

Jerome Cornil

List of Publications by Year in descending order

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163
papers

16,724
citations

47006

47
h-index

14208

128
g-index

165
all docs

165
docs citations

165
times ranked

16440
citing authors

#	ARTICLE	IF	CITATIONS
1	Gas-phase structure of polymer ions: Tying together theoretical approaches and ion mobility spectrometry. <i>Mass Spectrometry Reviews</i> , 2023, 42, 1129-1151.	5.4	4
2	Electronic transport through single-molecule oligophenyl-diethynyl junctions with direct gold-carbon bonds formed at low temperature. <i>Nanoscale Advances</i> , 2022, 4, 457-466.	4.6	4
3	On the Conformation of Anionic Peptoids in the Gas Phase. <i>Biomacromolecules</i> , 2022, 23, 1138-1147.	5.4	2
4	Photoluminescence and electrochemiluminescence of thermally activated delayed fluorescence (TADF) emitters containing diphenylphosphine chalcogenide-substituted carbazole donors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4646-4667.	5.5	20
5	Terphenylthiazole-based self-assembled monolayers on cobalt with high conductance photo-switching ratio for spintronics. <i>Nanoscale</i> , 2022, 14, 5725-5742.	5.6	2
6	Theoretical Comparison of a Longitudinal versus a Transverse Transport Path through Diarylethene Molecular Switches. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5675-5681.	3.1	0
7	Dinaphthotetrathienoacenes: Synthesis, Characterization, and Applications in Organic Field-Effect Transistors. <i>Advanced Science</i> , 2022, 9, e2105674.	11.2	6
8	MLCT Excited-State Behavior of Trinuclear Ruthenium(II) 2,2'-Bipyridine Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 366-379.	4.0	12
9	Insights into the growth of nanoparticles in liquid polyol by thermal annealing. <i>Nanoscale Advances</i> , 2021, 3, 4780-4789.	4.6	4
10	Thermal conductivity of benzothieno-benzothiophene derivatives at the nanoscale. <i>Nanoscale</i> , 2021, 13, 3800-3807.	5.6	12
11	Tuning the Electronic Bandgap of Graphdiyne by H-Substitution to Promote Interfacial Charge Carrier Separation for Enhanced Photocatalytic Hydrogen Production. <i>Advanced Functional Materials</i> , 2021, 31, 2100994.	14.9	41
12	Magnetron sputter deposition of silver onto castor oil: The effect of plasma parameters on nanoparticle properties. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 615, 126286.	4.7	10
13	Peptoids as a Chiral Stationary Phase for Liquid Chromatography: Insights from Molecular Dynamics Simulations. <i>Biomacromolecules</i> , 2021, 22, 2573-2581.	5.4	6
14	Challenges for Incorporating Optical Switchability in Organic-Based Electronic Devices. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27737-27748.	8.0	17
15	[4]Cyclo-N-alkyl-2,7-carbazoles: Influence of the Alkyl Chain Length on the Structural, Electronic, and Charge Transport Properties. <i>Journal of the American Chemical Society</i> , 2021, 143, 8804-8820.	13.7	19
16	Bias-Polarity-Dependent Direct and Inverted Marcus Charge Transport Affecting Rectification in a Redox-Active Molecular Junction. <i>Advanced Science</i> , 2021, 8, e2100055.	11.2	14
17	Photocatalysis: Tuning the Electronic Bandgap of Graphdiyne by H-Substitution to Promote Interfacial Charge Carrier Separation for Enhanced Photocatalytic Hydrogen Production (Adv. Funct. Mater.) Tj ETQq1 1 0.784314 rgBT\$Overlo	14.9	41
18	Helical Peptoid Ions in the Gas Phase: Thwarting the Charge Solvation Effect by H-Bond Compensation. <i>Biomacromolecules</i> , 2021, 22, 3543-3551.	5.4	3

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19	Insights on the Formation of Nanoparticles Prepared by Magnetron Sputtering Onto Liquids: Gold Sputtered Onto Castor Oil as a Case Study. <i>Frontiers in Nanotechnology</i> , 2021, 3, .	4.8	10
20	Strong Suppression of Thermal Conductivity in the Presence of Long Terminal Alkyl Chains in Low-Disorder Molecular Semiconductors. <i>Advanced Materials</i> , 2021, 33, e2008708.	21.0	12
21	Switching the electrical characteristics of TiO ₂ from n-type to p-type by ion implantation. <i>Applied Surface Science</i> , 2021, 563, 150274.	6.1	6
22	Conductance switching of azobenzene-based self-assembled monolayers on cobalt probed by UHV conductive-AFM. <i>Nanoscale</i> , 2021, 13, 6977-6990.	5.6	13
23	Solvent-Free Design of Biobased Non-isocyanate Polyurethanes with Ferroelectric Properties. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 14946-14958.	6.7	11
24	Quantifying Image Charge Effects in Molecular Tunnel Junctions Based on Self-Assembled Monolayers of Substituted Oligophenylene Ethynylene Dithiols. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 56404-56412.	8.0	6
25	White-light electroluminescence from a layer incorporating a single fully-organic spiro compound with phosphine oxide substituents. <i>Journal of Materials Chemistry C</i> , 2020, 8, 14462-14468.	5.5	15
26	Assessing the Structural Heterogeneity of Isomeric Homo and Copolymers: an Approach Combining Ion Mobility Mass Spectrometry and Molecular Dynamics Simulations. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 2379-2388.	2.8	1
27	Reversal of the Direction of Rectification Induced by Fermi Level Pinning at Molecule-Electrode Interfaces in Redox-Active Tunneling Junctions. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 55044-55055.	8.0	21
28	On the reliability of acquiring molecular junction parameters by Lorentzian fitting of I/V curves. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26702-26706.	2.8	5
29	Fine Control of the Chemistry of Nitrogen Doping in TiO ₂ : A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17401-17412.	3.1	17
30	Efficient Convergent Energy Transfer in a Stereoisomerically Pure Heptanuclear Luminescent Terpyridine-Based Ru(II)-Os(II) Dendrimer. <i>Inorganic Chemistry</i> , 2020, 59, 14536-14543.	4.0	5
31	Enhanced Adhesion Energy at Oxide/Ag Interfaces for Low-Emissivity Glasses: Theoretical Insight into Doping and Vacancy Effects. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 40838-40849.	8.0	5
32	Interlayer Bonding in Two-Dimensional Materials: The Special Case of SnP ₃ and GeP ₃ . <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4503-4510.	4.6	24
33	Theoretical characterization of the electronic properties of heterogeneous vertical stacks of 2D metal dichalcogenides containing one doped layer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14088-14098.	2.8	5
34	Sodium Coordination and Protonation of Poly(ethoxy phosphate) Chains in the Gas Phase Probed by Ion Mobility-Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 633-641.	2.8	4
35	Helicity of Peptoid Ions in the Gas Phase. <i>Biomacromolecules</i> , 2020, 21, 903-909.	5.4	7
36	Tuning Spin Current Injection at Ferromagnet-Nonmagnet Interfaces by Molecular Design. <i>Physical Review Letters</i> , 2020, 124, 027204.	7.8	19

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37	Effects of electrospray mechanisms and structural relaxation on polylactide ion conformations in the gas phase: insights from ion mobility spectrometry and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4193-4204.	2.8	9
38	Co-sputtering of gold and copper onto liquids: a route towards the production of porous gold nanoparticles. <i>Nanotechnology</i> , 2020, 31, 455303.	2.6	11
39	Influence of the nature of the anchoring group on the interfacial energy level alignment in dye-sensitized solar cells: A theoretical perspective. <i>Physical Review Materials</i> , 2020, 4, .	2.4	4
40	Ion mobility mass spectrometry of saponin ions. <i>Rapid Communications in Mass Spectrometry</i> , 2019, 33, 22-33.	1.5	17
41	Resilience to Conformational Fluctuations Controls Energetic Disorder in Conjugated Polymer Materials: Insights from Atomistic Simulations. <i>Chemistry of Materials</i> , 2019, 31, 6889-6899.	6.7	30
42	Tuning the Optical and Electrical Properties of Few-Layer Black Phosphorus via Physisorption of Small Solvent Molecules. <i>Small</i> , 2019, 15, e1903432.	10.0	21
43	Repurposing DNA-binding agents as H-bonded organic semiconductors. <i>Nature Communications</i> , 2019, 10, 4217.	12.8	28
44	Dynamically Switching the Electronic and Electrostatic Properties of Indium-Tin Oxide Electrodes with Photochromic Monolayers: Toward Photoswitchable Optoelectronic Devices. <i>ACS Applied Nano Materials</i> , 2019, 2, 1102-1110.	5.0	20
45	A tool box to ascertain the nature of doping and photoresponse in single-walled carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4063-4071.	2.8	9
46	Photomodulation of Two-Dimensional Self-Assembly of Azobenzene-Hexa-peri-hexabenzocoronene Azobenzene Triads. <i>Chemistry of Materials</i> , 2019, 31, 6979-6985.	6.7	18
47	One Step Further in the Characterization of Synthetic Polymers by Ion Mobility Mass Spectrometry: Evaluating the Contribution of End-groups. <i>Polymers</i> , 2019, 11, 688.	4.5	11
48	A New Class of Rigid Multi(azobenzene) Switches Featuring Electronic Decoupling: Unravelling the Isomerization in Individual Photochromes. <i>Journal of the American Chemical Society</i> , 2019, 141, 9273-9283.	13.7	43
49	Reversible switching of the Au(111) work function by near infrared irradiation with a bistable SAM based on a radical donor-acceptor dyad. <i>Journal of Materials Chemistry C</i> , 2019, 7, 7418-7426.	5.5	3
50	Glass Hardness Modification by Means of Ion Implantation: Electronic Doping versus Surface Composition Effect. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900039.	2.8	4
51	Simple Approach for a Self-Healable and Stiff Polymer Network from Iminoboronate-Based Boroxine Chemistry. <i>Chemistry of Materials</i> , 2019, 31, 3736-3744.	6.7	87
52	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4382-4391.	5.5	10
53	Switching the Electronic Properties of ZnO Surfaces with Negative Type Photochromic Pyridyl-dihydropyrene Layers and Impact of Fermi Level Pinning. <i>Advanced Materials Interfaces</i> , 2019, 6, 1900211.	3.7	13
54	Modelling Coupled Ion Motion in Electrolyte Solutions for Lithium-Sulfur Batteries. <i>Batteries and Supercaps</i> , 2019, 2, 473-481.	4.7	9

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55	Backbone Cleavages of Protonated Peptoids upon Collision-Induced Dissociation: Competitive and Consecutive B-Y and A ₁ -Y _X Reactions. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 2726-2740.	2.8	3
56	Mechanistic Insights on Spontaneous Moisture-Driven Healing of Urea-Based Polyurethanes. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 46176-46182.	8.0	18
57	Black Phosphorus: Tuning the Optical and Electrical Properties of Few-Layer Black Phosphorus via Physisorption of Small Solvent Molecules (Small 47/2019). <i>Small</i> , 2019, 15, 1970252.	10.0	3
58	Side-chain loss reactions of collisionally activated protonated peptoids: A mechanistic insight. <i>International Journal of Mass Spectrometry</i> , 2019, 435, 217-226.	1.5	4
59	Theoretical characterization of strain and interfacial electronic effects in donor-acceptor bilayers of 2D transition metal dichalcogenides. <i>2D Materials</i> , 2019, 6, 015025.	4.4	11
60	Doping of Monolayer Transition-Metal Dichalcogenides via Physisorption of Aromatic Solvent Molecules. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 540-547.	4.6	52
61	Effect of the Molecular Polarizability of SAMs on the Work Function Modification of Gold: Closed- versus Open-Shell Donor-Acceptor SAMs. <i>Advanced Materials Technologies</i> , 2019, 4, 1800152.	5.8	13
62	Discrimination of positional isomers by ion mobility mass spectrometry: application to organic semiconductors. <i>Analytical Methods</i> , 2018, 10, 2303-2306.	2.7	2
63	HOMO Level Pinning in Molecular Junctions: Joint Theoretical and Experimental Evidence. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2394-2403.	4.6	45
64	Energy Level Alignment at Interfaces Between Au (111) and Thiolated Oligophenylenes of Increasing Chain Size: Theoretical Evidence of Pinning Effects. <i>Advanced Theory and Simulations</i> , 2018, 1, 1700020.	2.8	13
65	Rotator side chains trigger cooperative transition for shape and function memory effect in organic semiconductors. <i>Nature Communications</i> , 2018, 9, 278.	12.8	90
66	Flying Cages in Traveling Wave Ion Mobility: Influence of the Instrumental Parameters on the Topology of the Host-Guest Complexes. <i>Journal of the American Society for Mass Spectrometry</i> , 2018, 29, 121-132.	2.8	9
67	PEPDROID: Development of a Generic DREIDING-Based Force Field for the Assessment of Peptoid Secondary Structures. <i>Advanced Theory and Simulations</i> , 2018, 1, 1800089.	2.8	21
68	Influence of the donor unit on the rectification ratio in tunnel junctions based on donor-acceptor SAMs using PTM units as acceptors. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25638-25647.	2.8	15
69	Electronic Decoupling in C ₃ -Symmetrical Light-Responsive Tris(Azobenzene) Scaffolds: Self-Assembly and Multiphotochromism. <i>Journal of the American Chemical Society</i> , 2018, 140, 16062-16070.	13.7	37
70	On the Sputtering of Titanium and Silver onto Liquids, Discussing the Formation of Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26605-26612.	3.1	17
71	Dynamic Photoswitching of Electron Energy Levels at Hybrid ZnO/Organic Photochromic Molecule Junctions. <i>Advanced Functional Materials</i> , 2018, 28, 1800716.	14.9	26
72	Design of Perchlorotriphenylmethyl (PTM) Radical-Based Compounds for Optoelectronic Applications: The Role of Orbital Delocalization. <i>ChemPhysChem</i> , 2018, 19, 2572-2578.	2.1	17

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73	Correlation between the shape of the ion mobility signals and the stepwise folding process of polylactide ions. <i>Journal of Mass Spectrometry</i> , 2017, 52, 133-138.	1.6	25
74	Tackling saponin diversity in marine animals by mass spectrometry: data acquisition and integration. <i>Analytical and Bioanalytical Chemistry</i> , 2017, 409, 3115-3126.	3.7	20
75	New Photomechanical Molecular Switch Based on a Linear π -Conjugated System. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12416-12425.	3.1	15
76	Which Oxide for Low-Emissivity Glasses? First-Principles Modeling of Silver Adhesion. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 18346-18354.	8.0	10
77	Estimation of π - π Electronic Couplings from Current Measurements. <i>Nano Letters</i> , 2017, 17, 3215-3224.	9.1	35
78	Influence of the nature of the anchoring group on electron injection processes at dye-titania interfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29389-29401.	2.8	18
79	Polymers for Traveling Wave Ion Mobility Spectrometry Calibration. <i>Journal of the American Society for Mass Spectrometry</i> , 2017, 28, 2483-2491.	2.8	36
80	Edge Functionalization of Structurally Defined Graphene Nanoribbons for Modulating the Self-Assembled Structures. <i>Journal of the American Chemical Society</i> , 2017, 139, 16454-16457.	13.7	43
81	Synthesis and Characterization of Ethylenedithio-MPTTF-PTM Radical Dyad as a Potential Neutral Radical Conductor. <i>Magnetochemistry</i> , 2016, 2, 46.	2.4	4
82	Influence of Equilibration Time in Solution on the Inclusion/Exclusion Topology Ratio of Host-Guest Complexes Probed by Ion Mobility and Collision-Induced Dissociation. <i>Chemistry - A European Journal</i> , 2016, 22, 4528-4534.	3.3	15
83	Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2- <i>b</i>][1]benzothiophene. <i>Advanced Materials</i> , 2016, 28, 7106-7114.	21.0	138
84	Design, synthesis, chemical stability, packing, cyclic voltammetry, ionisation potential, and charge transport of [1]benzothieno[3,2- <i>b</i>][1]benzothiophene derivatives. <i>Journal of Materials Chemistry C</i> , 2016, 4, 4863-4879.	5.5	33
85	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 433002.	1.8	131
86	Oxygen vacancy stabilized zirconia (OVSZ); a joint experimental and theoretical study. <i>Scripta Materialia</i> , 2016, 124, 26-29.	5.2	43
87	Charge Carrier Mobility: Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2- <i>b</i>][1]benzothiophene (Adv.) <i>Tj ETQq1 1 0.784314 rgBT /Over</i>	21.0	138
88	Structural Characterization of Alkylsilane and Fluoroalkylsilane Self-Assembled Monolayers on SiO ₂ by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14652-14662.	3.1	42
89	Partial vs. integer electron transfer in molecular assemblies: On the importance of multideterminant theoretical description and the necessity to find a solution within DFT. , 2015, , .		1
90	Modulating the charge injection in organic field-effect transistors: fluorinated oligophenyl self-assembled monolayers for high work function electrodes. <i>Journal of Materials Chemistry C</i> , 2015, 3, 3007-3015.	5.5	62

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91	Toward Fast and Accurate Evaluation of Charge On-Site Energies and Transfer Integrals in Supramolecular Architectures Using Linear Constrained Density Functional Theory (CDFT)-Based Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2077-2086.	5.3	38
92	Energy Level Alignment at Titanium Oxide–Dye Interfaces: Implications for Electron Injection and Light Harvesting. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9899-9909.	3.1	28
93	Bulky End-Capped [1]Benzothieno[3,2- <i>b</i>]benzothiophenes: Reaching High-Mobility Organic Semiconductors by Fine Tuning of the Crystalline Solid-State Order. <i>Advanced Materials</i> , 2015, 27, 3066-3072.	21.0	155
94	Thienoacene dimers based on the thieno[3,2- <i>b</i>]thiophene moiety: synthesis, characterization and electronic properties. <i>Journal of Materials Chemistry C</i> , 2015, 3, 674-685.	5.5	62
95	Work function modification of the (111) gold surface covered by long alkanethiol-based self-assembled monolayers. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2866.	2.8	26
96	25th Anniversary Article: High-Mobility Hole and Electron Transport Conjugated Polymers: How Structure Defines Function. <i>Advanced Materials</i> , 2014, 26, 2119-2136.	21.0	199
97	Approaching disorder-free transport in high-mobility conjugated polymers. <i>Nature</i> , 2014, 515, 384-388.	27.8	844
98	Light-induced reversible modification of the work function of a new perfluorinated biphenyl azobenzene chemisorbed on Au (111). <i>Nanoscale</i> , 2014, 6, 8969-8977.	5.6	31
99	Work function shifts of a zinc oxide surface upon deposition of self-assembled monolayers: a theoretical insight. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20887-20899.	2.8	33
100	Fermi Level Pinning and Orbital Polarization Effects in Molecular Junctions: The Role of Metal Induced Gap States. <i>Advanced Functional Materials</i> , 2014, 24, 6154-6165.	14.9	59
101	Photoswitching Azobenzene Derivatives in Single Molecule Junctions: A Theoretical Insight into the Characteristics. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18721-18729.	3.1	32
102	A one-pot two-step efficient metal-free process for the generation of PEO- <i>b</i> -PCL- <i>b</i> -PLA amphiphilic triblock copolymers. <i>RSC Advances</i> , 2014, 4, 10028.	3.6	28
103	Probing the Relation Between Charge Transport and Supramolecular Organization Down to Ångström Resolution in a Benzothiadiazole–Cyclopentadithiophene Copolymer. <i>Advanced Materials</i> , 2013, 25, 1939-1947.	21.0	84
104	Large Work Function Shift of Gold Induced by a Novel Perfluorinated Azobenzene-Based Self-Assembled Monolayer. <i>Advanced Materials</i> , 2013, 25, 432-436.	21.0	93
105	Tuning of the Photovoltaic Parameters of Molecular Donors by Covalent Bridging. <i>Advanced Functional Materials</i> , 2013, 23, 4854-4861.	14.9	20
106	Homotropic Allostery: In-Depth Structural Analysis of the Gas-Phase Noncovalent Complexes Associating a Double-Cavity Cucurbit[<i>n</i>]uril-Type Host and Size-Selected Protonated Amino Compounds. <i>ChemPlusChem</i> , 2013, 78, 959-969.	2.8	16
107	Work-function modification of the (111) gold surface upon deposition of self-assembled monolayers based on alkanethiol derivatives. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2013, 189, 32-38.	1.7	22
108	On the Supramolecular Packing of High Electron Mobility Naphthalene Diimide Copolymers: The Perfect Registry of Asymmetric Branched Alkyl Side Chains. <i>Macromolecules</i> , 2013, 46, 8171-8178.	4.8	44

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109	Impact of derivatization on electron transmission through dithienylethene-based photoswitches in molecular junctions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4392.	2.8	49
110	Exploring the Energy Landscape of the Charge Transport Levels in Organic Semiconductors at the Molecular Scale. <i>Accounts of Chemical Research</i> , 2013, 46, 434-443.	15.6	64
111	Work Function Modification of Au and Ag Surfaces upon Deposition of Self-Assembled Monolayers: Influence of the Choice of the Theoretical Approach and the Thiol Decomposition Scheme. <i>ChemPhysChem</i> , 2013, 14, 2939-2946.	2.1	14
112	Asymmetric electron and hole transport in a high-mobility n -type conjugated polymer. <i>Physical Review B</i> , 2012, 86,	3.2	63
113	Synthesis of poly(α -lactide) and gradient copolymers from α -lactide/trimethylene carbonate eutectic melt. <i>Chemical Science</i> , 2012, 3, 723-726.	7.4	45
114	Density functional theory for the description of charge-transfer processes at TTF/TCNQ interfaces. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	15
115	Photo-modulable molecular transport junctions based on organometallic molecular wires. <i>Chemical Science</i> , 2012, 3, 3113.	7.4	94
116	The Impact of Molecular Orientation on the Photovoltaic Properties of a Phthalocyanine/Fullerene Heterojunction. <i>Advanced Functional Materials</i> , 2012, 22, 2987-2995.	14.9	298
117	Electronic and structural characterisation of a tetrathiafulvalene compound as a potential candidate for ambipolar transport properties. <i>CrystEngComm</i> , 2011, 13, 6597.	2.6	19
118	Origin of the different transport properties of electron and hole polarons in an ambipolar polyselenophene-based conjugated polymer. <i>Physical Review B</i> , 2011, 84, .	3.2	39
119	Photoinduced work function changes by isomerization of a densely packed azobenzene-based SAM on Au: a joint experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14302.	2.8	61
120	Size Dependence of the Folding of Multiply Charged Sodium Cationized Polylactides Revealed by Ion Mobility Mass Spectrometry and Molecular Modelling. <i>Chemistry - A European Journal</i> , 2011, 17, 9738-9745.	3.3	41
121	Ferromagnetism in transparent thin films of MgO. <i>Physical Review B</i> , 2010, 82, .	3.2	91
122	On the Interface Dipole at the Pentacene/Fullerene Heterojunction: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3215-3224.	3.1	122
123	Bianthrone in a Single-Molecule Junction: Conductance Switching with a Bistable Molecule Facilitated by Image Charge Effects. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20686-20695.	3.1	19
124	Multideterminant assessment of mean-field methods for the description of electron transfer in the weak-coupling regime. <i>Physical Review B</i> , 2009, 80, .	3.2	19
125	Screening effects in a density functional theory based description of molecular junctions in the Coulomb blockade regime. <i>Physical Review B</i> , 2009, 79, .	3.2	17
126	Quantum-Chemical Characterization of the Origin of Dipole Formation at Molecular Organic/Organic Interfaces. <i>Advanced Functional Materials</i> , 2009, 19, 624-633.	14.9	63

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127	Electronic Structure and Geminate Pair Energetics at Organic/Organic Interfaces: The Case of Pentacene/C ₆₀ Heterojunctions. <i>Advanced Functional Materials</i> , 2009, 19, 3809-3814.	14.9	208
128	Solid-State Supramolecular Organization of Polythiophene Chains Containing Thienothiophene Units. <i>Advanced Materials</i> , 2009, 21, 1193-1198.	21.0	76
129	Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. <i>ChemPhysChem</i> , 2009, 10, 2265-2273.	2.1	77
130	Inside Cover: Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene (<i>ChemPhysChem</i> 13/2009). <i>ChemPhysChem</i> , 2009, 10, 2158-2158.	2.1	0
131	Tuning the Energy Levels of Photochromic Diarylethene Compounds for Opto-Electronic Switch Devices. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18396-18405.	3.1	44
132	Electronic structure of small band gap oligomers based on cyclopentadithiophenes and acceptor units. <i>Journal of Materials Chemistry</i> , 2009, 19, 5343.	6.7	63
133	Towards a theoretical description of molecular junctions in the Coulomb blockade regime based on density functional theory. <i>Physical Review B</i> , 2008, 78, .	3.2	21
134	A theoretical view of unimolecular rectification. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 374105.	1.8	50
135	Electronic polarization effects on charge carriers in anthracene: A valence bond study. <i>Physical Review B</i> , 2008, 77, .	3.2	72
136	Depolarization Effects in Self-Assembled Monolayers: A Quantum-Chemical Insight. <i>Advanced Functional Materials</i> , 2007, 17, 1143-1148.	14.9	97
137	Optical Bandgaps of π -Conjugated Organic Materials at the Polymer Limit: Experiment and Theory. <i>Advanced Materials</i> , 2007, 19, 173-191.	21.0	566
138	Ambipolar Transport in Organic Conjugated Materials. <i>Advanced Materials</i> , 2007, 19, 1791-1799.	21.0	296
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