

# Egbert Zojer

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

221  
papers

8,975  
citations

51  
h-index

87  
g-index

235  
ext. papers

9,544  
ext. citations

7  
avg, IF

5.87  
L-index

#	Paper	IF	Citations
221	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> , <b>2022</b> , 10, 2532-2543	7.1	0
220	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> , <b>2021</b> , 8, 2101039	4.6	1
219	Mechanism of mediated alkali peroxide oxidation and triplet versus singlet oxygen formation. <i>Nature Chemistry</i> , <b>2021</b> , 13, 465-471	17.6	18
218	Porous Honeycomb Self-Assembled Monolayers: Tripodal Adsorption and Hidden Chirality of Carboxylate Anchored Triptycenes on Ag. <i>ACS Nano</i> , <b>2021</b> ,	16.7	7
217	Maximizing the Carrier Mobilities of Metal-Organic Frameworks Comprising Stacked Pentacene Units. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 7002-7009	6.4	0
216	Identifying the Bottleneck for Heat Transport in Metal-Organic Frameworks. <i>Advanced Theory and Simulations</i> , <b>2021</b> , 4, 2000211	3.5	4
215	Understanding the origin of serrated stacking motifs in planar two-dimensional covalent organic frameworks. <i>Nanoscale</i> , <b>2021</b> , 13, 9339-9353	7.7	3
214	First-principles calculations of hybrid inorganic-organic interfaces: from state-of-the-art to best practice. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 8132-8180	3.6	11
213	Avoiding the Center-Symmetry Trap: Programmed Assembly of Dipolar Precursors into Porous, Crystalline Molecular Thin Films. <i>Advanced Materials</i> , <b>2021</b> , 33, e2103287	24	1
212	Strategies for Controlling Through-Space Charge Transport in Metal-Organic Frameworks via Structural Modifications. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	3
211	Electrostatic Design of Polar Metal-Organic Framework Thin Films. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	1
210	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> , <b>2020</b> , 6, 2000110	6.4	6
209	Evaluating Computational Shortcuts in Supercell-Based Phonon Calculations of Molecular Crystals: The Instructive Case of Naphthalene. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 2716-2735	6.4	10
208	Self-Assembled Monolayers with Distributed Dipole Moments Originating from Bipyrimidine Units. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 504-519	3.8	9
207	Exciton Coupling and Conformational Changes Impacting the Excited State Properties of Metal Organic Frameworks. <i>Molecules</i> , <b>2020</b> , 25,	4.8	4
206	Final-State Simulations of Core-Level Binding Energies at Metal-Organic Hybrid Interfaces: Artifacts Caused by Spurious Collective Electrostatic Effects. <i>ACS Omega</i> , <b>2020</b> , 5, 25868-25881	3.9	3
205	The Potential of X-ray Photoelectron Spectroscopy for Determining Interface Dipoles of Self-Assembled Monolayers. <i>Applied Sciences (Switzerland)</i> , <b>2020</b> , 10, 5735	2.6	3

204	Energy-level alignment at strongly coupled organic-metal interfaces. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 194002	1.8	8
203	Analyzing the Electronic Coupling in Molecular Crystals—The Instructive Case of Quinacridone. <i>Advanced Theory and Simulations</i> , <b>2019</b> , 2, 1800204	3.5	6
202	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> , <b>2019</b> , 141, 5995-6005	16.4	30
201	Understanding the Correlation between Electronic Coupling and Energetic Stability of Molecular Crystal Polymorphs: The Instructive Case of Quinacridone. <i>Chemistry of Materials</i> , <b>2019</b> , 31, 7054-7069	9.6	6
200	The Impact of Dipolar Layers on the Electronic Properties of Organic/Inorganic Hybrid Interfaces. <i>Advanced Materials Interfaces</i> , <b>2019</b> , 6, 1900581	4.6	75
199	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	2
198	Understanding phonon properties in isorecticular metal-organic frameworks from first principles. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	11
197	Modelling Organic-Inorganic Hybrid Interfaces. <i>World Scientific Series in Nanoscience and Nanotechnology</i> , <b>2019</b> , 3-40	0.1	1
196	A dithiocarbamate anchoring group as a flexible platform for interface engineering. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 22511-22525	3.6	9
195	Controlling the electronic properties of van der Waals heterostructures by applying electrostatic design. <i>2D Materials</i> , <b>2018</b> , 5, 035019	5.9	11
194	Structural, Spectroscopic, and Computational Characterization of the Concomitant Polymorphs of the Natural Semiconductor Indigo. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 18422-18431	3.8	14
193	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> , <b>2018</b> , 14, 4380-4390	6.4	20
192	Understanding the Properties of Tailor-Made Self-Assembled Monolayers with Embedded Dipole Moments for Interface Engineering. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 28757-28774	3.8	26
191	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> , <b>2018</b> , 28, 1804462	15.6	48
190	Tunneling Probability Increases with Distance in Junctions Comprising Self-Assembled Monolayers of Oligothiophenes. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 15048-15055	16.4	15
189	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> , <b>2018</b> , 122, 14621-14630	3.8	5
188	Distinguishing between Charge-Transfer Mechanisms at Organic/Inorganic Interfaces Employing Hybrid Functionals. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 14640-14653	3.8	9
187	Electrostatic Design of 3D Covalent Organic Networks. <i>Advanced Materials</i> , <b>2017</b> , 29, 1700888	24	4

186	Orientation-Dependent Work-Function Modification Using Substituted Pyrene-Based Acceptors. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 24657-24668	3.8	25
185	Unconventional Current Scaling and Edge Effects for Charge Transport through Molecular Clusters. <i>Nano Letters</i> , <b>2017</b> , 17, 7350-7357	11.5	12
184	Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface. <i>ACS Nano</i> , <b>2017</b> , 11, 10495-10508	16.7	14
183	DFT-Assisted Polymorph Identification from Lattice Raman Fingerprinting. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 3690-3695	6.4	29
182	Relative Thermal Stability of Thiolate- and Selenolate-Bonded Aromatic Monolayers on the Au(111) Substrate. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 28031-28042	3.8	27
181	Exploring the driving forces behind the structural assembly of biphenylthiolates on Au(111). <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 024706	3.9	8
180	Effects of Embedded Dipole Layers on Electrostatic Properties of Alkanethiolate Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 15815-15830	3.8	35
179	Employing X-ray Photoelectron Spectroscopy for Determining Layer Homogeneity in Mixed Polar Self-Assembled Monolayers. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 2994-3000	6.4	25
178	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. <i>RSC Advances</i> , <b>2016</b> , 6, 69479-69483	3.7	26
177	Electronic Properties of 1,2;8,9-Dibenzopentacene in Solutions, Solid Matrices, and Thin Films. <i>Journal of Applied Spectroscopy</i> , <b>2016</b> , 83, 20-26	0.7	1
176	Understanding Chemical versus Electrostatic Shifts in X-ray Photoelectron Spectra of Organic Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 3428-3437	3.8	84
175	Adsorption Behavior of Nonplanar Phthalocyanines: Competition of Different Adsorption Conformations. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 6869-6875	3.8	9
174	Sticking with the Pointy End? Molecular Configuration of Chloro Boron-Subphthalocyanine on Cu(111). <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 7113-7121	3.8	10
173	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. <i>Chemical Science</i> , <b>2016</b> , 7, 781-787	9.4	33
172	Complex Stoichiometry-Dependent Reordering of 3,4,9,10-Perylenetetracarboxylic Dianhydride on Ag(111) upon K Intercalation. <i>ACS Nano</i> , <b>2016</b> , 10, 2365-74	16.7	15
171	Electronic Properties of Biphenylthiolates on Au(111): The Impact of Coverage Revisited. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 7817-7825	3.8	19
170	Impact of Anchoring Groups on Ballistic Transport: Single Molecule vs Monolayer Junctions. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 21198-21208	3.8	36
169	Impact of the Capacitance of the Dielectric on the Contact Resistance of Organic Thin-Film Transistors. <i>Physical Review Applied</i> , <b>2015</b> , 4,	4.3	22

168	The Effects of Embedded Dipoles in Aromatic Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , <b>2015</b> , 25, 3943-3957	15.6	73
167	Tuning the Electronic Structure of Graphene through Collective Electrostatic Effects. <i>Advanced Materials Interfaces</i> , <b>2015</b> , 2, 1500323	4.6	8
166	Postadsorption Work Function Tuning via Hydrogen Pressure Control. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 27162-27172	3.8	11
165	A Toolbox for Controlling the Energetics and Localization of Electronic States in Self-Assembled Organic Monolayers. <i>Advanced Science</i> , <b>2015</b> , 2, 1400016	13.6	17
164	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 1934-1952	6.4	109
163	Impact of Collective Electrostatic Effects on Charge Transport through Molecular Monolayers. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 22395-22401	3.8	20
162	Understanding the adsorption of CuPc and ZnPc on noble metal surfaces by combining quantum-mechanical modelling and photoelectron spectroscopy. <i>Molecules</i> , <b>2014</b> , 19, 2969-92	4.8	66
161	Anticorrelation between the Evolution of Molecular Dipole Moments and Induced Work Function Modifications. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 3521-3526	6.4	19
160	X-ray based tools for the investigation of buried interfaces in organic electronic devices. <i>Organic Electronics</i> , <b>2013</b> , 14, 479-487	3.5	13
159	Impact of Materials versus Geometric Parameters on the Contact Resistance in Organic Thin-Film Transistors. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, 2941-2952	15.6	39
158	Understanding Structure and Bonding of Multilayered Metal-Organic Nanostructures. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 3055-3061	3.8	36
157	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> , <b>2012</b> , 213, 367-373	2.6	3
156	Characterisation of a dipolar chromophore with third-harmonic generation applications in the near-IR. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 4371		15
155	Radical self-assembled monolayers on Au(111) formed by the adsorption of closed-shell molecules. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 4269		12
154	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. <i>Organic Electronics</i> , <b>2012</b> , 13, 3165-3176	3.5	19
153	Density-functional theory with screened van der Waals interactions for the modeling of hybrid inorganic-organic systems. <i>Physical Review Letters</i> , <b>2012</b> , 108, 146103	7.4	467
152	Mechanism of surface proton transfer doping in pentacene based organic thin-film transistors. <i>Physica Status Solidi (A) Applications and Materials Science</i> , <b>2012</b> , 209, 181-192	1.6	14
151	Polarity switching of charge transport and thermoelectricity in self-assembled monolayer devices. <i>Advanced Materials</i> , <b>2012</b> , 24, 4403-7	24	21

150	Collectively induced quantum-confined Stark effect in monolayers of molecules consisting of polar repeating units. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 18634-45	16.4	31
149	Electronic structure of pyridine-based SAMs on flat Au(111) surfaces: extended charge rearrangements and Fermi level pinning. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 9747-60	3.6	24
148	Orientalional ordering of nonplanar phthalocyanines on Cu(111): strength and orientation of the electric dipole moment. <i>Physical Review Letters</i> , <b>2011</b> , 106, 156102	7.4	41
147	Photochemical control of the carrier mobility in pentacene-based organic thin-film transistors. <i>Applied Physics Letters</i> , <b>2010</b> , 96, 213303	3.4	16
146	Density-dependent reorientation and rehybridization of chemisorbed conjugated molecules for controlling interface electronic structure. <i>Physical Review Letters</i> , <b>2010</b> , 104, 246805	7.4	51
145	Work-function modification beyond pinning: when do molecular dipoles count?. <i>Nano Letters</i> , <b>2010</b> , 10, 4369-74	11.5	63
144	The electronic structure of mixed self-assembled monolayers. <i>ACS Nano</i> , <b>2010</b> , 4, 6735-46	16.7	34
143	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> , <b>2010</b> , 114, 2677-2684	3.8	32
142	Analysis of Bonding between Conjugated Organic Molecules and Noble Metal Surfaces Using Orbital Overlap Populations. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 3481-3489	6.4	9
141	A particularly strong organic acceptor for tuning the hole-injection barriers in modern organic devices. <i>Synthetic Metals</i> , <b>2010</b> , 160, 1456-1462	3.6	6
140	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 4291-4	3.6	24
139	Is there a Au-S bond dipole in self-assembled monolayers on gold?. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 4287-90	3.6	36
138	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. <i>MRS Bulletin</i> , <b>2010</b> , 35, 435-442	3.2	244
137	Efficient blue-light-emitting polymer heterostructure devices: the fabrication of multilayer structures from orthogonal solvents. <i>Advanced Materials</i> , <b>2010</b> , 22, 2087-91	24	81
136	Modeling the electronic properties of pi-conjugated self-assembled monolayers. <i>Advanced Materials</i> , <b>2010</b> , 22, 2494-513	24	107
135	Tuning the threshold voltage in organic thin-film transistors by local channel doping using photoreactive interfacial layers. <i>Advanced Materials</i> , <b>2010</b> , 22, 5361-5	24	38
134	A novel concept for humidity compensated sub-ppm ammonia detection. <i>Sensors and Actuators B: Chemical</i> , <b>2010</b> , 145, 181-184	8.5	19
133	F4TCNQ on Cu, Ag, and Au as prototypical example for a strong organic acceptor on coinage metals. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	108

132	Threshold Voltage Shifts in Organic Thin-Film Transistors Due to Self-Assembled Monolayers at the Dielectric Surface. <i>Advanced Functional Materials</i> , <b>2009</b> , 19, 958-967	15.6	95
131	Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. <i>Advanced Functional Materials</i> , <b>2009</b> , 19, 3766-3775	15.6	36
130	A high molecular weight donor for electron injection interlayers on metal electrodes. <i>ChemPhysChem</i> , <b>2009</b> , 10, 2947-54	3.2	14
129	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> , <b>2009</b> , 95, 43-48	2.6	12
128	Understanding the electronic structure of metal/SAM/organic-semiconductor heterojunctions. <i>ACS Nano</i> , <b>2009</b> , 3, 3513-20	16.7	45
127	Theoretical study of PTCDA adsorbed on the coinage metal surfaces, Ag(111), Au(111) and Cu(111). <i>New Journal of Physics</i> , <b>2009</b> , 11, 053010	2.9	175
126	Doping molecular wires. <i>Nano Letters</i> , <b>2009</b> , 9, 2559-64	11.5	29
125	Interface Modification of Pentacene OFET Gate Dielectrics. <i>Springer Proceedings in Physics</i> , <b>2009</b> , 185-187.2		3
124	The interface energetics of self-assembled monolayers on metals. <i>Accounts of Chemical Research</i> , <b>2008</b> , 41, 721-9	24.3	340
123	First-principles study of the geometric and electronic structure of Au <sub>13</sub> clusters: Importance of the prism motif. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	38
122	Synthesis of a Photosensitive Thiocyanate-Functionalized Trialkoxysilane and Its Application in Patterned Surface Modifications. <i>Chemistry of Materials</i> , <b>2008</b> , 20, 2009-2015	9.6	14
121	Defect chemistry of polyfluorenes: identification of the origin of "interface defects" in polyfluorene based light-emitting devices. <i>Chemical Communications</i> , <b>2008</b> , 5170-2	5.8	28
120	Odd-even effects in self-assembled monolayers of omega-(biphenyl-4-yl)alkanethiols: a first-principles study. <i>Langmuir</i> , <b>2008</b> , 24, 474-82	4	69
119	"Soft" metallic contact to isolated C <sub>60</sub> molecules. <i>Nano Letters</i> , <b>2008</b> , 8, 3825-9	11.5	45
118	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> , <b>2008</b> , 112, 20357-20365	3.8	42
117	A theoretical view on self-assembled monolayers in organic electronic devices <b>2008</b> ,		6
116	Gold work function reduction by 2.2eV with an air-stable molecular donor layer. <i>Applied Physics Letters</i> , <b>2008</b> , 93, 243303	3.4	71
115	Electronic structure of thiol-bonded self-assembled monolayers: Impact of coverage. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	71

114	Synthesis and Photophysical Properties of 3,6-Diphenyl-9-hexyl-9H-carbazole Derivatives Bearing Electron Withdrawing Groups. <i>Monatshefte Für Chemie</i> , <b>2008</b> , 139, 223-231	1.4	10
113	Understanding the properties of interfaces between organic self-assembled monolayers and noble metals – theoretical perspective. <i>Surface and Interface Analysis</i> , <b>2008</b> , 40, 371-378	1.5	39
112	The Effect of Protonation on the Optical Properties of Conjugated Fluorene-Pyridine Copolymers. <i>Macromolecular Chemistry and Physics</i> , <b>2008</b> , 209, 2122-2134	2.6	18
111	Order of Magnitude Effects of Thiazole Regioisomerism on the Near-IR Two-Photon Cross-Sections of Dipolar Chromophores. <i>Advanced Functional Materials</i> , <b>2008</b> , 18, 794-801	15.6	8
110	The Influence of UV Irradiation on Ketonic Defect Emission in Fluorene-Based Copolymers. <i>Advanced Functional Materials</i> , <b>2008</b> , 18, 2480-2488	15.6	12
109	The Dielectric Constant of Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , <b>2008</b> , 18, 3999-4006	15.6	95
108	Chemical Control of Local Doping in Organic Thin-Film Transistors: From Depletion to Enhancement. <i>Advanced Materials</i> , <b>2008</b> , 20, 3143-3148	24	61
107	High two-photon cross-sections in bis(diarylaminostyryl) chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. <i>Chemical Communications</i> , <b>2007</b> , 1372-4	5.8	51
106	Improving the Stability of Polymer FETs by Introducing Fixed Acceptor Units into the Main Chain: Application to Poly(alkylthiophenes). <i>Chemistry of Materials</i> , <b>2007</b> , 19, 1472-1481	9.6	20
105	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> , <b>2007</b> , 111, 8509-18	2.8	19
104	Characterizing Chemically Reactive Thin Layers: Surface Reaction of [2-[4-(Chlorosulfonyl)phenyl]ethyl]trichlorosilane with Ammonia. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 12407-12413	3.8	10
103	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> , <b>2007</b> , 7, 932-40	11.5	244
102	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> , <b>2007</b> , 17, 2687-2692	15.6	106
101	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> , <b>2007</b> , 208, 1458-1468	2.6	11
100	Two-Photon Absorption in Quadrupolar Bis(acceptor)-Terminated Chromophores with Electron-Rich Bis(heterocycle)vinylene Bridges. <i>Chemistry of Materials</i> , <b>2007</b> , 19, 432-442	9.6	62
99	Synthesis and Photo Physical Properties of 9,10-Bis(hydroxyphenyl)anthracene Derivatives. <i>Monatshefte Für Chemie</i> , <b>2007</b> , 138, 453-464	1.4	7
98	Comment on "Electron core-hole interaction and its induced ionic structural relaxation in molecular systems under x-ray irradiation". <i>Physical Review Letters</i> , <b>2007</b> , 99, 059601; discussion 059602	7.4	4
97	Impact of bidirectional charge transfer and molecular distortions on the electronic structure of a metal-organic interface. <i>Physical Review Letters</i> , <b>2007</b> , 99, 256801	7.4	186



96	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> , <b>2007</b> , 17, 2944-2949		35
95	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. <i>Surface Science</i> , <b>2006</b> , 600, 4548-4562	1.8	122
94	Molecular Origin of the Temperature-Dependent Energy Migration in a Rigid-Rod Ladder-Phenylene Molecular Host. <i>Advanced Materials</i> , <b>2006</b> , 18, 310-314	24	20
93	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> , <b>2006</b> , 124, 044510	3.9	34
92	Structure-property relationships for three-photon absorption in stilbene-based dipolar and quadrupolar chromophores. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 44101	3.9	17
91	Interface energetics and level alignment at covalent metal-molecule junctions: pi-conjugated thiols on gold. <i>Physical Review Letters</i> , <b>2006</b> , 96, 196806	7.4	243
90	Pyrroline Chromophores for Electro-Optics. <i>Chemistry of Materials</i> , <b>2006</b> , 18, 2982-2988	9.6	103
89	Extended squaraine dyes with large two-photon absorption cross-sections. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 14444-5	16.4	181
88	Molecular fluorescent pH-probes based on 8-hydroxyquinoline. <i>Organic and Biomolecular Chemistry</i> , <b>2006</b> , 4, 1503-11	3.9	22
87	Organoboron Quinolinolates with Extended Conjugated Chromophores: Synthesis, Structure, and Electronic and Electroluminescent Properties. <i>Chemistry of Materials</i> , <b>2006</b> , 18, 3539-3547	9.6	68
86	UVBzone treated Au for air-stable, low hole injection barrier electrodes in organic electronics. <i>Journal of Applied Physics</i> , <b>2006</b> , 100, 053701	2.5	90
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