitrile-based acceptor end groups and role of auxiliary donors and acceptors. <i>Journal of Chemical Physics</i> , 2006, 124, 044510.	1.2	36
84	Understanding Structure and Bonding of Multilayered Metal–Organic Nanostructures. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3055-3061.	1.5	36
85	First-principles calculations of hybrid inorganic–organic interfaces: from state-of-the-art to best practice. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8132-8180.	1.3	36
86	Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2677-2684.	1.5	34
87	Adsorption, initial growth and desorption kinetics of p-terphenyl on polycrystalline gold surfaces. <i>Applied Surface Science</i> , 2004, 221, 184-196.	3.1	33
88	Effective conjugation and Raman intensities in oligo(para-phenylene)s: A microscopic view from first-principles calculations. <i>Journal of Chemical Physics</i> , 2005, 122, 114511.	1.2	33
89	Collectively Induced Quantum-Confined Stark Effect in Monolayers of Molecules Consisting of Polar Repeating Units. <i>Journal of the American Chemical Society</i> , 2011, 133, 18634-18645.	6.6	33
90	Relative Thermal Stability of Thiolate- and Selenolate-Bonded Aromatic Monolayers on the Au(111) Substrate. <i>Journal of Physical Chemistry C</i> , 2017, 121, 28031-28042.	1.5	33

#	ARTICLE	IF	CITATIONS
91	Ab initio study of vibrational anharmonic coupling effects in oligo(para-phenylenes). Journal of Chemical Physics, 2002, 116, 10921-10931.	1.2	32
92	Doping Molecular Wires. Nano Letters, 2009, 9, 2559-2564.	4.5	32
93	Limitations of Essential-State Models for the Description of Two-Photon Absorption Processes: The Example of Bis(dioxaborine)-Substituted Chromophores. Journal of Physical Chemistry B, 2004, 108, 8641-8646.	1.2	31
94	Impact of the Capacitance of the Dielectric on the Contact Resistance of Organic Thin-Film Transistors. Physical Review Applied, 2015, 4, .	1.5	31
95	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. RSC Advances, 2016, 6, 69479-69483.	1.7	31
96	Momentum-dependent excitations in highly ordered films of para-hexaphenyl. Physical Review B, 1997, 56, 10138-10144.	1.1	29
97	Multicolor Organic Electroluminescent Devices Fabricated by a Reductive Photo-patterning Method. Advanced Materials, 2002, 14, 1722-1725.	11.1	29
98	Defect chemistry of polyfluorenes: identification of the origin of interface defects in polyfluorene based light-emitting devices. Chemical Communications, 2008, , 5170.	2.2	29
99	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. Physical Chemistry Chemical Physics, 2010, 12, 4291.	1.3	28
100	Employing X-ray Photoelectron Spectroscopy for Determining Layer Homogeneity in Mixed Polar Self-Assembled Monolayers. Journal of Physical Chemistry Letters, 2016, 7, 2994-3000.	2.1	28
101	On the polarization of the green emission of polyfluorenes. Journal of Chemical Physics, 2003, 119, 6832-6839.	1.2	26
102	Electronic structure of pyridine-based SAMs on flat Au(111) surfaces: extended charge rearrangements and Fermi level pinning. Physical Chemistry Chemical Physics, 2011, 13, 9747.	1.3	26
103	Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. Journal of Chemical Theory and Computation, 2018, 14, 4380-4390.	2.3	26
104	Two-Photon Absorption in Linear Bis-dioxaborine Compounds: The Impact of Correlation-Induced Oscillator-Strength Redistribution. ChemPhysChem, 2004, 5, 982-988.	1.0	25
105	Anticorrelation between the Evolution of Molecular Dipole Moments and Induced Work Function Modifications. Journal of Physical Chemistry Letters, 2013, 4, 3521-3526.	2.1	25
106	Porous Honeycomb Self-Assembled Monolayers: Tripodal Adsorption and Hidden Chirality of Carboxylate Anchored Triptycenes on Ag. ACS Nano, 2021, 15, 11168-11179.	7.3	25
107	Localized and delocalized singlet excitons in ladder-type poly(paraphenylene). Physical Review B, 1998, 57, R4202-R4205.	1.1	24
108	Tunneling Probability Increases with Distance in Junctions Comprising Self-Assembled Monolayers of Oligothiophenes. Journal of the American Chemical Society, 2018, 140, 15048-15055.	6.6	24

#	ARTICLE	IF	CITATIONS
109	Molecular Origin of the Temperature-Dependent Energy Migration in a Rigid-Rod Ladder-Phenylene Molecular Host. <i>Advanced Materials</i> , 2006, 18, 310-314.	11.1	23
110	Molecular fluorescent pH-probes based on 8-hydroxyquinoline. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 1503.	1.5	22
111	Polarity Switching of Charge Transport and Thermoelectricity in Self-Assembled Monolayer Devices. <i>Advanced Materials</i> , 2012, 24, 4403-4407.	11.1	22
112	Impact of Collective Electrostatic Effects on Charge Transport through Molecular Monolayers. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22395-22401.	1.5	22
113	Complex Stoichiometry-Dependent Reordering of 3,4,9,10-Perylenetetracarboxylic Dianhydride on Ag(111) upon K Intercalation. <i>ACS Nano</i> , 2016, 10, 2365-2374.	7.3	22
114	Structural, Spectroscopic, and Computational Characterization of the Concomitant Polymorphs of the Natural Semiconductor Indigo. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18422-18431.	1.5	22
115	Improving the Stability of Polymer FETs by Introducing Fixed Acceptor Units into the Main Chain: Application to Poly(alkylthiophenes). <i>Chemistry of Materials</i> , 2007, 19, 1472-1481.	3.2	21
116	A novel concept for humidity compensated sub-ppm ammonia detection. <i>Sensors and Actuators B: Chemical</i> , 2010, 145, 181-184.	4.0	21
117	Evaluating Computational Shortcuts in Supercell-Based Phonon Calculations of Molecular Crystals: The Instructive Case of Naphthalene. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2716-2735.	2.3	21
118	Structure to Property Relationships for Multiphoton Absorption in Covalently Linked Porphyrin Dimers: A Correction Vector INDO/MRDCI Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8509-8518.	1.1	20
119	The Effect of Protonation on the Optical Properties of Conjugated Fluorene-Pyridine Copolymers. <i>Macromolecular Chemistry and Physics</i> , 2008, 209, 2122-2134.	1.1	20
120	A Toolbox for Controlling the Energetics and Localization of Electronic States in Self-Assembled Organic Monolayers. <i>Advanced Science</i> , 2015, 2, 1400016.	5.6	20
121	Electronic Properties of Biphenylthiolates on Au(111): The Impact of Coverage Revisited. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7817-7825.	1.5	20
122	Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface. <i>ACS Nano</i> , 2017, 11, 10495-10508.	7.3	20
123	The influence of the counterion on the electronic structure in doped phenylene-based materials. <i>Surface Science</i> , 2000, 454-456, 1000-1004.	0.8	19
124	Structure-property relationships for three-photon absorption in stilbene-based dipolar and quadrupolar chromophores. <i>Journal of Chemical Physics</i> , 2006, 125, 044101.	1.2	19
125	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. <i>Organic Electronics</i> , 2012, 13, 3165-3176.	1.4	19
126	Synthesis and characterization of a novel side-chain liquid crystalline poly(p-phenylenevinylene). <i>Synthetic Metals</i> , 1996, 83, 177-180.	2.1	18

#	ARTICLE	IF	CITATIONS
127	Controlling the electronic properties of van der Waals heterostructures by applying electrostatic design. <i>2D Materials</i> , 2018, 5, 035019.	2.0	18
128	Interfacial Band Engineering of MoS ₂ /Gold Interfaces Using Pyrimidine-Containing Self-Assembled Monolayers: Toward Contact-Resistance-Free Bottom-Contacts. <i>Advanced Electronic Materials</i> , 2020, 6, 2000110.	2.6	18
129	Excited-state localization effects in alternating meta- and para-linked poly(phenylene-vinylene)s. <i>Chemical Physics</i> , 2004, 297, 143-151.	0.9	17
130	Photochemical control of the carrier mobility in pentacene-based organic thin-film transistors. <i>Applied Physics Letters</i> , 2010, 96, 213303.	1.5	17
131	Characterisation of a dipolar chromophore with third-harmonic generation applications in the near-IR. <i>Journal of Materials Chemistry</i> , 2012, 22, 4371.	6.7	17
132	Polymer-based red, green, and blue emitting devices fabricated by reductive photopatterning. <i>Applied Physics Letters</i> , 2002, 81, 4269-4271.	1.5	16
133	A High Molecular Weight Donor for Electron Injection Interlayers on Metal Electrodes. <i>ChemPhysChem</i> , 2009, 10, 2947-2954.	1.0	16
134	X-ray based tools for the investigation of buried interfaces in organic electronic devices. <i>Organic Electronics</i> , 2013, 14, 479-487.	1.4	16
135	Understanding phonon properties in isorecticular metal-organic frameworks from first principles. <i>Physical Review Materials</i> , 2019, 3, .	0.9	16
136	Dynamic structure factor and excitons in TPD. <i>Physical Review B</i> , 2000, 61, 1662-1665.	1.1	15
137	Three-photon absorption in anthracene-porphyrin-anthracene triads: A quantum-chemical study. <i>Journal of Chemical Physics</i> , 2004, 121, 11060.	1.2	15
138	Cross-section analysis of organic light-emitting diodes. <i>Ultramicroscopy</i> , 2004, 101, 123-128.	0.8	15
139	Synthesis of a Photosensitive Thiocyanate-Functionalized Trialkoxysilane and Its Application in Patterned Surface Modifications. <i>Chemistry of Materials</i> , 2008, 20, 2009-2015.	3.2	15
140	Self-Assembled Monolayers with Distributed Dipole Moments Originating from Bipyrimidine Units. <i>Journal of Physical Chemistry C</i> , 2020, 124, 504-519.	1.5	15
141	Concept of Embedded Dipoles as a Versatile Tool for Surface Engineering. <i>Accounts of Chemical Research</i> , 2022, 55, 1857-1867.	7.6	15
142	From molecular states to band structure: Theoretical investigation of momentum dependent excitations in phenylene based organic materials. <i>Journal of Chemical Physics</i> , 1999, 111, 1668-1675.	1.2	14
143	The Influence of UV Irradiation on Ketonic Defect Emission in Fluorene-Based Copolymers. <i>Advanced Functional Materials</i> , 2008, 18, 2480-2488.	7.8	14
144	Continuous tuning of the threshold voltage of organic thin-film transistors by a chemically reactive interfacial layer. <i>Applied Physics A: Materials Science and Processing</i> , 2009, 95, 43-48.	1.1	14

#	ARTICLE	IF	CITATIONS
145	Mechanism of surface proton transfer doping in pentacene based organic thin-film transistors. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2012, 209, 181-192.	0.8	14
146	Unconventional Current Scaling and Edge Effects for Charge Transport through Molecular Clusters. <i>Nano Letters</i> , 2017, 17, 7350-7357.	4.5	14
147	A dithiocarbamate anchoring group as a flexible platform for interface engineering. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22511-22525.	1.3	14
148	Identifying the Bottleneck for Heat Transport in Metal-Organic Frameworks. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000211.	1.3	14
149	Avoiding the Center-Symmetry Trap: Programmed Assembly of Dipolar Precursors into Porous, Crystalline Molecular Thin Films. <i>Advanced Materials</i> , 2021, 33, e2103287.	11.1	14
150	High pressure Raman studies on the structural conformation of oligophenyls. <i>Synthetic Metals</i> , 2001, 116, 163-166.	2.1	13
151	Combined photoelectron and metastable atom electron spectroscopy study of n-doped oligophenylene thin films. <i>Applied Surface Science</i> , 2001, 175-176, 764-768.	3.1	13
152	Ultrafast photoexcitation dynamics in a ladder-type oligophenyl. <i>Physical Review B</i> , 2002, 66, .	1.1	13
153	Synthesis and Photophysical Properties of 3,6-Diphenyl-9-hexyl-9H-carbazole Derivatives Bearing Electron Withdrawing Groups. <i>Monatshefte für Chemie</i> , 2008, 139, 223-231.	0.9	13
154	Radical self-assembled monolayers on Au(111) formed by the adsorption of closed-shell molecules. <i>Journal of Materials Chemistry</i> , 2012, 22, 4269.	6.7	13
155	Influence of the degree of conjugation on excited state lifetimes in phenylene-based materials. <i>Synthetic Metals</i> , 2002, 127, 241-245.	2.1	12
156	Main-Chain Liquid Crystalline Polymers Based on Bis-Etherified 9,9-Dihexyl-2,7-bis(4-hydroxy-1,1'-biphen-4-yl)fluorenes. <i>Macromolecular Chemistry and Physics</i> , 2007, 208, 1458-1468.	1.1	12
157	Analysis of Bonding between Conjugated Organic Molecules and Noble Metal Surfaces Using Orbital Overlap Populations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3481-3489.	2.3	12
158	Postadsorption Work Function Tuning via Hydrogen Pressure Control. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27162-27172.	1.5	12
159	Distinguishing between Charge-Transfer Mechanisms at Organic/Inorganic Interfaces Employing Hybrid Functionals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 14640-14653.	1.5	12
160	Energy-level alignment at strongly coupled organic-metal interfaces. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 194002.	0.7	12
161	Sticking with the Pointy End? Molecular Configuration of Chloro Boron-Subphthalocyanine on Cu(111). <i>Journal of Physical Chemistry C</i> , 2016, 120, 7113-7121.	1.5	11
162	Geometry-dependent absorption, and emission of para-hexaphenyl. <i>Synthetic Metals</i> , 1999, 101, 662-663.	2.1	10

#	ARTICLE	IF	CITATIONS
163	Characterizing Chemically Reactive Thin Layers: Surface Reaction of [2-[4-(Chlorosulfonyl)phenyl]ethyl]trichlorosilane with Ammonia. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12407-12413.	1.5	10
164	A theoretical view on self-assembled monolayers in organic electronic devices. <i>Proceedings of SPIE</i> , 2008, , .	0.8	10
165	Adsorption Behavior of Nonplanar Phthalocyanines: Competition of Different Adsorption Conformations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6869-6875.	1.5	10
166	Analyzing the Electronic Coupling in Molecular Crystals – The Instructive Case of Quinacridone. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800204.	1.3	10
167	The H ₂ -phase of the lyotropic liquid crystal sodium 3,4,5-tris(omega-acryloyloxyundecyloxy)benzoate. <i>Liquid Crystals</i> , 2000, 27, 407-411.	0.9	9
168	Albrecht theory and anharmonic coupling in polyphenyl Raman spectra. <i>Synthetic Metals</i> , 2003, 139, 823-825.	2.1	9
169	Synthesis and Photo Physical Properties of 9,10-Bis(hydroxyphenyl)anthracene Derivatives. <i>Monatshefte für Chemie</i> , 2007, 138, 453-464.	0.9	9
170	Understanding the Correlation between Electronic Coupling and Energetic Stability of Molecular Crystal Polymorphs: The Instructive Case of Quinacridone. <i>Chemistry of Materials</i> , 2019, 31, 7054-7069.	3.2	9
171	Exciton Coupling and Conformational Changes Impacting the Excited State Properties of Metal Organic Frameworks. <i>Molecules</i> , 2020, 25, 4230.	1.7	9
172	Understanding the origin of serrated stacking motifs in planar two-dimensional covalent organic frameworks. <i>Nanoscale</i> , 2021, 13, 9339-9353.	2.8	9
173	Synthesis and characterization of novel oligo(phenylenevinylene) derivatives. <i>Synthetic Metals</i> , 2001, 119, 183-184.	2.1	8
174	The size of electron-hole pairs in π -conjugated oligomers. <i>Synthetic Metals</i> , 2001, 119, 499-502.	2.1	8
175	Order of Magnitude Effects of Thiazole Regioisomerism on the Near-IR Two-Photon Cross-Sections of Dipolar Chromophores. <i>Advanced Functional Materials</i> , 2008, 18, 794-801.	7.8	8
176	A particularly strong organic acceptor for tuning the hole-injection barriers in modern organic devices. <i>Synthetic Metals</i> , 2010, 160, 1456-1462.	2.1	8
177	Tuning the Electronic Structure of Graphene through Collective Electrostatic Effects. <i>Advanced Materials Interfaces</i> , 2015, 2, 1500323.	1.9	8
178	Electrostatic Design of 3D Covalent Organic Networks. <i>Advanced Materials</i> , 2017, 29, 1700888.	11.1	8
179	Exploring the driving forces behind the structural assembly of biphenylthiolates on Au(111). <i>Journal of Chemical Physics</i> , 2017, 147, 024706.	1.2	8
180	Semi-Automatic Deposition of Oriented Cu(OH) ₂ Nanobelts for the Heteroepitaxial Growth of Metal-Organic Framework Films. <i>Advanced Materials Interfaces</i> , 2021, 8, 2101039.	1.9	8

#	ARTICLE	IF	CITATIONS
181	Bias-Triggered Conductivity Switching and High Effective Rectification in Metallocene-Based Molecular Junctions. <i>Advanced Electronic Materials</i> , 2022, 8, .	2.6	8
182	The quasi-band-structure description of conjugated oligomers. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 1753-1768.	0.7	7
183	High Pressure Studies of Polyaromatic Molecular Crystals: Optical and Electronic Properties from first Principles. <i>Materials Research Society Symposia Proceedings</i> , 2001, 665, 1.	0.1	7
184	Solid state effects in the electronic structure of ladder-type poly(p-phenylene)s and oligo(p-phenylene)s. <i>Synthetic Metals</i> , 2000, 111-112, 509-513.	2.1	6
185	van der Waals Interaction Activated Strong Electronic Coupling at the Interface between Chloro Boron-Subphthalocyanine and Cu(111). <i>Journal of Physical Chemistry C</i> , 2018, 122, 14621-14630.	1.5	6
186	Final-State Simulations of Core-Level Binding Energies at Metal-Organic Hybrid Interfaces: Artifacts Caused by Spurious Collective Electrostatic Effects. <i>ACS Omega</i> , 2020, 5, 25868-25881.	1.6	6
187	Maximizing the Carrier Mobilities of Metal-Organic Frameworks Comprising Stacked Pentacene Units. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7002-7009.	2.1	6
188	Discovering structure-property relationships for the phonon band structures of hydrocarbon-based organic semiconductor crystals: the instructive case of acenes. <i>Journal of Materials Chemistry C</i> , 2022, 10, 2532-2543.	2.7	6
189	Device characteristics of nanostructured Poly(p-phenylenevinylene). <i>Synthetic Metals</i> , 1999, 102, 1155-1156.	2.1	5
190	Reductive photo-patterning of conjugated thin films. <i>Synthetic Metals</i> , 2003, 138, 85-87.	2.1	5
191	Understanding the Anisotropic Elastic Properties of Metal-Organic Frameworks at the Nanoscale: The Instructive Example of MOF-74. <i>Journal of Physical Chemistry C</i> , 2021, 125, 24728-24745.	1.5	5
192	Understanding the Origin of the Particularly Small and Anisotropic Thermal Expansion of MOF-74. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	5
193	Exploring the Impact of the Linker Length on Heat Transport in Metal-Organic Frameworks. <i>Nanomaterials</i> , 2022, 12, 2142.	1.9	5
194	Photophysical properties of nanostructured PPV-composites. <i>Synthetic Metals</i> , 1999, 102, 1270-1271.	2.1	4
195	Comment on "Electron Core-Hole Interaction and Its Induced Ionic Structural Relaxation in Molecular Systems under X-Ray Irradiation". <i>Physical Review Letters</i> , 2007, 99, 059601; discussion 059602.	2.9	4
196	Strategies for Controlling Through-Space Charge Transport in Metal-Organic Frameworks via Structural Modifications. <i>Nanomaterials</i> , 2020, 10, 2372.	1.9	4
197	Electrostatic Design of Polar Metal-Organic Framework Thin Films. <i>Nanomaterials</i> , 2020, 10, 2420.	1.9	4
198	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. <i>Physical Review Materials</i> , 2019, 3, .	0.9	4

#	ARTICLE	IF	CITATIONS
199	Theoretical investigation of phenylene-based materials in their pristine and doped state. <i>Optical Materials</i> , 1999, 12, 307-310.	1.7	3
200	Momentum-dependent excitation processes in crystalline and amorphous films of conjugated oligomers. <i>Physical Review B</i> , 2000, 61, 16561-16569.	1.1	3
201	Patterned Immobilization of a Luminescent Ru(II) Complex in Polymer Films Using the Photoreaction of Benzyl thiocyanate: Toward Color Emission Tuning of Electroluminescent Devices. <i>Macromolecular Chemistry and Physics</i> , 2012, 213, 367-373.	1.1	3
202	Electronic Properties of 1,2;8,9-Dibenzopentacene in Solutions, Solid Matrices, and Thin Films. <i>Journal of Applied Spectroscopy</i> , 2016, 83, 20-26.	0.3	3
203	The Potential of X-ray Photoelectron Spectroscopy for Determining Interface Dipoles of Self-Assembled Monolayers. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 5735.	1.3	3
204	Electronic Properties of the Interfaces Between the Wide Bandgap Organic Semiconductor Para-Sexiphenyl and Samarium. <i>Advanced Functional Materials</i> , 2001, 11, 51-58.	7.8	3
205	Interface Modification of Pentacene OFET Gate Dielectrics. <i>Springer Proceedings in Physics</i> , 2009, , 185-187.	0.1	3
206	Application of new PPV precursor polymers in organic LEDs. <i>Synthetic Metals</i> , 1999, 102, 997.	2.1	2
207	Momentum dependent excitation processes in organic materials. <i>Synthetic Metals</i> , 1999, 101, 337-338.	2.1	2
208	Fluorescent Hexacatenar Liquid Crystals. <i>Materials Research Society Symposia Proceedings</i> , 1999, 560, 277.	0.1	2
209	Doping effects on the electronic and structural properties of poly(para-phenylene) investigated from first-principles. <i>Synthetic Metals</i> , 2001, 119, 211-212.	2.1	2
210	Tuning the emission color of conjugated organic materials by photochemical reactions. <i>Synthetic Metals</i> , 2003, 137, 1027-1028.	2.1	2
211	TEM Investigations of Cross-Sectional Prepared Organic Light Emitting Devices. <i>Microscopy and Microanalysis</i> , 2003, 9, 266-267.	0.2	2
212	Role of Dimensionality on the Two-Photon Absorption Response of Conjugated Molecules: The Case of Octupolar Compounds. , 2002, 12, 631.		2
213	Photochemical Patterning Approaches for Multicolor Polymer Light Emitting Devices. <i>Materials Research Society Symposia Proceedings</i> , 2003, 771, 991.	0.1	2
214	A New Alternative for the Low-Workfunction Electrode in Organic Devices. <i>Materials Research Society Symposia Proceedings</i> , 1999, 598, 23.	0.1	1
215	Influence of the Chemical Structure on the Luminescence Properties of Organic Dye Molecules. <i>Materials Research Society Symposia Proceedings</i> , 1999, 598, 339.	0.1	1
216	Structural Properties of Conjugated Molecular Crystals Under high Pressure. <i>Materials Research Society Symposia Proceedings</i> , 2001, 665, 1.	0.1	1

#	ARTICLE	IF	CITATIONS
217	Raman intensities in polyphenyls: An ab-initio study. Synthetic Metals, 2003, 135-136, 359-360.	2.1	1
218	Colorless Molecular Dopants for Low-Operating-Voltage Nematic Liquid Crystals. Molecular Crystals and Liquid Crystals, 2005, 428, 17-32.	0.4	1
219	2D Semiconductors: Interfacial Band Engineering of MoS ₂ /Gold Interfaces Using Pyrimidine-Containing Self-Assembled Monolayers: Toward Contact-Resistance-Free Bottom-Contacts (Adv. Electron. Mater. 5/2020). Advanced Electronic Materials, 2020, 6, 2070026.	2.6	1
220	Modelling Organic-Inorganic Hybrid Interfaces. World Scientific Series in Nanoscience and Nanotechnology, 2019, , 3-40.	0.1	1
221	Side Chain Influence on Main Chain Orientation of PPV-Type Oligomers. Materials Research Society Symposia Proceedings, 1999, 598, 173.	0.1	0
222	Reductive Photopatterning of Phenylene-Vinylene-Based Polymers. Materials Research Society Symposia Proceedings, 2001, 707, 1131.	0.1	0
223	Reductive photopatterning of phenylene-vinylene-based polymers. Materials Research Society Symposia Proceedings, 2001, 708, 1131/AA11.3.1.	0.1	0
224	Ab Initio Study of Vibrational Anharmonic Coupling Effects in Oligo(para-phenylenes). Materials Research Society Symposia Proceedings, 2001, 708, 3101.	0.1	0
225	Exciton-Phonon Coupling in Conjugated Organic Molecules. Physica Scripta, 2004, T109, 156.	1.2	0
226	Computational Modelling of Organic Semiconductors: From the Quantum World to Actual Devices. Advanced Functional Materials, 2015, 25, 1913-1914.	7.8	0
227	Polymers and Organic Materials, Electronic States of. , 2005, , 375-386.		0
228	(Invited) Understanding Phonons and Thermal Transport in Metal-Organic Frameworks. ECS Meeting Abstracts, 2020, MA2020-02, 2019-2019.	0.0	0