

# Egbert Zojer

## List of Publications by Year in descending order

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228  
papers

10,134  
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31949

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42364

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all docs

235  
docs citations

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times ranked

9525  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	Bias-Triggered Conductivity Switching and High Effective Rectification in Metallocene-Based Molecular Junctions. <i>Advanced Electronic Materials</i> , 2022, 8, .	2.6	8
4	Concept of Embedded Dipoles as a Versatile Tool for Surface Engineering. <i>Accounts of Chemical Research</i> , 2022, 55, 1857-1867.	7.6	15
5	Exploring the Impact of the Linker Length on Heat Transport in Metal–Organic Frameworks. <i>Nanomaterials</i> , 2022, 12, 2142.	1.9	5
6	Identifying the Bottleneck for Heat Transport in Metal–Organic Frameworks. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000211.	1.3	14
7	Understanding the origin of serrated stacking motifs in planar two-dimensional covalent organic frameworks. <i>Nanoscale</i> , 2021, 13, 9339-9353.	2.8	9
8	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
9	Mechanism of mediated alkali peroxide oxidation and triplet versus singlet oxygen formation. <i>Nature Chemistry</i> , 2021, 13, 465-471.	6.6	41
10	Porous Honeycomb Self-Assembled Monolayers: Tripodal Adsorption and Hidden Chirality of Carboxylate Anchored Triptycenes on Ag. <i>ACS Nano</i> , 2021, 15, 11168-11179.	7.3	25
11	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
12	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
13	Semi-Automatic Deposition of Oriented Cu(OH) <sub>2</sub> Nanobelts for the Heteroepitaxial Growth of Metal–Organic Framework Films. <i>Advanced Materials Interfaces</i> , 2021, 8, 2101039.	1.9	8
14	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
15	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
16	Exciton Coupling and Conformational Changes Impacting the Excited State Properties of Metal Organic Frameworks. <i>Molecules</i> , 2020, 25, 4230.	1.7	9
17	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
18	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

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19	Strategies for Controlling Through-Space Charge Transport in Metal-Organic Frameworks via Structural Modifications. <i>Nanomaterials</i> , 2020, 10, 2372.	1.9	4
20	Electrostatic Design of Polar Metal-Organic Framework Thin Films. <i>Nanomaterials</i> , 2020, 10, 2420.	1.9	4
21	2D Semiconductors: Interfacial Band Engineering of MoS <sub>2</sub> /Gold Interfaces Using Pyrimidine-Containing Self-Assembled Monolayers: Toward Contact-Resistance-Free Bottom-Contacts ( <i>Adv. Electron. Mater.</i> 5/2020). <i>Advanced Electronic Materials</i> , 2020, 6, 2070026.	2.6	1
22	Interfacial Band Engineering of MoS <sub>2</sub> /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
23	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
24	(Invited) Understanding Phonons and Thermal Transport in Metal-Organic Frameworks. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 2019-2019.	0.0	0
25	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
26	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
27	Energy-level alignment at strongly coupled organic-metal interfaces. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 194002.	0.7	12
28	Analyzing the Electronic Coupling in Molecular Crystals—The Instructive Case of Quinacridone. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800204.	1.3	10
29	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
30	A dithiocarbamate anchoring group as a flexible platform for interface engineering. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22511-22525.	1.3	14
31	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
32	Understanding phonon properties in isorecticular metal-organic frameworks from first principles. <i>Physical Review Materials</i> , 2019, 3, .	0.9	16
33	Modelling Organic-Inorganic Hybrid Interfaces. <i>World Scientific Series in Nanoscience and Nanotechnology</i> , 2019, , 3-40.	0.1	1
34	Controlling the electronic properties of van der Waals heterostructures by applying electrostatic design. <i>2D Materials</i> , 2018, 5, 035019.	2.0	18
35	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
36	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.	7.8	66

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37	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.	6.6	24
38	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
39	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
40	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
41	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.	2.3	26
42	Electrostatic Design of 3D Covalent Organic Networks. <i>Advanced Materials</i> , 2017, 29, 1700888.	11.1	8
43	Orientation-Dependent Work-Function Modification Using Substituted Pyrene-Based Acceptors. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24657-24668.	1.5	39
44	Unconventional Current Scaling and Edge Effects for Charge Transport through Molecular Clusters. <i>Nano Letters</i> , 2017, 17, 7350-7357.	4.5	14
45	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
46	DFT-Assisted Polymorph Identification from Lattice Raman Fingerprinting. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3690-3695.	2.1	42
47	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
48	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
49	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
50	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.	2.1	28
51	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. <i>RSC Advances</i> , 2016, 6, 69479-69483.	1.7	31
52	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
53	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
54	Adsorption Behavior of Nonplanar Phthalocyanines: Competition of Different Adsorption Conformations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6869-6875.	1.5	10

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55	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
56	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. <i>Chemical Science</i> , 2016, 7, 781-787.	3.7	46
57	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
58	Impact of the Capacitance of the Dielectric on the Contact Resistance of Organic Thin-Film Transistors. <i>Physical Review Applied</i> , 2015, 4, .	1.5	31
59	The Effects of Embedded Dipoles in Aromatic Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2015, 25, 3943-3957.	7.8	90
60	Tuning the Electronic Structure of Graphene through Collective Electrostatic Effects. <i>Advanced Materials Interfaces</i> , 2015, 2, 1500323.	1.9	8
61	Postadsorption Work Function Tuning via Hydrogen Pressure Control. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27162-27172.	1.5	12
62	Computational Modelling of Organic Semiconductors: From the Quantum World to Actual Devices. <i>Advanced Functional Materials</i> , 2015, 25, 1913-1914.	7.8	0
63	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
64	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
65	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
66	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
67	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
68	Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy. <i>Molecules</i> , 2014, 19, 2969-2992.	1.7	69
69	Anticorrelation between the Evolution of Molecular Dipole Moments and Induced Work Function Modifications. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3521-3526.	2.1	25
70	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
71	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
72	Understanding Structure and Bonding of Multilayered Metal-Organic Nanostructures. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3055-3061.	1.5	36

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73	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
74	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
75	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
76	Density-Functional Theory with Screened vanÂderÂWaal's Interactions for the Modeling of Hybrid Inorganic-Organic Systems. <i>Physical Review Letters</i> , 2012, 108, 146103.	2.9	503
77	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
78	Polarity Switching of Charge Transport and Thermoelectricity in Self-Assembled Monolayer Devices. <i>Advanced Materials</i> , 2012, 24, 4403-4407.	11.1	22
79	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
80	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.	1.3	26
81	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
82	Orientational 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
83	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
84	Modeling the Electronic Properties of $\pi$ -Conjugated Self-Assembled Monolayers. <i>Advanced Materials</i> , 2010, 22, 2494-2513.	11.1	126
85	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
86	A novel concept for humidity compensated sub-ppm ammonia detection. <i>Sensors and Actuators B: Chemical</i> , 2010, 145, 181-184.	4.0	21
87	Photochemical control of the carrier mobility in pentacene-based organic thin-film transistors. <i>Applied Physics Letters</i> , 2010, 96, 213303.	1.5	17
88	Density-Dependent Reorientation and Rehybridization of Chemisorbed Conjugated Molecules for Controlling Interface Electronic Structure. <i>Physical Review Letters</i> , 2010, 104, 246805.	2.9	55
89	Work-Function Modification beyond Pinning: When Do Molecular Dipoles Count?. <i>Nano Letters</i> , 2010, 10, 4369-4374.	4.5	70
90	The Electronic Structure of Mixed Self-Assembled Monolayers. <i>ACS Nano</i> , 2010, 4, 6735-6746.	7.3	43

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91	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
92	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
93	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
94	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4291.	1.3	28
95	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
96	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. <i>MRS Bulletin</i> , 2010, 35, 435-442.	1.7	257
97	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
98	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
99	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
100	A High Molecular Weight Donor for Electron Injection Interlayers on Metal Electrodes. <i>ChemPhysChem</i> , 2009, 10, 2947-2954.	1.0	16
101	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
102	Understanding the Electronic Structure of Metal/SAM/Organic Semiconductor Heterojunctions. <i>ACS Nano</i> , 2009, 3, 3513-3520.	7.3	48
103	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
104	Doping Molecular Wires. <i>Nano Letters</i> , 2009, 9, 2559-2564.	4.5	32
105	Interface Modification of Pentacene OFET Gate Dielectrics. <i>Springer Proceedings in Physics</i> , 2009, , 185-187.	0.1	3
106	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
107	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
108	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

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109	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
110	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
111	The Dielectric Constant of Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2008, 18, 3999-4006.	7.8	101
112	Chemical Control of Local Doping in Organic Thin-Film Transistors: From Depletion to Enhancement. <i>Advanced Materials</i> , 2008, 20, 3143-3148.	11.1	62
113	The Interface Energetics of Self-Assembled Monolayers on Metals. <i>Accounts of Chemical Research</i> , 2008, 41, 721-729.	7.6	371
114	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
115	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
116	Defect chemistry of polyfluorenes: identification of the origin of interface defects in polyfluorene based light-emitting devices. <i>Chemical Communications</i> , 2008, , 5170.	2.2	29
117	Odd-Even Effects in Self-Assembled Monolayers of $\omega$ -(Biphenyl-4-yl)alkanethiols: A First-Principles Study. <i>Langmuir</i> , 2008, 24, 474-482.	1.6	75
118	Soft-Metallic Contact to Isolated $C_{60}$ Molecules. <i>Nano Letters</i> , 2008, 8, 3825-3829.	4.5	50
119	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
120	A theoretical view on self-assembled monolayers in organic electronic devices. <i>Proceedings of SPIE</i> , 2008, , .	0.8	10
121	Gold work function reduction by 2.2eV with an air-stable molecular donor layer. <i>Applied Physics Letters</i> , 2008, 93, .	1.5	75
122	Electronic structure of thiol-bonded self-assembled monolayers: Impact of coverage. <i>Physical Review B</i> , 2008, 77, .	1.1	80
123	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
124	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
125	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
126	High two-photon cross-sections in bis(diarylaminostyryl) chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. <i>Chemical Communications</i> , 2007, , 1372-1374.	2.2	52

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127	Improving the Stability of Polymer FETs by Introducing Fixed Acceptor Units into the Main Chain: A Application to Poly(alkylthiophenes). <i>Chemistry of Materials</i> , 2007, 19, 1472-1481.	3.2	21
128	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
129	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
130	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, 932-940.	4.5	257
131	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
132	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
133	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.	3.2	66
134	Synthesis and Photo Physical Properties of 9,10-Bis(hydroxyphenyl)anthracene Derivatives. <i>Monatshefte für Chemie</i> , 2007, 138, 453-464.	0.9	9
135	Interface Energetics and Level Alignment at Covalent Metal-Molecule Junctions: $\pi$ -Conjugated Thiols on Gold. <i>Physical Review Letters</i> , 2006, 96, 196806.	2.9	258
136	Pyrraline Chromophores for Electro-Optics. <i>Chemistry of Materials</i> , 2006, 18, 2982-2988.	3.2	114
137	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
138	Molecular fluorescent pH-probes based on 8-hydroxyquinoline. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 1503.	1.5	22
139	Organoboron Quinolinolates with Extended Conjugated Chromophores: Synthesis, Structure, and Electronic and Electroluminescent Properties. <i>Chemistry of Materials</i> , 2006, 18, 3539-3547.	3.2	72
140	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
141	Stretching and Breaking of a Molecular Junction. <i>Small</i> , 2006, 2, 1468-1475.	5.2	44
142	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
143	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
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.	1.2	36

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145	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
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