Alessandro Troisi

List of Publications by Year
in descending order

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182 papers	11,422 citations	22132 59 h-index	32815 100 g-index
190 all docs	190 docs citations	190 times ranked	9218 citing authors

#	Article	IF	Citations
1	Charge-Transport Regime of Crystalline Organic Semiconductors: Diffusion Limited by Thermal Off-Diagonal Electronic Disorder. Physical Review Letters, 2006, 96, 086601.	2.9	523
2	Charge transport in high mobility molecular semiconductors: classical models and new theories. Chemical Society Reviews, 2011, 40, 2347.	18.7	395
3	Dynamics of the Intermolecular Transfer Integral in Crystalline Organic Semiconductors. Journal of Physical Chemistry A, 2006, 110, 4065-4070.	1.1	345
4	Evaluation of the External Reorganization Energy of Polyacenes. Journal of Physical Chemistry Letters, 2010, 1, 941-946.	2.1	286
5	Nuclear Coupling and Polarization in Molecular Transport Junctions: Beyond Tunneling to Function. Science, 2008, 319, 1056-1060.	6.0	273
6	What Makes Fullerene Acceptors Special as Electron Acceptors in Organic Solar Cells and How to Replace Them. Advanced Materials, 2013, 25, 1038-1041.	11.1	273
7	Absolute Rate of Charge Separation and Recombination in a Molecular Model of the P3HT/PCBM Interface. Journal of Physical Chemistry C, 2011, 115, 2406-2415.	1.5	241
8	Prediction of the Absolute Charge Mobility of Molecular Semiconductors: the Case of Rubrene. Advanced Materials, 2007, 19, 2000-2004.	11.1	223
9	Hole Migration in DNA:Â a Theoretical Analysis of the Role of Structural Fluctuations. Journal of Physical Chemistry B, 2002, 106, 2093-2101.	1.2	215
10	The hole transfer in DNA: calculation of electron coupling between close bases. Chemical Physics Letters, 2001, 344, 509-518.	1.2	198
11	Theoretical studies of dye-sensitised solar cells: from electronic structure to elementary processes. Energy and Environmental Science, 2011, 4, 4473.	15.6	187
12	A map of high-mobility molecular semiconductors. Nature Materials, 2017, 16, 998-1002.	13.3	182
13	Theoretical Study of the Organic Photovoltaic Electron Acceptor PCBM: Morphology, Electronic Structure, and Charge Localization. Journal of Physical Chemistry C, 2010, 114, 20479-20488.	1.5	181
14	Why Holes and Electrons Separate So Well in Polymer/Fullerene Photovoltaic Cells. Journal of Physical Chemistry Letters, 2011, 2, 2737-2741.	2.1	175
15	Band Structure of the Four Pentacene Polymorphs and Effect on the Hole Mobility at Low Temperature. Journal of Physical Chemistry B, 2005, 109, 1849-1856.	1.2	164
16	Parallel (Face-to-Face) Versus Perpendicular (Edge-to-Face) Alignment of Electron Donors and Acceptors in Fullerene Porphyrin Dyads:Â The Importance of Orientation in Electron Transfer. Journal of the American Chemical Society, 2001, 123, 9166-9167.	6.6	157
17	Charge Transport in Organic Crystals: Role of Disorder and Topological Connectivity. Journal of the American Chemical Society, 2010, 132, 11702-11708.	6.6	157
18	Toward Predicting Efficiency of Organic Solar Cells via Machine Learning and Improved Descriptors. Advanced Energy Materials, 2018, 8, 1801032.	10.2	154

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19	Long-range exciton dissociation in organic solar cells. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 13498-13502.	3.3	153
20	What Is the Best Anchoring Group for a Dye in a Dye-Sensitized Solar Cell?. Journal of Physical Chemistry Letters, 2012, 3, 1531-1535.	2.1	151
21	Reducing dynamic disorder in small-molecule organic semiconductors by suppressing large-amplitude thermal motions. Nature Communications, 2016, 7, 10736.	5.8	147
22	Modelling charge transport in organic semiconductors: from quantum dynamics to soft matter. Physical Chemistry Chemical Physics, 2008, 10, 5941.	1.3	134
23	Electronic Structure of TiO₂ Surfaces and Effect of Molecular Adsorbates Using Different DFT Implementations. Journal of Physical Chemistry C, 2010, 114, 22659-22670.	1.5	134
24	A rate constant expression for charge transfer through fluctuating bridges. Journal of Chemical Physics, 2003, 119, 5782-5788.	1.2	133
25	Conformational Molecular Rectifiers. Nano Letters, 2004, 4, 591-595.	4.5	131
26	Combining electronic and structural features in machine learning models to predict organic solar cells properties. Materials Horizons, 2019, 6, 343-349.	6.4	124
27	Vibronic effects in off-resonant molecular wire conduction. Journal of Chemical Physics, 2003, 118, 6072-6082.	1.2	122
28	Electronic Interactions and Thermal Disorder in Molecular Crystals Containing Cofacial Pentacene Units. Chemistry of Materials, 2005, 17, 5024-5031.	3.2	120
29	Molecular Signatures in the Transport Properties of Molecular Wire Junctions: What Makes a Junction â€œMolecularâ€?. Small, 2006, 2, 172-181.	5.2	120
30	High-Throughput Computational Screening of Chromophores for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2011, 115, 11781-11792.	1.5	120
31	Molecular Transport Junctions:â€‰ Propensity Rules for Inelastic Electron Tunneling Spectra. Nano Letters, 2006, 6, 1784-1788.	4.5	111
32	Charge Transport in Semiconductors with Multiscale Conformational Dynamics. Physical Review Letters, 2009, 102, 116602.	2.9	111
33	Dynamics of the Excitonic Coupling in Organic Crystals. Physical Review Letters, 2015, 114, 026402.	2.9	111
34	Modulating Charge-Transfer Interactions in Topologically Different Porphyrinâ€“C60 Dyads. Chemistry - A European Journal, 2003, 9, 4968-4979.	1.7	110
35	Effects of hydration on molecular junction transport. Nature Materials, 2006, 5, 901-908.	13.3	110
36	Hall-Effect Measurements Probing the Degree of Charge-Carrier Delocalization in Solution-Processed Crystalline Molecular Semiconductors. Physical Review Letters, 2011, 107, 066601.	2.9	101

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37	Computational Study of the Structure and Charge-Transfer Parameters in Low-Molecular-Mass P3HT. Journal of Physical Chemistry B, 2009, 113, 9393-9401.	1.2	100
38	Molecular Rectification through Electric Field Induced Conformational Changes. Journal of the American Chemical Society, 2002, 124, 14528-14529.	6.6	99
39	Structural variability and dynamics of the P3HT/PCBM interface and its effects on the electronic structure and the charge-transfer rates in solar cells. Physical Chemistry Chemical Physics, 2011, 13, 21461.	1.3	97
40	Tracing electronic pathways in molecules by using inelastic tunneling spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14255-14259.	3.3	95
41	Trends in the electronic and geometric structure of non-fullerene based acceptors for organic solar cells. Energy and Environmental Science, 2017, 10, 395-401.	15.6	94
42	Ethylene Glycol-Based Side Chain Length Engineering in Polythiophenes and its Impact on Organic Electrochemical Transistor Performance. Chemistry of Materials, 2020, 32, 6618-6628.	3.2	92
43	Measurement of molecular motion in organic semiconductors by thermal diffuse electron scattering. Nature Materials, 2013, 12, 1045-1049.	13.3	91
44	Effect of the Anchoring Group on Electron Injection: Theoretical Study of Phosphonated Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2012, 116, 2622-2629.	1.5	90
45	From The Cover: An agent-based approach for modeling molecular self-organization. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 255-260.	3.3	88
46	Modeling the inelastic electron tunneling spectra of molecular wire junctions. Physical Review B, 2005, 72, .	1.1	86
47	Relation between Microstructure and Charge Transport in Polymers of Different Regioregularity. Journal of Physical Chemistry C, 2011, 115, 19386-19393.	1.5	85
48	Evaluating Charge Recombination Rate in Dye-Sensitized Solar Cells from Electronic Structure Calculations. Journal of Physical Chemistry C, 2012, 116, 7638-7649.	1.5	85
49	Dynamic disorder in molecular semiconductors: Charge transport in two dimensions. Journal of Chemical Physics, 2011, 134, 034702.	1.2	82
50	Organic Semiconductors: Impact of Disorder at Different Timescales. ChemPhysChem, 2010, 11, 2067-2074.	1.0	77
51	Reducing Molecular Shuttling to a Single Dimension. Angewandte Chemie - International Edition, 2000, 39, 350-353.	7.2	74
52	Singlet fission molecules among known compounds: finding a few needles in a haystack. Energy and Environmental Science, 2019, 12, 2412-2416.	15.6	74
53	Relation between Structure and Electronic Properties of Amorphous MEH-PPV Polymers. Journal of the American Chemical Society, 2013, 135, 11247-11256.	6.6	65
54	Regimes of Exciton Transport in Molecular Crystals in the Presence of Dynamic Disorder. Advanced Functional Materials, 2016, 26, 2316-2325.	7.8	65

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55	Propensity rules for inelastic electron tunneling spectroscopy of single-molecule transport junctions. Journal of Chemical Physics, 2006, 125, 214709.	1.2	64
56	A Realistic Description of the Charge Carrier Wave Function in Microcrystalline Polymer Semiconductors. Journal of the American Chemical Society, 2009, 131, 11179-11186.	6.6	64
57	Dynamic Nature of the Intramolecular Electronic Coupling Mediated by a Solvent Molecule:â€‰ A Computational Study. Journal of the American Chemical Society, 2004, 126, 2215-2224.	6.6	62
58	A method to rapidly predict the charge injection rate in dye sensitized solar cells. Physical Chemistry Chemical Physics, 2010, 12, 4625.	1.3	62
59	Effective Polarization in Pairwise Potentials at the Grapheneâ€“Electrolyte Interface. Journal of Physical Chemistry Letters, 2017, 8, 703-708.	2.1	62
60	Morphology and Charge Transport in P3HT: A Theoristâ€™s Perspective. Advances in Polymer Science, 2014, , 139-180.	0.4	61
61	Understanding the Microscopic Origin of the Very High Charge Mobility in PBTTT: Tolerance of Thermal Disorder. Advanced Functional Materials, 2014, 24, 925-933.	7.8	59
62	Strong optical response and light emission from a monolayer molecular crystal. Nature Communications, 2019, 10, 5589.	5.8	59
63	Effect of Increasing the Descriptor Set on Machine Learning Prediction of Small Molecule-Based Organic Solar Cells. Chemistry of Materials, 2020, 32, 7777-7787.	3.2	58
64	How TiO2 crystallographic surfaces influence charge injection rates from a chemisorbed dye sensitiser. Physical Chemistry Chemical Physics, 2012, 14, 13392.	1.3	57
65	Direct Optical Generation of Longâ€Range Chargeâ€Transfer States in Organic Photovoltaics. Advanced Materials, 2014, 26, 6163-6167.	11.1	57
66	Theory of charge hopping along a disordered polymer chain. Physical Chemistry Chemical Physics, 2014, 16, 9997.	1.3	55
67	Modeling the Self-Assembly of Benzenedicarboxylic Acids Using Monte Carlo and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2010, 114, 4376-4388.	1.5	54
68	How quasi-free holes and electrons are generated in organic photovoltaic interfaces. Faraday Discussions, 2013, 163, 377.	1.6	54
69	Concurrent Optimization of Organic Donorâ€“Acceptor Pairs through Machine Learning. Advanced Energy Materials, 2019, 9, 1902463.	10.2	54
70	Direct probe of the nuclear modes limiting charge mobility in molecular semiconductors. Materials Horizons, 2019, 6, 182-191.	6.4	53
71	The speed limit for sequential charge hopping in molecular materials. Organic Electronics, 2011, 12, 1988-1991.	1.4	52
72	Charge Diffusion in Semiconducting Polymers: Analytical Relation between Polymer Rigidity and Time Scales for Intrachain and Interchain Hopping. Journal of Physical Chemistry Letters, 2014, 5, 2637-2641.	2.1	47

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73	On the Structure and Stability of Self-Assembled Zwitterionic Peptide Amphiphiles:â€‰ A Theoretical Study. Nano Letters, 2004, 4, 427-431.	4.5	46
74	On the mechanism of charge transport in pentacene. Journal of Chemical Physics, 2008, 129, 044704.	1.2	46
75	All-Atom Numerical Studies of Self-Assembly of Zwitterionic Peptide Amphiphiles. Journal of Physical Chemistry B, 2004, 108, 15278-15284.	1.2	45
76	On the Largest Possible Mobility of Molecular Semiconductors and How to Achieve It. Advanced Functional Materials, 2020, 30, 2001906.	7.8	45
77	Charge Transport in Self-Assembled Semiconducting Organic Layers: Role of Dynamic and Static Disorder. Journal of Physical Chemistry C, 2010, 114, 10592-10597.	1.5	44
78	Packing Patterns of Silica Nanoparticles on Surfaces of Armored Polystyrene Latex Particles. Langmuir, 2009, 25, 12399-12403.	1.6	43
79	How Many Parameters Actually Affect the Mobility of Conjugated Polymers?. Physical Review Letters, 2017, 118, 086601.	2.9	43
80	Practical Computation of the Charge Mobility in Molecular Semiconductors Using Transient Localization Theory. Journal of Physical Chemistry C, 2019, 123, 6989-6997.	1.5	40
81	Transition from dynamic to static disorder in one-dimensional organic semiconductors. Journal of Chemical Physics, 2009, 131, 014703.	1.2	39
82	Nonlocal Electronâ€“Phonon Coupling in Prototypical Molecular Semiconductors from First Principles. Journal of Chemical Theory and Computation, 2018, 14, 3752-3762.	2.3	38
83	Rapid Evaluation of Dynamic Electronic Disorder in Molecular Semiconductors. Journal of Physical Chemistry C, 2018, 122, 18336-18345.	1.5	37
84	Using Orbital Symmetry to Minimize Charge Recombination in Dyeâ€Sensitized Solar Cells. Angewandte Chemie - International Edition, 2013, 52, 973-975.	7.2	36
85	Nanoscale Electrical Investigation of Layerâ€byâ€Layer Grown Molecular Wires. Advanced Materials, 2014, 26, 1688-1693.	11.1	36
86	Single Molecule Conductance of Linear Dithioalkanes in the Liquid Phase:â€‰ Apparently Activated Transport Due to Conformational Flexibility. Journal of Physical Chemistry C, 2007, 111, 14567-14573.	1.5	35
87	Calculation of rates of exciton dissociation into hot charge-transfer states in model organic photovoltaic interfaces. Physical Review B, 2013, 88, .	1.1	35
88	Exploiting Quantum Interference in Dye Sensitized Solar Cells. ACS Nano, 2014, 8, 409-418.	7.3	35
89	Sequencing conjugated polymers by eye. Science Advances, 2018, 4, eaas9543.	4.7	35
90	Modulating the Exciton Dissociation Rate by up to More than Two Orders of Magnitude by Controlling the Alignment of LUMO + 1 in Organic Photovoltaics. Journal of Physical Chemistry C, 2014, 118, 27272-27280.	1.5	34

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91	Inelastic insights for molecular tunneling pathways: Bypassing the terminal groups. Physical Chemistry Chemical Physics, 2007, 9, 2421.	1.3	33
92	Modeling charge transport in high-mobility molecular semiconductors: Balancing electronic structure and quantum dynamics methods with the help of experiments. Journal of Chemical Physics, 2020, 152, 190902.	1.2	33
93	Charge transport perpendicular to the high mobility plane in organic crystals: Bandlike temperature dependence maintained despite hundredfold anisotropy. Physical Review B, 2016, 93, .	1.1	32
94	Negative Isotope Effect on Fieldâ€Effect Hole Transport in Fully Substituted ¹³Câ€Rubrene. Advanced Electronic Materials, 2017, 3, 1700018.	2.6	32
95	Very Large Ï€-Conjugation Despite Strong Nonplanarity: A Path for Designing New Semiconducting Polymers. Journal of Physical Chemistry Letters, 2016, 7, 4689-4694.	2.1	31
96	Excitonâ€“Phonon Interaction Model for Singlet Fission in Prototypical Molecular Crystals. Journal of Chemical Theory and Computation, 2019, 15, 3721-3729.	2.3	31
97	An ad hoc tight binding method to study the electronic structure of semiconducting polymers. Chemical Physics Letters, 2009, 480, 210-214.	1.2	30
98	Electronic Excited States in Amorphous MEH-PPV Polymers from Large-Scale First Principles Calculations. Journal of Chemical Theory and Computation, 2014, 10, 1272-1282.	2.3	30
99	A very general rate expression for charge hopping in semiconducting polymers. Journal of Chemical Physics, 2015, 142, 184105.	1.2	30
100	Quantitative Prediction of the Electroâ€Mechanical Response in Organic Crystals. Advanced Materials, 2021, 33, e2008049.	11.1	29
101	Adsorption and electron injection of the N3 metalâ€“organic dye on the TiO2 rutile (110) surface. Physical Chemistry Chemical Physics, 2012, 14, 16668.	1.3	28
102	Narrower Bands with Better Charge Transport: The Counterintuitive Behavior of Semiconducting Copolymers. Advanced Materials, 2014, 26, 7627-7631.	11.1	28
103	Inelastic Electron Tunneling Spectroscopy of Alkane Monolayers with Dissimilar Attachment Chemistry to Gold. Journal of the American Chemical Society, 2007, 129, 15303-15310.	6.6	27
104	Exciton Dynamics in Phthalocyanine Molecular Crystals. Journal of Physical Chemistry C, 2016, 120, 7987-7996.	1.5	27
105	Vibronic enhancement of excitation energy transport: Interplay between local and non-local exciton-phonon interactions. Journal of Chemical Physics, 2017, 146, 075101.	1.2	27
106	Novel thermally activated delayed fluorescence materials by high-throughput virtual screening: going beyond donorâ€“acceptor design. Journal of Materials Chemistry C, 2021, 9, 3324-3333.	2.7	27
107	The heptakisoctahedral group and its relevance to carbon allotropes with negative curvature. Journal of Mathematical Chemistry, 1999, 26, 101-123.	0.7	26
108	A Quantum-Mechanical Description of Macrocyclic Ring Rotation in Benzylic Amide [2]Catenanes. Chemistry - A European Journal, 2001, 7, 1450-1454.	1.7	26

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109	Self-assembly of sparsely distributed molecules: An efficient cluster algorithm. Chemical Physics Letters, 2008, 458, 210-213.	1.2	26
110	Efficient Electronic Tunneling Governs Transport in Conducting Polymer-Insulator Blends. Journal of the American Chemical Society, 2022, 144, 10368-10376.	6.6	26
111	Hexagonal Lattice Model of the Patterns Formed by Hydrogen-Bonded Molecules on the Surface. Journal of Physical Chemistry B, 2010, 114, 1849-1858.	1.2	25
112	Importance and Nature of Short-Range Excitonic Interactions in Light Harvesting Complexes and Organic Semiconductors. Journal of Chemical Theory and Computation, 2017, 13, 3754-3763.	2.3	25
113	Charge Dynamics in Organic Photovoltaic Materials: Interplay between Quantum Diffusion and Quantum Relaxation. Journal of Physical Chemistry C, 2015, 119, 14989-14998.	1.5	24
114	Chromophore-Dependent Intramolecular Excitonâ€“Vibrational Coupling in the FMO Complex: Quantification and Importance for Exciton Dynamics. Journal of Physical Chemistry B, 2017, 121, 10026-10035.	1.2	24
115	Excitonic couplings between molecular crystal pairs by a multistate approximation. Journal of Chemical Physics, 2015, 142, 164107.	1.2	23
116	Valencies of a small fullerene: structures and energetics of C24H2m. Chemical Physics Letters, 1999, 312, 77-84.	1.2	22
117	Charge dynamics through pi-stacked arrays of conjugated molecules: effect of dynamic disorder in different transport/transfer regimes. Molecular Simulation, 2006, 32, 707-716.	0.9	22
118	Synthesis and isomerization of N-Î±-aza-heteroaryl-Î²-lactams. Tetrahedron, 2006, 62, 12064-12070.	1.0	22
119	Molecular structure and phase behaviour of hairy-rod polymers. Physical Chemistry Chemical Physics, 2009, 11, 2105.	1.3	22
120	Explaining different experimental hole mobilities: influence of polymorphism on dynamic disorder in pentacene. Journal of Materials Chemistry C, 2019, 7, 9665-9670.	2.7	22
121	Relation between Local Structure, Electric Dipole, and Charge Carrier Dynamics in DHICA Melanin: A Model for Biocompatible Semiconductors. Journal of Physical Chemistry Letters, 2020, 11, 1045-1051.	2.1	22
122	Bright Frenkel Excitons in Molecular Crystals: A Survey. Chemistry of Materials, 2021, 33, 3368-3378.	3.2	22
123	Developing accurate molecular mechanics force fields for conjugated molecular systems. Physical Chemistry Chemical Physics, 2015, 17, 25123-25132.	1.3	21
124	Developing Consistent Molecular Dynamics Force Fields for Biological Chromophores via Force Matching. Journal of Physical Chemistry B, 2019, 123, 428-438.	1.2	21
125	Simulation of STM Images from Commercially Available Software. Journal of the American Chemical Society, 1999, 121, 5392-5395.	6.6	20
126	Construction of electronic diabatic states within a molecular orbital scheme. Journal of Chemical Physics, 2003, 118, 5356-5363.	1.2	20

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127	Persistence time of charge carriers in defect states of molecular semiconductors. Physical Chemistry Chemical Physics, 2011, 13, 10241.	1.3	20
128	Theoretical study of charge recombination at the TiO2-electrolyte interface in dye sensitised solar cells. Journal of Chemical Physics, 2012, 137, 22A508.	1.2	20
129	Systematic Study of the Effect of Auxiliary Acceptors in Dâ€“Aâ€²â^Ï€â€“A Sensitizers Used on Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2018, 122, 23890-23898.	1.5	20
130	A QM/MD Coupling Method to Model the Ion-Induced Polarization of Graphene. Journal of Chemical Theory and Computation, 2020, 16, 5253-5263.	2.3	20
131	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. Journal of Materials Chemistry C, 2021, 9, 13557-13583.	2.7	20
132	Predicting with confidence the efficiency of new dyes in dye sensitized solar cells. Physical Chemistry Chemical Physics, 2014, 16, 19106.	1.3	19
133	Computational Identification of Novel Families of Nonfullerene Acceptors by Modification of Known Compounds. Journal of Physical Chemistry Letters, 2021, 12, 5009-5015.	2.1	19
134	A computational study of the competing reaction mechanisms of the photo-catalytic reduction of CO₂ on anatase(101). Physical Chemistry Chemical Physics, 2016, 18, 25010-25021.	1.3	18
135	Theoretical evidence of multiple dye regeneration mechanisms in dye-sensitized solar cells. Chemical Physics Letters, 2013, 570, 159-162.	1.2	17
136	Elucidating the Relationship between Multiradical Character and Predicted Singlet Fission Activity. ChemPhotoChem, 2020, 4, 5223-5229.	1.5	17
137	Independent sets and the prediction of addition patterns for higher fullerenes. Journal of the Chemical Society Perkin Transactions II, 1999, , 2023-2027.	0.9	16
138	Quantum dynamic localization in the Holstein Hamiltonian at finite temperatures. Physical Review B, 2010, 82, .	1.1	16
139	Singlet fission in linear chains of molecules. Journal of Chemical Physics, 2014, 141, 204703.	1.2	16
140	Organic materials repurposing, a data set for theoretical predictions of new applications for existing compounds. Scientific Data, 2022, 9, 54.	2.4	16
141	Theory of the Charge Recombination Reaction at the Semiconductorâ€“Adsorbate Interface in the Presence of Defects. Journal of Physical Chemistry C, 2013, 117, 24196-24205.	1.5	15
142	Probing local electric field and conformational switching in single-molecule break junctions. Physical Review B, 2009, 79, .	1.1	14
143	Unexpected Like-Charge Self-Assembly of a Biguanide-Based Antimicrobial Polyelectrolyte. Journal of Physical Chemistry Letters, 2016, 7, 3730-3735.	2.1	14
144	Structure-Dynamics Relation in Physically-Plausible Multi-Chromophore Systems. Journal of Physical Chemistry Letters, 2017, 8, 2328-2333.	2.1	14

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145	Quantifying the â€œSubtle Interplayâ€•between Intermolecular and Moleculeâ€“Substrate Interactions in Molecular Assembly on Surfaces. Journal of Physical Chemistry C, 2018, 122, 17954-17962.	1.5	14
146	Strategies to reduce the dynamic disorder in molecular semiconductors. Materials Horizons, 2020, 7, 2922-2928.	6.4	14
147	Effect of the intermolecular thermal motions on the tail ofÂtheÂelectronic density of states in polyacene crystals. Applied Physics A: Materials Science and Processing, 2009, 95, 147-152.	1.1	13
148	Agent-Based Modeling for the 2D Molecular Self-Organization of Realistic Molecules. Journal of Physical Chemistry B, 2010, 114, 10151-10159.	1.2	13
149	Determining usefulness of machine learning in materials discovery using simulated research landscapes. Physical Chemistry Chemical Physics, 2021, 23, 14156-14163.	1.3	13
150	Performance Prediction and Experimental Optimization Assisted by Machine Learning for Organic Photovoltaics. Advanced Intelligent Systems, 2022, 4, .	3.3	13
151	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. Journal of Chemical Theory and Computation, 2020, 16, 3494-3503.	2.3	12
152	Self-assembly on multiple length scales: A Monte Carlo algorithm with data augmentation. Journal of Chemical Physics, 2005, 122, 024102.	1.2	11
153	Determination of kinetic parameters of enantiomerization of benzothiadiazines by DCXplorer. Chirality, 2010, 22, 789-797.	1.3	11
154	Structure and Photophysics of an Old, New Molecule:Â 1,3,6,8-Tetraazatricyclo[4.4.1.13,8]dodecane. Journal of the American Chemical Society, 2002, 124, 149-158.	6.6	10
155	Effect of Infrared Pulse Excitation on the Bound Charge-Transfer State of Photovoltaic Interfaces. Journal of Physical Chemistry Letters, 2017, 8, 4872-4877.	2.1	10
156	An Artificial Intelligence Approach for Modeling Molecular Self-assembly: Agent-based Simulations of Rigid Molecules. Journal of Physical Chemistry B, 2009, 113, 9877-9885.	1.2	9
157	Does the Donor-Ï€-Acceptor Character of Dyes Improve the Efficiency of Dye-Sensitized Solar Cells?. Journal of Physical Chemistry Letters, 2016, 7, 2989-2993.	2.1	9
158	Rapid Method for Calculating the Conformationally Averaged Electronic Structure of Conjugated Polymers. Journal of Physical Chemistry B, 2021, 125, 6338-6348.	1.2	9
159	Local structuring of diketopyrrolopyrrole (DPP)-based oligomers from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 19693-19707.	1.3	9
160	Theories of the Charge Transport Mechanism in Ordered Organic Semiconductors. Advances in Polymer Science, 2009, , 213-258.	0.4	8
161	Charge generation mechanism in organic solar cells. Physical Chemistry Chemical Physics, 2014, 16, 20277-20278.	1.3	8
162	Excitonic Coupling Modulated by Mechanical Stimuli. Journal of Physical Chemistry Letters, 2017, 8, 4326-4332.	2.1	8

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163	Limitations of machine learning models when predicting compounds with completely new chemistries: possible improvements applied to the discovery of new non-fullerene acceptors. , 2022, 1, 266-276.		8
164	How fine-tuned for energy transfer is the environmental noise produced by proteins around biological chromophores?. Physical Chemistry Chemical Physics, 2018, 20, 17279-17288.	1.3	7
165	Quantitative Hole Mobility Simulation and Validation in Substituted Acenes. Journal of Physical Chemistry Letters, 2022, 13, 5530-5537.	2.1	7
166	Inelastic electron tunnelling in saturated molecules with different functional groups: correlations and symmetry considerations from a computational study. Journal of Physics Condensed Matter, 2008, 20, 374111.	0.7	6
167	Chiral Semiconductor Phases: The Optically Pure D₃[M^{III}(S,S-EDDS)]₂ (D = TTF, TSF) Family. Inorganic Chemistry, 2011, 50, 4039-4046.	1.9	6
168	Charge Injection Rates in Hybrid Nanosiliconâ€“Polythiophene Bulk Heterojunction Solar Cells. Journal of Physical Chemistry C, 2013, 117, 110-115.	1.5	6
169	Quantum dynamics of a vibronically coupled linear chain using a surrogate Hamiltonian approach. Journal of Chemical Physics, 2016, 144, 214106.	1.2	6
170	On the arrangement of chromophores in light harvesting complexes: chance versus design. Faraday Discussions, 2019, 221, 133-149.	1.6	6
171	Exploring Charge Dissociation in a Statistical Sample of Active-Layer Models of an Organic Solar Cell. Journal of Physical Chemistry C, 2020, 124, 18840-18846.	1.5	6
172	Continuum and atomistic description of excess electrons in TiO₂. Journal of Physics Condensed Matter, 2016, 28, 074004.	0.7	5
173	Quantum coherence in complex environments: general discussion. Faraday Discussions, 2019, 221, 168-201.	1.6	5
174	Evaluating the Electronic Structure of Coexisting Excitonic and Multiexcitonic States in Periodic Systems: Significance for Singlet Fission. Journal of Chemical Theory and Computation, 2022, 18, 394-405.	2.3	4
175	Polymers as one-dimensional metals. Nature Materials, 2009, 8, 538-539.	13.3	3
176	An expression for the bridge-mediated electron transfer rate in dye-sensitized solar cells. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130011.	1.6	3
177	Development of hybrid coarse-grained atomistic models for rapid assessment of local structuring of polymeric semiconductors. Molecular Systems Design and Engineering, 2022, 7, 294-305.	1.7	3
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