

Egbert Zojer

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221
papers

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51
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235
ext. papers

9,544
ext. citations

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avg, IF

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#	Paper	IF	Citations
221	Density-functional theory with screened van der Waals interactions for the modeling of hybrid inorganic-organic systems. <i>Physical Review Letters</i> , 2012 , 108, 146103	7.4	467
220	The interface energetics of self-assembled monolayers on metals. <i>Accounts of Chemical Research</i> , 2008 , 41, 721-9	24.3	340
219	Role of Dimensionality on the Two-Photon Absorption Response of Conjugated Molecules: The Case of Octupolar Compounds. <i>Advanced Functional Materials</i> , 2002 , 12, 631-641	15.6	334
218	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. <i>MRS Bulletin</i> , 2010 , 35, 435-442	3.2	244
217	Toward control of the metal-organic interfacial electronic structure in molecular electronics: a first-principles study on self-assembled monolayers of pi-conjugated molecules on noble metals. <i>Nano Letters</i> , 2007 , 7, 932-40	11.5	244
216	Interface energetics and level alignment at covalent metal-molecule junctions: pi-conjugated thiols on gold. <i>Physical Review Letters</i> , 2006 , 96, 196806	7.4	243
215	The Origin of Green Emission in Polyfluorene-Based Conjugated Polymers: On-Chain Defect Fluorescence. <i>Advanced Functional Materials</i> , 2003 , 13, 597-601	15.6	243
214	Metal-ion sensing fluorophores with large two-photon absorption cross sections: aza-crown ether substituted donor-acceptor-donor distyrylbenzenes. <i>Journal of the American Chemical Society</i> , 2004 , 126, 9291-306	16.4	193
213	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	7.4	186
212	Green emission from poly(fluorene)s: The role of oxidation. <i>Journal of Chemical Physics</i> , 2002 , 117, 6794-6802	5.9	183
211	Extended squaraine dyes with large two-photon absorption cross-sections. <i>Journal of the American Chemical Society</i> , 2006 , 128, 14444-5	16.4	181
210	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	2.9	175
209	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, 7282-3	16.4	142
208	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. <i>Surface Science</i> , 2006 , 600, 4548-4562	1.8	122
207	Aromatic amines: a comparison of electron-donor strengths. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 9346-52	2.8	118
206	Tuning the two-photon absorption response of quadrupolar organic molecules. <i>Journal of Chemical Physics</i> , 2002 , 116, 3646-3658	3.9	110
205	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	6.4	109

204	F4TCNQ on Cu, Ag, and Au as prototypical example for a strong organic acceptor on coinage metals. <i>Physical Review B</i> , 2009 , 79,	3.3	108
203	Modeling the electronic properties of pi-conjugated self-assembled monolayers. <i>Advanced Materials</i> , 2010 , 22, 2494-513	24	107
202	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	15.6	106
201	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, 54501	3.9	105
200	Pyrroline Chromophores for Electro-Optics. <i>Chemistry of Materials</i> , 2006 , 18, 2982-2988	9.6	103
199	Resonant enhancement of two-photon absorption in substituted fluorene molecules. <i>Journal of Chemical Physics</i> , 2004 , 121, 3152-60	3.9	97
198	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	15.6	95
197	The Dielectric Constant of Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2008 , 18, 3999-4006	15.6	95
196	UVzone treated Au for air-stable, low hole injection barrier electrodes in organic electronics. <i>Journal of Applied Physics</i> , 2006 , 100, 053701	2.5	90
195	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	3.8	84
194	Efficient blue-light-emitting polymer heterostructure devices: the fabrication of multilayer structures from orthogonal solvents. <i>Advanced Materials</i> , 2010 , 22, 2087-91	24	81
193	Bis(dioxaborine) compounds with large two-photon cross sections, and their use in the photodeposition of silver. <i>Chemical Communications</i> , 2003 , 1490-1491	5.8	80
192	Theoretical investigation of the geometric and optical properties of neutral and charged oligophenylenes. <i>Physical Review B</i> , 1999 , 59, 7957-7968	3.3	79
191	The Impact of Dipolar Layers on the Electronic Properties of Organic/Inorganic Hybrid Interfaces. <i>Advanced Materials Interfaces</i> , 2019 , 6, 1900581	4.6	75
190	The Effects of Embedded Dipoles in Aromatic Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2015 , 25, 3943-3957	15.6	73
189	Gold work function reduction by 2.2eV with an air-stable molecular donor layer. <i>Applied Physics Letters</i> , 2008 , 93, 243303	3.4	71
188	Electronic structure of thiol-bonded self-assembled monolayers: Impact of coverage. <i>Physical Review B</i> , 2008 , 77,	3.3	71
187	Quantitative prediction of optical excitations in conjugated organic oligomers: A density functional theory study. <i>Journal of Chemical Physics</i> , 2002 , 117, 5921-5928	3.9	70

186	Odd-even effects in self-assembled monolayers of omega-(biphenyl-4-yl)alkanethiols: a first-principles study. <i>Langmuir</i> , 2008 , 24, 474-82	4	69
185	Two-photon absorption in quadrupolar pi-conjugated molecules: influence of the nature of the conjugated bridge and the donor-acceptor separation. <i>Chemistry - A European Journal</i> , 2004 , 10, 2668-80 ^{4.8}	4.8	69
184	Structure, morphology, and optical properties of highly ordered films of para-sexiphenyl. <i>Physical Review B</i> , 2000 , 61, 16538-16549	3.3	69
183	Organoboron Quinolinolates with Extended Conjugated Chromophores: Synthesis, Structure, and Electronic and Electroluminescent Properties. <i>Chemistry of Materials</i> , 2006 , 18, 3539-3547	9.6	68
182	Understanding the adsorption of CuPc and ZnPc on noble metal surfaces by combining quantum-mechanical modelling and photoelectron spectroscopy. <i>Molecules</i> , 2014 , 19, 2969-92	4.8	66
181	Influence of molecular conformation on organic/metal interface energetics. <i>Chemical Physics Letters</i> , 2005 , 413, 390-395	2.5	66
180	Work-function modification beyond pinning: when do molecular dipoles count?. <i>Nano Letters</i> , 2010 , 10, 4369-74	11.5	63
179	Two-Photon Absorption in Quadrupolar Bis(acceptor)-Terminated Chromophores with Electron-Rich Bis(heterocycle)vinylene Bridges. <i>Chemistry of Materials</i> , 2007 , 19, 432-442	9.6	62
178	Chemical Control of Local Doping in Organic Thin-Film Transistors: From Depletion to Enhancement. <i>Advanced Materials</i> , 2008 , 20, 3143-3148	24	61
177	Continuously Color-Tunable Rubber Laser. <i>Advanced Materials</i> , 2004 , 16, 130-133	24	61
176	Universal exciton size scaling in π -conjugated systems. <i>Chemical Physics Letters</i> , 2000 , 318, 585-589	2.5	61
175	Limitations of the F \ddot{u} ster Description of Singlet Exciton Migration: The Illustrative Example of Energy Transfer to Ketonic Defects in Ladder-type Poly(para-phenylenes). <i>Advanced Functional Materials</i> , 2005 , 15, 155-160	15.6	60
174	Localized triplet excitations and the effect of photo-oxidation in ladder-type poly(p-phenylene) and oligo(p-phenylene). <i>Physical Review B</i> , 2000 , 61, 10807-10814	3.3	52
173	Pressure studies on the intermolecular interactions in biphenyl. <i>Synthetic Metals</i> , 2001 , 116, 327-331	3.6	52
172	Density-dependent reorientation and rehybridization of chemisorbed conjugated molecules for controlling interface electronic structure. <i>Physical Review Letters</i> , 2010 , 104, 246805	7.4	51
171	High two-photon cross-sections in bis(diarylaminostyryl) chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. <i>Chemical Communications</i> , 2007 , 1372-4	5.8	51
170	Excited state localization in organic molecules consisting of conjugated and nonconjugated segments. <i>Journal of Chemical Physics</i> , 2000 , 113, 10002-10012	3.9	49
169	Embedded Dipole Self-Assembled Monolayers for Contact Resistance Tuning in p-Type and n-Type Organic Thin Film Transistors and Flexible Electronic Circuits. <i>Advanced Functional Materials</i> , 2018 , 28, 1804462	15.6	48

168	Suppression of the Keto-Emission in Polyfluorene Light-Emitting Diodes: Experiments and Models. <i>Advanced Functional Materials</i> , 2004 , 14, 1097-1104	15.6	47
167	Ketonic Defects in Ladder-type Poly(p-phenylene)s. <i>Chemistry of Materials</i> , 2004 , 16, 4667-4674	9.6	47
166	Twisted π -System electro-optic chromophores. A CIS vs. MRD-CI theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2003 , 633, 227-235		46
165	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	3.4	46
164	Understanding the electronic structure of metal/SAM/organic-semiconductor heterojunctions. <i>ACS Nano</i> , 2009 , 3, 3513-20	16.7	45
163	"Soft" metallic contact to isolated C60 molecules. <i>Nano Letters</i> , 2008 , 8, 3825-9	11.5	45
162	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	3.8	42
161	Orientalional ordering of nonplanar phthalocyanines on Cu(111): strength and orientation of the electric dipole moment. <i>Physical Review Letters</i> , 2011 , 106, 156102	7.4	41
160	Stretching and breaking of a molecular junction. <i>Small</i> , 2006 , 2, 1468-75	11	40
159	Theoretical characterization of phenylene-based oligomers, polymers, and dendrimers. <i>Synthetic Metals</i> , 1999 , 100, 141-162	3.6	40
158	Impact of Materials versus Geometric Parameters on the Contact Resistance in Organic Thin-Film Transistors. <i>Advanced Functional Materials</i> , 2013 , 23, 2941-2952	15.6	39
157	Understanding the properties of interfaces between organic self-assembled monolayers and noble metals: theoretical perspective. <i>Surface and Interface Analysis</i> , 2008 , 40, 371-378	1.5	39
156	Tuning the Electroluminescence Color in Polymer Light-Emitting Devices Using the Thiol-Ene Photoreaction. <i>Advanced Functional Materials</i> , 2005 , 15, 403-409	15.6	39
155	Tuning the threshold voltage in organic thin-film transistors by local channel doping using photoreactive interfacial layers. <i>Advanced Materials</i> , 2010 , 22, 5361-5	24	38
154	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,	3.3	38
153	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	2.3	38
152	Electronic Properties of the Interfaces Between the Wide Bandgap Organic Semiconductor Para-Sexiphenyl and Samarium. <i>Advanced Functional Materials</i> , 2001 , 11, 51-58	15.6	37
151	Impact of Anchoring Groups on Ballistic Transport: Single Molecule vs Monolayer Junctions. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 21198-21208	3.8	36

150	Understanding Structure and Bonding of Multilayered Metal-Organic Nanostructures. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 3055-3061	3.8	36
149	Is there a Au-S bond dipole in self-assembled monolayers on gold?. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 4287-90	3.6	36
148	Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. <i>Advanced Functional Materials</i> , 2009 , 19, 3766-3775	15.6	36
147	Effects of Embedded Dipole Layers on Electrostatic Properties of Alkanethiolate Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 15815-15830	3.8	35
146	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		35
145	The electronic structure of mixed self-assembled monolayers. <i>ACS Nano</i> , 2010 , 4, 6735-46	16.7	34
144	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	3.9	34
143	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. <i>Chemical Science</i> , 2016 , 7, 781-787	9.4	33
142	Adsorption, initial growth and desorption kinetics of p-quaterphenyl on polycrystalline gold surfaces. <i>Applied Surface Science</i> , 2004 , 221, 184-196	6.7	33
141	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	3.8	32
140	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	3.9	32
139	Ab initio study of vibrational anharmonic coupling effects in oligo(para-phenylenes). <i>Journal of Chemical Physics</i> , 2002 , 116, 10921-10931	3.9	32
138	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, 18634-45	16.4	31
137	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	16.4	30
136	DFT-Assisted Polymorph Identification from Lattice Raman Fingerprinting. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 3690-3695	6.4	29
135	Doping molecular wires. <i>Nano Letters</i> , 2009 , 9, 2559-64	11.5	29
134	Momentum-dependent excitations in highly ordered films of para-hexaphenyl. <i>Physical Review B</i> , 1997 , 56, 10138-10144	3.3	29
133	Limitations of Essential-State Models for the Description of Two-Photon Absorption Processes: The Example of Bis(dioxaborine)-Substituted Chromophores. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 8641-8646	3.4	29

132	Defect chemistry of polyfluorenes: identification of the origin of "interface defects" in polyfluorene based light-emitting devices. <i>Chemical Communications</i> , 2008 , 5170-2	5.8	28
131	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	3.8	27
130	Multicolor Organic Electroluminescent Devices Fabricated by a Reductive Photo-patterning Method. <i>Advanced Materials</i> , 2002 , 14, 1722-1725	24	27
129	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. <i>RSC Advances</i> , 2016 , 6, 69479-69483	3.7	26
128	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	3.8	26
127	Orientation-Dependent Work-Function Modification Using Substituted Pyrene-Based Acceptors. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 24657-24668	3.8	25
126	Employing X-ray Photoelectron Spectroscopy for Determining Layer Homogeneity in Mixed Polar Self-Assembled Monolayers. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2994-3000	6.4	25
125	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 4291-4	3.6	24
124	Electronic structure of pyridine-based SAMs on flat Au(111) surfaces: extended charge rearrangements and Fermi level pinning. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 9747-60	3.6	24
123	On the polarization of the green emission of polyfluorenes. <i>Journal of Chemical Physics</i> , 2003 , 119, 6832-6839	5.9	24
122	Two-photon absorption in linear bis-dioxaborine compounds-the impact of correlation-induced oscillator-strength redistribution. <i>ChemPhysChem</i> , 2004 , 5, 982-8	3.2	23
121	Localized and delocalized singlet excitons in ladder-type poly(paraphenylene). <i>Physical Review B</i> , 1998 , 57, R4202-R4205	3.3	23
120	Impact of the Capacitance of the Dielectric on the Contact Resistance of Organic Thin-Film Transistors. <i>Physical Review Applied</i> , 2015 , 4,	4.3	22
119	Molecular fluorescent pH-probes based on 8-hydroxyquinoline. <i>Organic and Biomolecular Chemistry</i> , 2006 , 4, 1503-11	3.9	22
118	Polarity switching of charge transport and thermoelectricity in self-assembled monolayer devices. <i>Advanced Materials</i> , 2012 , 24, 4403-7	24	21
117	Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4380-4390	6.4	20
116	Impact of Collective Electrostatic Effects on Charge Transport through Molecular Monolayers. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 22395-22401	3.8	20
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	9.6	20

114	Molecular Origin of the Temperature-Dependent Energy Migration in a Rigid-Rod Ladder-Phenylene Molecular Host. <i>Advanced Materials</i> , 2006 , 18, 310-314	24	20
113	Electronic Properties of Biphenylthiolates on Au(111): The Impact of Coverage Revisited. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 7817-7825	3.8	19
112	Anticorrelation between the Evolution of Molecular Dipole Moments and Induced Work Function Modifications. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3521-3526	6.4	19
111	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. <i>Organic Electronics</i> , 2012 , 13, 3165-3176	3.5	19
110	A novel concept for humidity compensated sub-ppm ammonia detection. <i>Sensors and Actuators B: Chemical</i> , 2010 , 145, 181-184	8.5	19
109	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, 8509-18	2.8	19
108	The influence of the counterion on the electronic structure in doped phenylene-based materials. <i>Surface Science</i> , 2000 , 454-456, 1000-1004	1.8	19
107	The Effect of Protonation on the Optical Properties of Conjugated FluoreneByridine Copolymers. <i>Macromolecular Chemistry and Physics</i> , 2008 , 209, 2122-2134	2.6	18
106	Mechanism of mediated alkali peroxide oxidation and triplet versus singlet oxygen formation. <i>Nature Chemistry</i> , 2021 , 13, 465-471	17.6	18
105	A Toolbox for Controlling the Energetics and Localization of Electronic States in Self-Assembled Organic Monolayers. <i>Advanced Science</i> , 2015 , 2, 1400016	13.6	17
104	Structure-property relationships for three-photon absorption in stilbene-based dipolar and quadrupolar chromophores. <i>Journal of Chemical Physics</i> , 2006 , 125, 44101	3.9	17
103	Excited-state localization effects in alternating meta- and para-linked poly(phenylene-vinylene)s. <i>Chemical Physics</i> , 2004 , 297, 143-151	2.3	17
102	Photochemical control of the carrier mobility in pentacene-based organic thin-film transistors. <i>Applied Physics Letters</i> , 2010 , 96, 213303	3.4	16
101	Complex Stoichiometry-Dependent Reordering of 3,4,9,10-Perylenetetracarboxylic Dianhydride on Ag(111) upon K Intercalation. <i>ACS Nano</i> , 2016 , 10, 2365-74	16.7	15
100	Characterisation of a dipolar chromophore with third-harmonic generation applications in the near-IR. <i>Journal of Materials Chemistry</i> , 2012 , 22, 4371		15
99	Tunneling Probability Increases with Distance in Junctions Comprising Self-Assembled Monolayers of Oligothiophenes. <i>Journal of the American Chemical Society</i> , 2018 , 140, 15048-15055	16.4	15
98	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	3.8	14
97	Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface. <i>ACS Nano</i> , 2017 , 11, 10495-10508	16.7	14

96	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	1.6	14
95	A high molecular weight donor for electron injection interlayers on metal electrodes. <i>ChemPhysChem</i> , 2009 , 10, 2947-54	3.2	14
94	Synthesis of a Photosensitive Thiocyanate-Functionalized Trialkoxysilane and Its Application in Patterned Surface Modifications. <i>Chemistry of Materials</i> , 2008 , 20, 2009-2015	9.6	14
93	Polymer-based red, green, and blue emitting devices fabricated by reductive photopatterning. <i>Applied Physics Letters</i> , 2002 , 81, 4269-4271	3.4	14
92	Dynamic structure factor and excitons in TPD. <i>Physical Review B</i> , 2000 , 61, 1662-1665	3.3	14
91	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	3.9	14
90	Synthesis and characterization of a novel side-chain liquid crystalline poly(p-phenylenevinylene). <i>Synthetic Metals</i> , 1996 , 83, 177-180	3.6	14
89	X-ray based tools for the investigation of buried interfaces in organic electronic devices. <i>Organic Electronics</i> , 2013 , 14, 479-487	3.5	13
88	Three-photon absorption in anthracene-porphyrin-anthracene triads: a quantum-chemical study. <i>Journal of Chemical Physics</i> , 2004 , 121, 11060-7	3.9	13
87	Cross-section analysis of organic light-emitting diodes. <i>Ultramicroscopy</i> , 2004 , 101, 123-8	3.1	13
86	High pressure Raman studies on the structural conformation of oligophenylys. <i>Synthetic Metals</i> , 2001 , 116, 163-166	3.6	13
85	Unconventional Current Scaling and Edge Effects for Charge Transport through Molecular Clusters. <i>Nano Letters</i> , 2017 , 17, 7350-7357	11.5	12
84	Radical self-assembled monolayers on Au(111) formed by the adsorption of closed-shell molecules. <i>Journal of Materials Chemistry</i> , 2012 , 22, 4269		12
83	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	2.6	12
82	The Influence of UV Irradiation on Ketonic Defect Emission in Fluorene-Based Copolymers. <i>Advanced Functional Materials</i> , 2008 , 18, 2480-2488	15.6	12
81	Combined photoelectron and metastable atom electron spectroscopy study of n-doped oligophenylene thin films. <i>Applied Surface Science</i> , 2001 , 175-176, 764-768	6.7	12
80	Ultrafast photoexcitation dynamics in a ladder-type oligophenyl. <i>Physical Review B</i> , 2002 , 66,	3.3	12
79	Controlling the electronic properties of van der Waals heterostructures by applying electrostatic design. <i>2D Materials</i> , 2018 , 5, 035019	5.9	11

78	Postadsorption Work Function Tuning via Hydrogen Pressure Control. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 27162-27172	3.8	11
77	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	2.6	11
76	Influence of the degree of conjugation on excited state lifetimes in phenylene-based materials. <i>Synthetic Metals</i> , 2002 , 127, 241-245	3.6	11
75	Understanding phonon properties in isorecticular metal-organic frameworks from first principles. <i>Physical Review Materials</i> , 2019 , 3,	3.2	11
74	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	3.6	11
73	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	6.4	10
72	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	3.8	10
71	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	3.8	10
70	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	1.4	10
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