Chad Risko

List of Publications by Year
in descending order

189 papers	8,877 citations	36087 51 h-index	49007 88 g-index
202 all docs	202 docs citations	202 times ranked	11948 citing authors

#	Article	IF	Citations
1	Design, Synthesis, and Characterization of Ladder-Type Molecules and Polymers. Air-Stable, Solution-Processable n-Channel and Ambipolar Semiconductors for Thin-Film Transistors via Experiment and Theory. Journal of the American Chemical Society, 2009, 131, 5586-5608.	14.6	490
2	Synthesis, Characterization, and Transistor Response of Semiconducting Silole Polymers with Substantial Hole Mobility and Air Stability. Experiment and Theory. Journal of the American Chemical Society, 2008, 130, 7670-7685.	14.6	345
3	A molecular interactionâ€“diffusion framework for predicting organic solar cell stability. Nature Materials, 2021, 20, 525-532.	26.6	251
4	A quantum-chemical perspective into low optical-gap polymers for highly-efficient organic solar cells. Chemical Science, 2011, 2, 1200-1218.	7.8	242
5	Solution-Processed Organic Solar Cells with Power Conversion Efficiencies of 2.5% using Benzothiadiazole/Imide-Based Acceptors. Chemistry of Materials, 2011, 23, 5484-5490.	7.1	232
6	Noncovalent Intermolecular Interactions in Organic Electronic Materials: Implications for the Molecular Packing vs Electronic Properties of Acenes. Chemistry of Materials, 2016, 28, 3-16.	7.1	226
7	Transition from Tunneling to Hopping Transport in Long, Conjugated Oligo-imine Wires Connected to Metals. Journal of the American Chemical Society, 2010, 132, 4358-4368.	14.6	220
8	Donorâ€“Acceptor Copolymers of Relevance for Organic Photovoltaics: A Theoretical Investigation of the Impact of Chemical Structure Modifications on the Electronic and Optical Properties. Macromolecules, 2012, 45, 6405-6414.	5.1	205
9	High current density, long duration cycling of soluble organic active species for non-aqueous redox flow batteries. Energy and Environmental Science, 2016, 9, 3531-3543.	32.2	203
10	Controlled Conjugated Backbone Twisting for an Increased Open-Circuit Voltage while Having a High Short-Circuit Current in Poly(hexylthiophene) Derivatives. Journal of the American Chemical Society, 2012, 134, 5222-5232.	14.6	189
11	Electron Affinities of 1,1-Diaryl-2,3,4,5-tetraphenylsiloles:Â Direct Measurements and Comparison with Experimental and Theoretical Estimates. Journal of the American Chemical Society, 2005, 127, 9021-9029.	14.6	156
12	Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties. Chemistry of Materials, 2013, 25, 2254-2263.	7.1	145
13	Intervalence Transitions in the Mixed-Valence Monocations of Bis(triarylamines) Linked with Vinylene and Phenyleneâ^Vinylene Bridges. Journal of the American Chemical Society, 2005, 127, 16900-16911.	14.6	135
14	Heteroannulated acceptors based on benzothiadiazole. Materials Horizons, 2015, 2, 22-36.	12.8	130
15	Use of Xâ€Ray Diffraction, Molecular Simulations, and Spectroscopy to Determine the Molecular Packing in a Polymerâ€Fullerene Bimolecular Crystal. Advanced Materials, 2012, 24, 6071-6079.	24.3	127
16	Synthetic Principles Directing Charge Transport in Low-Band-Gap Dithienosiloleâ€“Benzothiadiazole Copolymers. Journal of the American Chemical Society, 2012, 134, 8944-8957.	14.6	125
17	Ring Substituents Mediate the Morphology of PBDTTPD-PCBM Bulk-Heterojunction Solar Cells. Chemistry of Materials, 2014, 26, 2299-2306.	7.1	121
18	Engineering ligand reactivity enables high-temperature operation of stable perovskite solar cells. Science, 2023, 381, 209-215.	20.9	121

#	Article	IF	Citations
19	Impact of Molecular Packing on Electronic Polarization in Organic Crystals: The Case of Pentacene vs TIPS-Pentacene. Journal of the American Chemical Society, 2014, 136, 6421-6427.	14.6	117
20	A stable two-electron-donating phenothiazine for application in nonaqueous redox flow batteries. Journal of Materials Chemistry A, 2017, 5, 24371-24379.	10.5	114
21	Three-Dimensional Packing Structure and Electronic Properties of Biaxially Oriented Poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene) Films. Journal of the American Chemical Society, 2012, 134, 6177-6190.	14.6	113
22	Electronic Coupling in Tetraanisylarylenediamine Mixed-Valence Systems:Â The Interplay between Bridge Energy and Geometric Factors. Journal of the American Chemical Society, 2005, 127, 8508-8516.	14.6	110
23	Exploiting Excited-State Aromaticity To Design Highly Stable Singlet Fission Materials. Journal of the American Chemical Society, 2019, 141, 13867-13876.	14.6	109
24	Solution-Processed Molecular Bis(Naphthalene Diimide) Derivatives with High Electron Mobility. Chemistry of Materials, 2011, 23, 3408-3410.	7.1	107
25	Indacenodibenzothiophenes: synthesis, optoelectronic properties and materials applications of molecules with strong antiaromatic character. Chemical Science, 2016, 7, 5547-5558.	7.8	105
26	25th Anniversary Article: Design of Polymethine Dyes for Allâ€Optical Switching Applications: Guidance from Theoretical and Computational Studies. Advanced Materials, 2014, 26, 68-84.	24.3	99
27	High Charge-Carrier Mobility in an Amorphous Hexaazatrinaphthylene Derivative. Journal of the American Chemical Society, 2005, 127, 16358-16359.	14.6	97
28	Factors Governing Intercalation of Fullerenes and Other Small Molecules Between the Side Chains of Semiconducting Polymers Used in Solar Cells. Advanced Energy Materials, 2012, 2, 1208-1217.	22.2	97
29	Characterization of Charge-Carrier Transport in Semicrystalline Polymers: Electronic Couplings, Site Energies, and Charge-Carrier Dynamics in Poly(bithiophene-alt-thienothiophene) [PBTTT]. Journal of Physical Chemistry C, 2013, 117, 1633-1640.	3.3	94
30	Intermixing at the Pentaceneâ€Fullerene Bilayer Interface: A Molecular Dynamics Study. Advanced Materials, 2013, 25, 878-882.	24.3	92
31	Synthesis, Ionisation Potentials and Electron Affinities of Hexaazatrinaphthylene Derivatives. Chemistry - A European Journal, 2007, 13, 3537-3547.	3.9	91
32	Benzothiadiazole-Dithienopyrrole Donorâ€“Acceptorâ€“Donor and Acceptorâ€“Donorâ€“Acceptor Triads: Synthesis and Optical, Electrochemical, and Charge-Transport Properties. Journal of Physical Chemistry C, 2011, 115, 23149-23163.	3.3	90
33	Tuning the Optoelectronic Properties of Vinylene-Linked Donorâ”Acceptor Copolymers for Organic Photovoltaics. Macromolecules, 2010, 43, 6685-6698.	5.1	86
34	To bend or not to bend â€“ are heteroatom interactions within conjugated molecules effective in dictating conformation and planarity?. Materials Horizons, 2016, 3, 333-339.	12.8	84
35	Isolation and Crystal Structures of Two Singlet Bis(Triarylamine) Dications with Nonquinoidal Geometries. Journal of the American Chemical Society, 2006, 128, 1812-1817.	14.6	79
36	Crossover from band-like to thermally activated charge transport in organic transistors due to strain-induced traps. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6739-E6748.	7.6	79

#	Article	IF	Citations
37	n-type charge transport in heavily p-doped polymers. Nature Materials, 2021, 20, 518-524.	26.6	79
38	Distinguishing the Effects of Bond-Length Alternation versus Bond-Order Alternation on the Nonlinear Optical Properties of Ï€-Conjugated Chromophores. Journal of Physical Chemistry Letters, 2015, 6, 2158-2162.	4.9	78
39	Strain effects on the work function of an organic semiconductor. Nature Communications, 2016, 7, 10270.	13.2	78
40	Bis(carbazolyl) derivatives of pyrene and tetrahydropyrene: synthesis, structures, optical properties, electrochemistry, and electroluminescence. Journal of Materials Chemistry C, 2013, 1, 1638.	5.6	77
41	Polymethine dyes for all-optical switching applications: a quantum-chemical characterization of counter-ion and aggregation effects on the third-order nonlinear optical response. Chemical Science, 2012, 3, 3103.	7.8	76
42	Tuning Delocalization in the Radical Cations of 1,4-Bis[4-(diarylamino)styryl]benzenes, 2,5-Bis[4-(diarylamino)styryl]thiophenes, and 2,5-Bis[4-(diarylamino)styryl]pyrroles through Substituent Effects. Journal of the American Chemical Society, 2012, 134, 10146-10155.	14.6	73
43	nâ€Doping of Organic Electronic Materials Using Airâ€Stable Organometallics: A Mechanistic Study of Reduction by Dimeric Sandwich Compounds. Chemistry - A European Journal, 2012, 18, 14760-14772.	3.9	67
44	Understanding the Electronic Structure of Isoindigo in Conjugated Systems: A Combined Theoretical and Experimental Approach.. Macromolecules, 2013, 46, 8832-8844.	5.1	65
45	Fullereneâ€“Carbene Lewis Acidâ€“Base Adducts. Journal of the American Chemical Society, 2011, 133, 12410-12413.	14.6	64
46	Nâ€Substituted Phenothiazine Derivatives: How the Stability of the Neutral and Radical Cation Forms Affects Overcharge Performance in Lithiumâ€ion Batteries. ChemPhysChem, 2015, 16, 1179-1189.	2.3	62
47	Polymethine materials with solid-state third-order optical susceptibilities suitable for all-optical signal-processing applications. Materials Horizons, 2014, 1, 577-581.	12.8	60
48	Entanglements in <scp>P3HT</scp> and their influence on thinâ€film mechanical properties: Insights from molecular dynamics simulations. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 934-942.	2.4	60
49	Molecular-Scale Understanding of Cohesion and Fracture in P3HT:Fullerene Blends. ACS Applied Materials & Interfaces, 2015, 7, 9957-9964.	8.3	60
50	Rubrene: The Interplay between Intramolecular and Intermolecular Interactions Determines the Planarization of Its Tetracene Core in the Solid State. Journal of the American Chemical Society, 2015, 137, 8775-8782.	14.6	59
51	Suppressing bias stress degradation in high performance solution processed organic transistors operating in air. Nature Communications, 2021, 12, 2352.	13.2	57
52	Rational Functionalization of a C₇₀ Buckybowl To Enable a C₇₀:Buckybowl Cocrystal for Organic Semiconductor Applications. Journal of the American Chemical Society, 2020, 142, 2460-2470.	14.6	55
53	Understanding the effect of host structure of nitrogen doped ultrananocrystalline diamond electrode on electrochemical carbon dioxide reduction. Carbon, 2020, 157, 408-419.	10.7	53
54	On the Molecular Origin of Charge Separation at the Donorâ€“Acceptor Interface. Advanced Energy Materials, 2018, 8, 1702232.	22.2	52

#	Article	IF	Citations
55	A mixed-valence bis(diarylamino)stilbene: crystal structure and comparison of electronic coupling with biphenyl and tolane analogues. Chemical Communications, 2005, , 764-766.	4.2	51
56	Electronic Polarization Effects upon Charge Injection in Oligoacene Molecular Crystals: Description via a Polarizable Force Field. Journal of Physical Chemistry C, 2013, 117, 13853-13860.	3.3	51
57	Near-Infrared-Absorbing Indolizine-Porphyrin Pushâ€“Pull Dye for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 16474-16489.	8.3	49
58	Fabrication and characterization of metal-molecule-silicon devices. Applied Physics Letters, 2007, 91, 033508.	3.2	48
59	Reactivity of an air-stable dihydrobenzoimidazole n-dopant with organic semiconductor molecules. CheM, 2021, 7, 1050-1065.	12.2	48
60	Structure and Disorder in Squaraineâ€“C₆₀ Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donorâ€“Acceptor Interface. Advanced Functional Materials, 2014, 24, 3790-3798.	16.5	45
61	Materialsâ€Scale Implications of Solvent and Temperature on [6,6]â€Phenylâ€C61â€butyric Acid Methyl Ester (PCBM): A Theoretical Perspective. Advanced Functional Materials, 2013, 23, 5800-5813.	16.5	44
62	Dimers of Nineteenâ€Electron Sandwich Compounds: Crystal and Electronic Structures, and Comparison of Reducing Strengths. Chemistry - A European Journal, 2014, 20, 15385-15394.	3.9	43
63	Fluorenyl-substituted silole molecules: geometric, electronic, optical, and device properties. Journal of Materials Chemistry, 2008, 18, 3157.	6.7	41
64	Synthesis, experimental and theoretical characterization, and field-effect transistor properties of a new class of dibenzothiophene derivatives: From linear to cyclic architectures. Journal of Materials Chemistry, 2012, 22, 1313-1325.	6.7	41
65	Tuning the electronic and photophysical properties of heteroleptic iridium(iii) phosphorescent emitters through ancillary ligand substitution: a theoretical perspective. Physical Chemistry Chemical Physics, 2013, 15, 6293.	2.9	41
66	Influence of Molecular Shape on Solid-State Packing in Disordered PC₆₁BM and PC₇₁BM Fullerenes. Journal of Physical Chemistry Letters, 2014, 5, 3427-3433.	4.9	41
67	The fate of phenothiazine-based redox shuttles in lithium-ion batteries. Physical Chemistry Chemical Physics, 2015, 17, 6905-6912.	2.9	41
68	Organic Semiconductors Derived from Dinaphtho-Fused s-Indacenes: How Molecular Structure and Film Morphology Influence Thin-Film Transistor Performance. Chemistry of Materials, 2019, 31, 6962-6970.	7.1	41
69	Impact of Molecular Orientation and Packing Density on Electronic Polarization in the Bulk and at Surfaces of Organic Semiconductors. ACS Applied Materials & Interfaces, 2016, 8, 14053-14062.	8.3	40
70	Noncovalent Interactions and Impact of Charge Penetration Effects in Linear Oligoacene Dimers and Single Crystals. Chemistry of Materials, 2016, 28, 3990-4000.	7.1	39
71	Impact of the Nature of the Excited-State Transition Dipole Moments on the Third-Order Nonlinear Optical Response of Polymethine Dyes for All-Optical Switching Applications. ACS Photonics, 2014, 1, 261-269.	6.9	36
72	nâ€Dopants Based on Dimers of Benzimidazoline Radicals: Structures and Mechanism of Redox Reactions. Chemistry - A European Journal, 2015, 21, 10878-10885.	3.9	36

#	Article	IF	Citations
73	Structural dependence of the optical properties of narrow bandgap semiconductors with orthogonal donorâ€“acceptor geometries. Chemical Science, 2013, 4, 1807.	7.8	35
74	Donor or Acceptor? How Selection of the Rylene Imide End Cap Impacts the Polarity of Ï€-Conjugated Molecules for Organic Electronics. ACS Applied Energy Materials, 2018, 1, 4906-4916.	5.3	34
75	Mono- and Dicarbonyl-Bridged Tricyclic Heterocyclic Acceptors: Synthesis and Electronic Properties. Journal of Organic Chemistry, 2011, 76, 2660-2671.	3.3	33
76	An unsymmetrical non-fullerene acceptor: synthesis via direct heteroarylation, self-assembly, and utility as a low energy absorber in organic photovoltaic cells. Chemical Communications, 2017, 53, 10168-10171.	4.2	32
77	Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. Chemistry of Materials, 2019, 31, 1507-1519.	7.1	32
78	Theory-Driven Insight into the Crystal Packing of Trialkylsilylethynyl Pentacenes. Chemistry of Materials, 2017, 29, 2502-2512.	7.1	30
79	Polarization Energies at Organicâ€“Organic Interfaces: Impact on the Charge Separation Barrier at Donorâ€“Acceptor Interfaces in Organic Solar Cells. ACS Applied Materials & Interfaces, 2016, 8, 15524-15534.	8.3	29
80	On the impact of isomer structure and packing disorder in thienoacene organic semiconductors. Journal of Materials Chemistry C, 2016, 4, 4040-4048.	5.6	29
81	Presence of Short Intermolecular Contacts Screens for Kinetic Stability in Packing Polymorphs. Journal of the American Chemical Society, 2018, 140, 7519-7525.	14.6	29
82	Noncovalent Close Contacts in Fluorinated Thiopheneâ€“Phenyleneâ€“Thiophene Conjugated Units: Understanding the Nature and Dominance of OÂ·Â·Â·H versus SÂ·Â·Â·F and OÂ·Â·Â·F Interactions with Respect to the Control of Polymer Conformation. Chemistry of Materials, 2019, 31, 7070-7079.	7.1	29
83	Effect of Solvent Additives on the Solution Aggregation of Phenyl-C₆₁â€“Butyl Acid Methyl Ester (PCBM). Chemistry of Materials, 2015, 27, 8261-8272.	7.1	28
84	Packing and Disorder in Substituted Fullerenes. Journal of Physical Chemistry C, 2016, 120, 17242-17250.	3.3	28
85	OCELOT: An infrastructure for data-driven research to discover and design crystalline organic semiconductors. Journal of Chemical Physics, 2021, 154, 174705.	3.1	28
86	Delimited Polyacenes: Edge Topology as a Tool To Modulate Carbon Nanoribbon Structure, Conjugation, and Mobility. Chemistry of Materials, 2018, 30, 947-957.	7.1	27
87	Acid dyeing for green solvent processing of solvent resistant semiconducting organic thin films. Materials Horizons, 2020, 7, 2959-2969.	12.8	27
88	Substrate-Induced Variations of Molecular Packing, Dynamics, and Intermolecular Electronic Couplings in Pentacene Monolayers on the Amorphous Silica Dielectric. ACS Nano, 2014, 8, 690-700.	15.3	26
89	Interplay of alternative conjugated pathways and steric interactions on the electronic and optical properties of donorâ€“acceptor conjugated polymers. Journal of Materials Chemistry C, 2014, 2, 8873-8879.	5.6	25
90	Overcharge protection of lithium-ion batteries above 4 V with a perfluorinated phenothiazine derivative. Journal of Materials Chemistry A, 2016, 4, 5410-5414.	10.5	25

#	Article	IF	Citations
91	Impact of Atomistic Substitution on Thin-Film Structure and Charge Transport in a Germanyl-ethynyl Functionalized Pentacene. Chemistry of Materials, 2019, 31, 6615-6623.	7.1	25
92	An anionic organic mixed-valence system with a remarkably well-resolved vibrational structure in its intervalence band. Chemical Communications, 2003, , 194-195.	4.2	24
93	Trends in Electron-Vibration and Electronic Interactions in Bis(dimethylamino) Mixed-Valence Systems: A Joint Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2008, 112, 7959-7967.	3.3	24
94	Synthesis and characterization of naphthalene diimide/diethynylbenzene copolymers. Polymer, 2012, 53, 1072-1078.	3.9	24
95	Computational Approaches for Organic Semiconductors: From Chemical and Physical Understanding to Predicting New Materials. Chemical Reviews, 2023, 123, 7498-7547.	51.4	24
96	Benzo[1,2-b:6,5-bâ€²]dithiophene(dithiazole)-4,5-dione derivatives: synthesis, electronic properties, crystal packing and charge transport. Journal of Materials Chemistry C, 2013, 1, 1467.	5.6	23
97	Charge Delocalization through Benzene, Naphthalene, and Anthracene Bridges in Ï€-Conjugated Oligomers: An Experimental and Quantum Chemical Study. Journal of Physical Chemistry B, 2013, 117, 6304-6317.	2.7	23
98	Bond Ellipticity Alternation: An Accurate Descriptor of the Nonlinear Optical Properties of Ï€-Conjugated Chromophores. Journal of Physical Chemistry Letters, 2018, 9, 1377-1383.	4.9	23
99	Bromination of the benzothioxanthene Bloc: toward new Ï€-conjugated systems for organic electronic applications. Journal of Materials Chemistry C, 2018, 6, 761-766.	5.6	23
100	Evenâ€“Odd Alkyl Chain-Length Alternation Regulates Oligothiophene Crystal Structure. Chemistry of Materials, 2019, 31, 6900-6907.	7.1	23
101	Computationally aided design of a high-performance organic semiconductor: the development of a universal crystal engineering core. Chemical Science, 2019, 10, 10543-10549.	7.8	23
102	Structureâ€“processingâ€“property correlations in solution-processed, small-molecule, organic solar cells. Journal of Materials Chemistry C, 2013, 1, 5250.	5.6	22
103	Nonlinear Optical Properties of X(C₆H₅)₄ (X = B^{â€“}, C,) Tj ETQq1 1 0.784314 rgBT Journal of the American Chemical Society, 2015, 137, 9635-9642.	14.6	22
104	Triperyleno[3,3,3]propellane triimides: achieving a new generation of quasi-D_{3h} symmetric nanostructures in organic electronics. Chemical Science, 2019, 10, 4951-4958.	7.8	22
105	Experimental and Theoretical Identification of Valence Energy Levels and Interface Dipole Trends for a Family of (Oligo)Phenylene-ethynylenethiols Adsorbed on Gold. Journal of Physical Chemistry C, 2008, 112, 13215-13225.	3.3	21
106	Impact of Bulk Aggregation on the Electronic Structure of Streptocyanines: Implications for the Solid-State Nonlinear Optical Properties and All-Optical Switching Applications. Journal of Physical Chemistry C, 2014, 118, 23575-23585.	3.3	20
107	Characterizing the Polymer:Fullerene Intermolecular Interactions. Chemistry of Materials, 2016, 28, 1446-1452.	7.1	20
108	Mixed-Valence Cations of Di(carbazol-9-yl) Biphenyl, Tetrahydropyrene, and Pyrene Derivatives. Journal of Physical Chemistry C, 2016, 120, 3156-3166.	3.3	20

#	Article	IF	Citations
109	Comparative studies of the geometric and electronic properties of 1,1-disubstituted-2,3,4,5-tetraphenylsiloles and 1,1,2,2-tetramethyl-3,4,5,6-tetraphenyl-1,2-disila-3,5-cyclohexadiene. Journal of Materials Chemistry, 2006, 16, 3814-3822.	6.7	19
110	Positional Effects from Ïƒ-Bonded Platinum(II) on Intersystem Crossing Rates in Perylenediimide Complexes: Synthesis, Structures, and Photophysical Properties. Journal of Physical Chemistry C, 2018, 122, 13848-13862.	3.3	19
111	Impact of rotamer diversity on the self-assembly of nearly isostructural molecular semiconductors. Journal of Materials Chemistry A, 2018, 6, 383-394.	10.5	19
112	Effect of Bulky Substituents on Thiopyrylium Polymethine Aggregation in the Solid State: A Theoretical Evaluation of the Implications for All-Optical Switching Applications. Chemistry of Materials, 2014, 26, 6439-6447.	7.1	18
113	Dynamics, Miscibility, and Morphology in Polymer:Molecule Blends: The Impact of Chemical Functionality. Chemistry of Materials, 2015, 27, 7643-7651.	7.1	18
114	Lowering Electrocatalytic CO₂ Reduction Overpotential Using N-Annulated Perylene Diimide Rhenium Bipyridine Dyads with Variable Tether Length. Journal of the American Chemical Society, 2021, 143, 16849-16864.	14.6	18
115	The Solution is the Solution: Data-Driven Elucidation of Solution-to-Device Feature Transfer for Ï€-Conjugated Polymer Semiconductors. ACS Applied Materials & Interfaces, 2022, 14, 3613-3620.	8.3	18
116	Bis(tercarbazole) pyrene and tetrahydropyrene derivatives: photophysical and electrochemical properties, theoretical modeling, and OLEDs. Journal of Materials Chemistry C, 2019, 7, 5009-5018.	5.6	16
117	Unusual Electronic Structure of the Donorâ€“Acceptor Cocrystal Formed by Dithieno[3,2-a:2â€²,3â€²-c]phenazine and 7,7,8,8-Tetracyanoquinodimethane. Journal of Physical Chemistry Letters, 2017, 8, 4510-4515.	4.9	16
118	Molecular modulation of Schottky barrier height in metal-molecule-silicon diodes: Capacitance and simulation results. Journal of Applied Physics, 2010, 107, 024505.	2.3	15
119	Small Optical Gap Molecules and Polymers: Using Theory to Design More Efficient Materials for Organic Photovoltaics. Topics in Current Chemistry, 2013, 352, 1-38.	0.0	14
120	Mapping the configuration dependence of electronic coupling in organic semiconductors. Journal of Materials Chemistry C, 2016, 4, 3825-3832.	5.6	14
121	Unveiling the structural, electronic, and optical effects of carbon-doping on multi-layer anatase TiO2 (1 0 1) and the impact on photocatalysis. Applied Surface Science, 2022, 586, 152641.	6.3	14
122	Nitration of benzothioxanthene: towards a new class of dyes with versatile photophysical properties. New Journal of Chemistry, 2020, 44, 900-905.	2.7	13
123	Evolution of Chain Dynamics and Oxidation States with Increasing Chain Length for a Donorâ€“Acceptor-Conjugated Oligomer Series. Macromolecules, 2021, 54, 8207-8219.	5.1	13
124	Genetic Algorithms and Machine Learning for Predicting Surface Composition, Structure, and Chemistry: A Historical Perspective and Assessment. Chemistry of Materials, 2021, 33, 6589-6615.	7.1	12
125	Reconsidering the Roles of Noncovalent Intramolecular â€œLocksâ€•in Ï€-Conjugated Molecules. Chemistry of Materials, 2021, 33, 9139-9151.	7.1	12
126	Assessment of Front-Substituted Zwitterionic Cyanine Polymethines for All-Optical Switching Applications. Journal of Physical Chemistry C, 2017, 121, 14166-14175.	3.3	11

#	Article	IF	Citations
127	Enhancing CO2 absorption for post-combustion carbon capture via zinc-based biomimetic catalysts in industrially relevant amine solutions. International Journal of Greenhouse Gas Control, 2019, 85, 156-165.	4.6	11
128	Deconstructing the behavior of donorâ€“acceptor copolymers in solution & the melt: the case of PTB7. Physical Chemistry Chemical Physics, 2019, 21, 7802-7813.	2.9	11
129	Steric Manipulation as a Mechanism for Tuning the Reduction and Oxidation Potentials of Phenothiazines. Journal of Physical Chemistry A, 2021, 125, 272-278.	2.6	11
130	Modification of the LiFePO₄ (010) Surface Due to Exposure to Atmospheric Gases. ACS Applied Materials & Interfaces, 2021, 13, 29034-29040.	8.3	11
131	Electronic, redox, and optical property prediction of organic Ï€-conjugated molecules through a hierarchy of machine learning approaches. Chemical Science, 2022, 14, 203-213.	7.8	11
132	Beyond the Hammett Effect: Using Strain to Alter the Landscape of Electrochemical Potentials. ChemPhysChem, 2017, 18, 2142-2146.	2.3	10
133	Noncovalent Interactions in Organic Electronic Materials. , 2017, , 277-302.		10
134	What is special about silicon in functionalised organic semiconductors?. Materials Advances, 2021, 2, 5415-5421.	5.2	10
135	Twisted Crystalline Organic Semiconductor Photodetectors. Advanced Functional Materials, 2023, 33, .	16.5	10
136	Dimers of Nineteen-Electron Sandwich Compounds: An Electrochemical Study of the Kinetics of Their Formation. Organometallics, 2015, 34, 3706-3712.	2.6	9
137	Intrinsic Properties of Two Benzodithiophene-Based Donorâ€“Acceptor Copolymers Used in Organic Solar Cells: A Quantum-Chemical Approach. Journal of Physical Chemistry A, 2016, 120, 1051-1064.	2.6	9
138	Data storage architectures to accelerate chemical discovery: data accessibility for individual laboratories and the community. Chemical Science, 2022, 13, 13646-13656.	7.8	9
139	Geometric and Chelation Influences on the Electronic Structure and Optical Properties of Tetra(carboxylic acid)phenyleneethynylene Dyes. Journal of Physical Chemistry A, 2008, 112, 4202-4208.	2.6	8
140	Effect of Halogenation on the Energetics of Pure and Mixed Phases in Model Organic Semiconductors Composed of Anthradithiophene Derivatives and C₆₀. Journal of Physical Chemistry C, 2018, 122, 4757-4767.	3.3	8
141	Oxidation Pathways Involving a Sulfide-Endcapped Donorâ€“Acceptorâ€“Donor Ï€-Conjugated Molecule and Antimony(V) Chloride. Journal of Physical Chemistry B, 2019, 123, 3866-3874.	2.7	8
142	Organometallic hydride-transfer agents as reductants for organic semiconductor molecules. Inorganica Chimica Acta, 2019, 489, 67-77.	2.5	8
143	Chalcocarbogels as High-Capacity and Cycle-Stable Electrode Materials for Lithium and Sodium Ion Batteries. ACS Energy Letters, 2024, 9, 1-9.	18.4	8
144	Solventâ€“Molecule Interactions Govern Crystal-Habit Selection in Naphthalene Tetracarboxylic Diimides. Chemistry of Materials, 2019, 31, 9691-9698.	7.1	7

#	Article	IF	Citations
145	The impact of symmetric modes on intramolecular electron transfer: A semi-classical approach. Chemical Physics, 2006, 326, 107-114.	2.0	6
146	Theoretical description of the geometric and electronic structures of organic-organic interfaces in organic solar cells: a brief review. Science China Chemistry, 2014, 57, 1330-1339.	8.8	6
147	Determination of the Free Energies of Mixing of Organic Solutions through a Combined Molecular Dynamics and Bayesian Statistics Approach. Journal of Chemical Information and Modeling, 2020, 60, 1424-1431.	5.7	6
148	Parallel and Perpendicular Packing in Mixed-Stack Cocrystals of Trimeric Perfluoro-ortho-phenylene Mercury and Benzo[1,2-b:6,5-bâ€²]dithiophene-4,5-dione Derivatives. Crystal Growth and Design, 2016, 16, 2190-2200.	3.2	5
149	Thermomechanical enhancement of <scp>DPPâ€4T</scp> through purposeful <scp>Ï€â€conjugation</scp> disruption. Journal of Polymer Science, 2022, 60, 559-568.	4.2	5
150	Biotinylation as a tool to enhance the uptake of small molecules in Gram-negative bacteria. PLoS ONE, 2021, 16, e0260023.	2.5	5
151	Nanoribbons or weakly connected acenes? The influence of pyrene insertion on linearly extended ring systems. Journal of Materials Chemistry C, 2021, 9, 16929-16934.	5.6	5
152	Challenges in Information-Mining the Materials Literature: A Case Study and Perspective. Chemistry of Materials, 2022, 34, 4821-4827.	7.1	5
153	Relating reorganization energies, exciton diffusion length and non-radiative recombination to the room temperature UV-vis absorption spectra of NF-SMA. Materials Horizons, 2023, 10, 443-453.	12.8	5
154	Resonant X-ray Diffraction Reveals the Location of Counterions in Doped Organic Mixed Ionic Conductors. Chemistry of Materials, 2023, 35, 3960-3967.	7.1	5
155	Towards a comprehensive data infrastructure for redox-active organic molecules targeting non-aqueous redox flow batteries. Digital Discovery, 2023, 2, 1152-1162.	5.7	5
156	Magnetic ordering in a vanadium-organic coordination polymer using a pyrrolo[2,3-d:5,4-dâ€²]bis(thiazole)-based ligand. RSC Advances, 2018, 8, 36223-36232.	3.7	4
157	Exploring thermal transitions in anthradithiophene-based organic semiconductors to reveal structure-packing relationships. Journal of Materials Chemistry C, 2018, 6, 10924-10934.	5.6	4
158	A Genetic Algorithmic Approach to Determine the Structure of Liâ€“Al Layered Double Hydroxides. Journal of Chemical Information and Modeling, 2020, 60, 4845-4855.	5.7	4
159	Synthesis and electronic properties of a linearly fused anthracene dimer. Tetrahedron Letters, 2020, 61, 152182.	1.4	4
160	Synthesis, structures, and reactivity of isomers of [RuCp*(1,4-(Me₂N)₂C₆H₄)]₂. Dalton Transactions, 2021, 50, 13020-13030.	3.4	4
161	Large variability and complexity of isothermal solubility for a series of redox-active phenothiazines. Materials Advances, 2022, 3, 8705-8715.	5.2	4
162	Healing contact. Nature Materials, 2013, 12, 1084-1085.	26.6	3

#	Article	IF	Citations
163	Work function reduction by a redox-active organometallic sandwich complex. Organic Electronics, 2016, 37, 263-270.	2.8	3
164	The role of crystal packing on the optical response of trialkyltetrelethynyl acenes. Journal of Chemical Physics, 2022, 157, .	3.1	3
165	Probing Redox Properties of Extreme Concentrations Relevant for Nonaqueous Redox-Flow Batteries. ACS Applied Energy Materials, 2023, 6, 2819-2831.	5.3	3
166	Impact of Molecular Geometry and Functionalization on Solution Complexation of Coronene-Based Buckybowls and Fullerenes. Chemistry of Materials, 2023, 35, 5524-5531.	7.1	3
167	Colloidal Stability and Solubility of Metalâ€“Organic Framework Particles. Chemistry of Materials, 2024, 36, 3673-3682.	7.1	3
168	Festschrift in Honor of Prof. Jean-Luc BrÃ©das on His 65th Birthday. Chemistry of Materials, 2019, 31, 6307-6308.	7.1	2
169	AlgorithmÂ1025: PARyOpt: A Software for <u>P</u> arallel <u>A</u> synchronous <u>R</u> emote Ba <u>y</u> esian <u>Opt</u> imization. ACM Transactions on Mathematical Software, 2022, 48, 1-15.	3.1	2
170	Carboxylic Acid Decarbonylation on Nickel: The Critical Role of the Acid Binding Geometry. ACS Catalysis, 2023, 13, 9102-9112.	11.7	2
171	Multiexciton quintet state populations in a rigid pyrene-bridged parallel tetracene dimer. Chemical Science, 2023, 14, 11554-11565.	7.8	2
172	Chain Conformation and Exciton Delocalization in a Pushâ€“Pull Conjugated Polymer. Chemistry of Materials, 2023, 35, 10258-10267.	7.1	2
173	ExpFlow: a graphical user interface for automated reproducible electrochemistry. Digital Discovery, 2024, 3, 163-172.	5.7	2
174	Understanding the Relationships Among Molecular Structure, Excited-State Properties, and Polarizabilities of Ï€-Conjugated Chromophores. Materials and Energy, 2016, , 393-419.	0.0	1
175	Following the crystal growth of anthradithiophenes through atomistic molecular dynamics simulations and graph characterization. Molecular Systems Design and Engineering, 2022, 7, 112-122.	3.3	1
176	Computational characterization of charge transport resiliency in molecular solids. Molecular Systems Design and Engineering, 2022, 7, 651-660.	3.3	1
177	Shear-aligned large-area organic semiconductor crystals through extended Ï€â€“Ï€ interaction. Journal of Materials Chemistry C, 2023, 11, 8992-9001.	5.6	1
178	Factors Impacting Dihedral Angle Rotation and Classification in Ï€-Conjugated Systems. Macromolecules, 2023, 56, 5259-5267.	5.1	1
179	Thank You, Elsa! A Virtual Special Issue in Honor of Professor Elsa Reichmanis. Chemistry of Materials, 2023, 35, 9819-9820.	7.1	1
180	Beyond n-dopants for organic semiconductors: use of bibenzo[d]imidazoles in UV-promoted dehalogenation reactions of organic halides. Beilstein Journal of Organic Chemistry, 0, 19, 1912-1922.	2.4	1

#	Article	IF	Citations
181	Barrier height modulation and dipole moments in metal-molecule-silicon diodes. , 2007, , .		0
182	Group 14 effects in alkynyl acene small molecule semiconductors. , 2021, , .		0
183	Combined Computational and Experimental Approach to Determine and Understand the Solubility of Phenothiazines as Redoxmers. ECS Meeting Abstracts, 2021, MA2021-02, 1679-1679.	0.0	0
184	Hydrogen-Bonding Trends in a Bithiophene with 3- and/or 4-Pyridyl Substituents. ACS Omega, 2023, 8, 24485-24494.	3.6	0
185	Atomistic Perspective of the Crystallization of Naphthodithiophene in Two Hydrocarbon Solvents. Chemistry of Materials, 0, , .	7.1	0
186	Promises and Perils of Big Data: Philosophical Constraints on Chemical Ontologies. Journal of the American Chemical Society, 2024, 146, 11579-11591.	14.6	0
187	Rapid Estimation of the Intermolecular Electronic Couplings and Charge-Carrier Mobilities of Crystalline Molecular Organic Semiconductors through a Machine Learning Pipeline. Journal of Physical Chemistry Letters, 0, , 7206-7213.	4.9	0
188	A 3D Printed Pumpless Nonaqueous Organic Redox Flow Cell. ECS Meeting Abstracts, 2024, MA2024-01, 768-768.	0.0	0
189	Temperature-dependent Stress-Strain Behavior of Amorphous and Crystalline P3HT. Journal of Materials Chemistry C, 0, , .	5.6	0