

# Denis Andrienko

## List of Publications by Year in descending order

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156  
papers

9,123  
citations

28190

55  
h-index

45213

90  
g-index

160  
all docs

160  
docs citations

160  
times ranked

8859  
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards high charge-carrier mobilities by rational design of the shape and periphery of discotics. <i>Nature Materials</i> , 2009, 8, 421-426.	13.3	555
2	Versatile Object-Oriented Toolkit for Coarse-Graining Applications. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3211-3223.	2.3	390
3	Microscopic Simulations of Charge Transport in Disordered Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3335-3345.	2.3	345
4	Barrierless Free Charge Generation in the High-Performance PM6:Y6 Bulk Heterojunction Non-Fullerene Solar Cell. <i>Advanced Materials</i> , 2020, 32, e1906763.	11.1	258
5	Intrinsic efficiency limits in low-bandgap non-fullerene acceptor organic solar cells. <i>Nature Materials</i> , 2021, 20, 378-384.	13.3	257
6	Band structure engineering in organic semiconductors. <i>Science</i> , 2016, 352, 1446-1449.	6.0	239
7	Introduction to liquid crystals. <i>Journal of Molecular Liquids</i> , 2018, 267, 520-541.	2.3	233
8	Density-functional based determination of intermolecular charge transfer properties for large-scale morphologies. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11103.	1.3	222
9	Long-range exciton diffusion in molecular non-fullerene acceptors. <i>Nature Communications</i> , 2020, 11, 5220.	5.8	204
10	Impact of mesoscale order on open-circuit voltage in organic solar cells. <i>Nature Materials</i> , 2015, 14, 434-439.	13.3	184
11	Charge Mobility of Discotic Mesophases: A Multiscale Quantum and Classical Study. <i>Physical Review Letters</i> , 2007, 98, 227402.	2.9	172
12	Universal strategy for Ohmic hole injection into organic semiconductors with high ionization energies. <i>Nature Materials</i> , 2018, 17, 329-334.	13.3	168
13	Charge Transport in Organic Crystals: Role of Disorder and Topological Connectivity. <i>Journal of the American Chemical Society</i> , 2010, 132, 11702-11708.	6.6	157
14	Efficient and stable perovskite-silicon tandem solar cells through contact displacement by MgF <sub>2</sub> . <i>Science</i> , 2022, 377, 302-306.	6.0	141
15	Modeling of Organic Light Emitting Diodes: From Molecular to Device Properties. <i>Advanced Functional Materials</i> , 2015, 25, 1955-1971.	7.8	135
16	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 433002.	0.7	131
17	A window to trap-free charge transport in organic semiconducting thin films. <i>Nature Materials</i> , 2019, 18, 1182-1186.	13.3	131
18	Effect of Polymorphism, Regioregularity and Paracrystallinity on Charge Transport in Poly(3-hexylthiophene) [P3HT] Nanofibers. <i>Macromolecules</i> , 2013, 46, 8941-8956.	2.2	130

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19	Elasticity of polyelectrolyte multilayer microcapsules. <i>Journal of Chemical Physics</i> , 2004, 120, 3822-3826.	1.2	117
20	Charge Transport in Semiconductors with Multiscale Conformational Dynamics. <i>Physical Review Letters</i> , 2009, 102, 116602.	2.9	111
21	Electron-Deficient N-Heteroaromatic Linkers for the Elaboration of Large, Soluble Polycyclic Aromatic Hydrocarbons and Their Use in the Synthesis of Some Very Large Transition Metal Complexes. <i>Journal of the American Chemical Society</i> , 2007, 129, 11743-11749.	6.6	107
22	Unicolored phosphor-sensitized fluorescence for efficient and stable blue OLEDs. <i>Nature Communications</i> , 2018, 9, 4990.	5.8	107
23	Impact of molecular quadrupole moments on the energy levels at organic heterojunctions. <i>Nature Communications</i> , 2019, 10, 2466.	5.8	101
24	Bilayer order in a polycarbazole-conjugated polymer. <i>Nature Communications</i> , 2012, 3, 795.	5.8	100
25	Frenkel and Charge-Transfer Excitations in Donor-acceptor Complexes from Many-Body Green's Functions Theory. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2790-2795.	2.3	98
26	Design Rules for Organic Donor-Acceptor Heterojunctions: Pathway for Charge Splitting and Detrapping. <i>Journal of the American Chemical Society</i> , 2015, 137, 6320-6326.	6.6	97
27	Young's Modulus of Polyelectrolyte Multilayers from Microcapsule Swelling. <i>Macromolecules</i> , 2004, 37, 1113-1117.	2.2	94
28	Characterization of Charge-Carrier Transport in Semicrystalline Polymers: Electronic Couplings, Site Energies, and Charge-Carrier Dynamics in Poly(bithiophene-alt-thienothiophene) [PBTTT]. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1633-1640.	1.5	92
29	Transferable Atomic Multipole Machine Learning Models for Small Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3225-3233.	2.3	91
30	Computer simulation of topological defects around a colloidal particle or droplet dispersed in a nematic host. <i>Physical Review E</i> , 2001, 63, 041701.	0.8	86
31	Understanding Structure-Mobility Relations for Perylene Tetracarboxydiimide Derivatives. <i>Journal of the American Chemical Society</i> , 2009, 131, 11426-11432.	6.6	86
32	Excited States of Dicyanovinyl-Substituted Oligothiophenes from Many-Body Green's Functions Theory. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 997-1002.	2.3	86
33	Design Rules for Charge-Transport Efficient Host Materials for Phosphorescent Organic Light-Emitting Diodes. <i>Journal of the American Chemical Society</i> , 2012, 134, 13818-13822.	6.6	85
34	Light-Induced Surface Sliding of the Nematic Director in Liquid Crystals. <i>Physical Review Letters</i> , 1999, 82, 1855-1858.	2.9	83
35	Defect structures and torque on an elongated colloidal particle immersed in a liquid crystal host. <i>Physical Review E</i> , 2002, 65, 041702.	0.8	81
36	Graphitic Nanoribbons with Dibenzo[ <i>a,h</i> ]pyrene Repeat Units: Synthesis and Self-Assembly. <i>Macromolecules</i> , 2009, 42, 6878-6884.	2.2	81

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37	Charge Carrier Transport and Photogeneration in P3HT:PCBM Photovoltaic Blends. <i>Macromolecular Rapid Communications</i> , 2015, 36, 1001-1025.	2.0	80
38	Comparative Study of Microscopic Charge Dynamics in Crystalline Acceptor-Substituted Oligothiophenes. <i>Journal of the American Chemical Society</i> , 2012, 134, 6052-6056.	6.6	78
39	A multiscale description of charge transport in conjugated oligomers. <i>Journal of Chemical Physics</i> , 2010, 132, 134103.	1.2	76
40	Electrochemical TERS Elucidates Potential-Induced Molecular Reorientation of Adenine/Au(111). <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9796-9801.	7.2	76
41	Atomistic simulation of structure and dynamics of columnar phases of hexabenzocoronene derivatives. <i>Journal of Chemical Physics</i> , 2006, 125, 124902.	1.2	70
42	Electron Trapping in Conjugated Polymers. <i>Chemistry of Materials</i> , 2019, 31, 6380-6386.	3.2	70
43	Sub-ns triplet state formation by non-geminate recombination in PSBTBT:PC <sub>70</sub> BM and PCPDTBT:PC <sub>60</sub> BM organic solar cells. <i>Energy and Environmental Science</i> , 2015, 8, 1511-1522.	15.6	67
44	Boundary slip as a result of a prewetting transition. <i>Journal of Chemical Physics</i> , 2003, 119, 13106-13112.	1.2	65
45	Drag on particles in a nematic suspension by a moving nematic-isotropic interface. <i>Physical Review E</i> , 2002, 66, 012702.	0.8	64
46	Columnar mesophases of hexabenzocoronene derivatives. II. Charge carrier mobility. <i>Journal of Chemical Physics</i> , 2008, 129, 094506.	1.2	64
47	Entropic Torque. <i>Physical Review Letters</i> , 2002, 89, 088301.	2.9	62
48	Morphology and Charge Transport in P3HT: A Theorist's Perspective. <i>Advances in Polymer Science</i> , 2014, , 139-180.	0.4	61
49	Relationship between supramolecular assembly and charge-carrier mobility in perylene diimide derivatives: The impact of side chains. <i>Journal of Materials Chemistry</i> , 2011, 21, 9538.	6.7	60
50	Extracting nondispersive charge carrier mobilities of organic semiconductors from simulations of small systems. <i>Physical Review B</i> , 2010, 82, .	1.1	58
51	Capillary bridging and long-range attractive forces in a mean-field approach. <i>Journal of Chemical Physics</i> , 2004, 121, 4414-4423.	1.2	57
52	Challenges for in silico design of organic semiconductors. <i>Journal of Materials Chemistry</i> , 2012, 22, 10971.	6.7	57
53	Nematic Ordering, Conjugation, and Density of States of Soluble Polymeric Semiconductors. <i>Macromolecules</i> , 2013, 46, 5762-5774.	2.2	56
54	Can Lattice Models Predict the Density of States of Amorphous Organic Semiconductors?. <i>Physical Review Letters</i> , 2012, 109, 136401.	2.9	55

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55	Electronic Excitations in Push-Pull Oligomers and Their Complexes with Fullerene from Many-Body Green's Functions Theory with Polarizable Embedding. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3104-3110.	2.3	55
56	Stochastic modeling of molecular charge transport networks. <i>Physical Review B</i> , 2012, 86, .	1.1	48
57	Coarse-grained interaction potentials for polyaromatic hydrocarbons. <i>Journal of Chemical Physics</i> , 2006, 124, 054307.	1.2	47
58	The PCPDTBT Family: Correlations between Chemical Structure, Polymorphism, and Device Performance. <i>Macromolecules</i> , 2017, 50, 1402-1414.	2.2	47
59	Long-Range Embedding of Molecular Ions and Excitations in a Polarizable Molecular Environment. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4516-4523.	2.3	46
60	Impact of Nonfullerene Acceptor Core Structure on the Photophysics and Efficiency of Polymer Solar Cells. <i>ACS Energy Letters</i> , 2018, 3, 802-811.	8.8	46
61	Structure-charge mobility relation for hexabenzocoronene derivatives. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 830-834.	0.7	44
62	Charge Transport in Self-Assembled Semiconducting Organic Layers: Role of Dynamic and Static Disorder. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10592-10597.	1.5	44
63	Kernel-Based Machine Learning for Efficient Simulations of Molecular Liquids. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3194-3204.	2.3	44
64	Amorphous films of tris(8-hydroxyquinolino)aluminium: Force-field, morphology, and charge transport. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2009, 206, 2737-2742.	0.8	43
65	Mechanistic study on the hydrolytic degradation of polyphosphates. <i>European Polymer Journal</i> , 2018, 108, 286-294.	2.6	43
66	Forces between elongated particles in a nematic colloid. <i>Physical Review E</i> , 2003, 68, 051702.	0.8	42
67	Structure-based coarse-graining in liquid slabs. <i>Journal of Chemical Physics</i> , 2012, 137, 064102.	1.2	41
68	Twist-bend instability for toroidal DNA condensates. <i>Europhysics Letters</i> , 2004, 67, 418-424.	0.7	40
69	Columnar mesophases of hexabenzocoronene derivatives. I. Phase transitions. <i>Journal of Chemical Physics</i> , 2008, 129, 094505.	1.2	40
70	Charge transport in amorphous and smectic mesophases of dicyanovinyl-substituted oligothiophenes. <i>Journal of Materials Chemistry</i> , 2012, 22, 22258.	6.7	40
71	Polaron spin dynamics in high-mobility polymeric semiconductors. <i>Nature Physics</i> , 2019, 15, 814-822.	6.5	40
72	Chemical Design Rules for Non-Fullerene Acceptors in Organic Solar Cells. <i>Advanced Energy Materials</i> , 2021, 11, 2102363.	10.2	38

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73	Toward Quantitative Structure–Property Relationships for Charge Transfer Rates of Polycyclic Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2549-2555.	2.3	37
74	Generic Model for Lamellar Self-Assembly in Conjugated Polymers: Linking Mesoscopic Morphology and Charge Transport in P3HT. <i>Macromolecules</i> , 2019, 52, 968-981.	2.2	36
75	Effect of Mesoscale Ordering on the Density of States of Polymeric Semiconductors. <i>Macromolecular Rapid Communications</i> , 2015, 36, 1047-1053.	2.0	35
76	Supramolecular structure of perylene tetracarboxydiimides. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 820-824.	0.7	34
77	Research Update: Computational materials discovery in soft matter. <i>APL Materials</i> , 2016, 4, .	2.2	34
78	Modeling of Spatially Correlated Energetic Disorder in Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 36-40.	2.3	34
79	Understanding three-body contributions to coarse-grained force fields. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22387-22394.	1.3	34
80	Interaction of colloids with a nematic-isotropic interface. <i>Physical Review E</i> , 2004, 69, 021706.	0.8	33
81	Macroscopic Structural Compositions of $\pi$ -Conjugated Polymers: Combined Insights from Solid-State NMR and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4155-4160.	2.1	31
82	Charge Photogeneration in Non-Fullerene Organic Solar Cells: Influence of Excess Energy and Electrostatic Interactions. <i>Advanced Functional Materials</i> , 2021, 31, 2007479.	7.8	31
83	Measurement of Azimuthal Anchoring Energy of Nematic Liquid Crystal on Photoaligning Polymer Surface. <i>Molecular Crystals and Liquid Crystals</i> , 1998, 321, 271-281.	0.3	30
84	Tuning electronic eigenvalues of benzene via doping. <i>Journal of Chemical Physics</i> , 2007, 127, 064305.	1.2	30
85	Control of the Anchoring Energy of Rubbed Polyimide Layers by Irradiation with Depolarized UV-Light. <i>Japanese Journal of Applied Physics</i> , 2000, 39, 1217-1220.	0.8	29
86	Rigorous Characterization and Predictive Modeling of Hole Transport in Amorphous Organic Semiconductors. <i>Advanced Electronic Materials</i> , 2018, 4, 1800366.	2.6	29
87	Alcohol- and Water-Tolerant Living Anionic Polymerization of Aziridines. <i>Macromolecules</i> , 2018, 51, 5713-5719.	2.2	29
88	Tilted photoalignment of a nematic liquid crystal induced by a magnetic field. <i>Journal of Applied Physics</i> , 1998, 83, 50-55.	1.1	28
89	Molecular simulation and theory of a liquid crystalline disclination core. <i>Physical Review E</i> , 2000, 61, 504-510.	0.8	28
90	Reduced Intrinsic Non-Radiative Losses Allow Room-Temperature Triplet Emission from Purely Organic Emitters. <i>Advanced Materials</i> , 2021, 33, e2101844.	11.1	28

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91	Parametrization of Extended Gaussian Disorder Models from Microscopic Charge Transport Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2508-2513.	2.3	27
92	Influence of orientation mismatch on charge transport across grain boundaries in tri-isopropylsilylethynyl (TIPS) pentacene thin films. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10854-10862.	1.3	27
93	Polymerizing Phostones: A Fast Way to In-Chain Poly(phosphonate)s with Adjustable Hydrophilicity. <i>Macromolecules</i> , 2018, 51, 1272-1279.	2.2	27
94	Molecular library of OLED host materialsâ€”Evaluating the multiscale simulation workflow. <i>Chemical Physics Reviews</i> , 2021, 2, .	2.6	24
95	Impact of Acceptor Quadrupole Moment on Charge Generation and Recombination in Blends of IDTâ€”Based Nonâ€”Fullerene Acceptors with PCE10 as Donor Polymer. <i>Advanced Energy Materials</i> , 2021, 11, 2100839.	10.2	23
96	Solvated poly-(phenylene vinylene) derivatives: conformational structure and aggregation behavior. <i>Journal of Materials Chemistry</i> , 2010, 20, 10475.	6.7	22
97	Charge transport in highly ordered organic nanofibrils: lessons from modelling. <i>Journal of Materials Chemistry C</i> , 2017, 5, 350-361.	2.7	22
98	Perspectives of Unicolored Phosphorâ€”Sensitized Fluorescence. <i>Advanced Electronic Materials</i> , 2019, 5, 1900646.	2.6	21
99	Liquid crystal director fluctuations and surface anchoring by molecular simulation. <i>Physical Review E</i> , 2000, 62, 6688-6693.	0.8	20
100	Effective pair interactions between colloidal particles at a nematic-isotropic interface. <i>Europhysics Letters</i> , 2005, 70, 95-101.	0.7	20
101	Molecular ordering and charge transport in a dicyanovinyl-substituted quaterthiophene thin film. <i>RSC Advances</i> , 2013, 3, 12117.	1.7	20
102	Charge Carrier Generation, Recombination, and Extraction in Polymerâ€”Fullerene Bulk Heterojunction Organic Solar Cells. <i>Advances in Polymer Science</i> , 2017, , 267-291.	0.4	20
103	Adhesion of Polycarbonate Blends on a Nickel Surface. <i>Macromolecules</i> , 2005, 38, 5810-5816.	2.2	19
104	Parameter-free continuous driftâ€”diffusion models of amorphous organic semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22778-22783.	1.3	19
105	Electrically controlled director slippage over a photosensitive aligning surface; in-plane sliding mode. <i>Liquid Crystals</i> , 2000, 27, 365-370.	0.9	18
106	Two Channels of Charge Generation in Perylene Monoimide Solidâ€”State Dyeâ€”Sensitized Solar Cells. <i>Advanced Energy Materials</i> , 2014, 4, 1300640.	10.2	18
107	Finite-size scaling of charge carrier mobility in disordered organic semiconductors. <i>Physical Review B</i> , 2016, 94, .	1.1	18
108	Selfâ€”Organization and Charge Transport Properties of Selenium and Tellurium Analogues of Polythiophene. <i>Macromolecular Rapid Communications</i> , 2019, 40, e1800596.	2.0	18

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109	Theory and simulation of the nematic zenithal anchoring coefficient. <i>Physical Review E</i> , 2002, 65, 021704.	0.8	17
110	Dynamic surface decoupling in a sheared polymer melt. <i>Europhysics Letters</i> , 2005, 70, 264-270.	0.7	17
111	Colloidal particles at a nematic-isotropic interface: Effects of confinement. <i>European Physical Journal E</i> , 2006, 20, 237-242.	0.7	17
112	Comparison of systematic coarse-graining strategies for soluble conjugated polymers. <i>European Physical Journal: Special Topics</i> , 2016, 225, 1441-1461.	1.2	17
113	N-Doping improves charge transport and morphology in the organic non-fullerene acceptor O-IDTBR. <i>Journal of Materials Chemistry C</i> , 2021, 9, 4486-4495.	2.7	17
114	Charge transport parameters of HBC at different temperatures. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 835-838.	0.7	16
115	Charge transport in columnar mesophases of carbazole macrocycles. <i>Journal of Chemical Physics</i> , 2010, 133, 134901.	1.2	16
116	Water-Free Proton Conduction in Hexakis( <i>i</i> -Phosphonatophenyl)benzene Nanochannels. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12366-12372.	1.5	16
117	Coarse-grained modelling of polypyrrole morphologies. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 844-848.	0.7	15
118	Ultra-coarse-graining of homopolymers in inhomogeneous systems. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 254002.	0.7	15
119	Spatially resolved fluorescence of caesium lead halide perovskite supercrystals reveals quasi-atomic behavior of nanocrystals. <i>Nature Communications</i> , 2022, 13, 892.	5.8	15
120	Observing Charge Dynamics in Surface Reactions by Time-Resolved Stark Effects. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9171-9177.	1.5	14
121	Computer aided design of stable and efficient OLEDs. <i>Journal of Applied Physics</i> , 2020, 128, .	1.1	14
122	Density of States of OLED Host Materials from Thermally Stimulated Luminescence. <i>Physical Review Applied</i> , 2021, 15, .	1.5	14
123	A General Framework for Consistent Estimation of Charge Transport Properties via Random Walks in Random Environments. <i>Multiscale Modeling and Simulation</i> , 2014, 12, 1108-1134.	0.6	13
124	Virtual Screening for Organic Solar Cells and Light Emitting Diodes. <i>Advanced Science</i> , 2022, 9, e2200825.	5.6	13
125	Flow boundary conditions for chain-end adsorbing polymer blends. <i>Journal of Chemical Physics</i> , 2005, 123, 104904.	1.2	12
126	Electrochemical TERS Elucidates Potential-Induced Molecular Reorientation of Adenine/Au(111). <i>Angewandte Chemie</i> , 2017, 129, 9928-9933.	1.6	12



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127	Efficiency-limiting processes in cyclopentadithiophene-bridged donor-acceptor-type dyes for solid-state dye-sensitized solar cells. <i>Journal of Chemical Physics</i> , 2018, 148, 044703.	1.2	12
128	Stark effect of hybrid charge transfer states at planar ZnO/organic interfaces. <i>Physical Review B</i> , 2018, 98, .	1.1	12
129	Efficient Simulation of Markov Chains Using Segmentation. <i>Methodology and Computing in Applied Probability</i> , 2014, 16, 465-484.	0.7	11
130	Direct and Energy-Transfer-Mediated Charge-Transfer State Formation and Recombination in Triangulene-Spacer-Perylenediimide Multichromophores: Lessons for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16602-16613.	1.5	11
131	Tuning Single-Molecule Conductance by Controlled Electric Field-Induced trans-to-cis Isomerisation. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 3317.	1.3	11
132	Glass transition temperature prediction of disordered molecular solids. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	11
133	Improvement of Photophysical Properties of CsPbBr <sub>3</sub> and Mn <sup>2+</sup> :CsPb(Br,Cl) <sub>3</sub> Perovskite Nanocrystals by Sr <sup>2+</sup> Doping for White Light-Emitting Diodes. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11277-11284.	1.5	10
134	Molecular scale simulation of hole mobility and current densities in amorphous tridecane. , 2015, , .		9
135	Molecular Origin of Balanced Bipolar Transport in Neat Layers of the Emitter CzDBA. <i>Advanced Materials Technologies</i> , 2021, 6, 2000120.	3.0	9
136	Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 28985-28996.	4.0	9
137	Effective triplet interactions in nematic colloids. <i>European Physical Journal E</i> , 2006, 21, 277-282.	0.7	8
138	Solid-State Electron Affinity Analysis of Amorphous Fluorinated Polymer Electret. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10507-10513.	1.2	8
139	Computing inelastic neutron scattering spectra from molecular dynamics trajectories. <i>Scientific Reports</i> , 2021, 11, 7938.	1.6	7
140	Virtual Screening of TADF Emitters for Single-Layer OLEDs. <i>Frontiers in Chemistry</i> , 2021, 9, 800027.	1.8	7
141	Atomistic force field and electronic properties of carbazole: from monomer to macrocycle. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 839-843.	0.7	6
142	Mechanism of Formation of Three Dimensional Structures of Particles in a Liquid Crystal. <i>Molecular Crystals and Liquid Crystals</i> , 2004, 410, 83-93.	0.4	5
143	Multiscale Concepts in Simulations of Organic Semiconductors. , 2018, , 1-12.		5
144	Tuning interfacial charge transfer in atomically precise nanographeneâ€“graphene heterostructures by engineering van der Waals interactions. <i>Journal of Chemical Physics</i> , 2022, 156, 074702.	1.2	5

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145	Drag of Micro-Particles by an Extended Nematic-Isotropic Interface. <i>Molecular Crystals and Liquid Crystals</i> , 2004, 422, 73-82.	0.4	4
146	Simulations of Morphology and Charge Transport in Supramolecular Organic Materials. <i>RSC Smart Materials</i> , 2014, , 309-362.	0.1	4
147	Organic Light-Emitting Diodes. , 2017, , 473-522.		4
148	Light-induced Freedericksz transition in a nematic liquid crystal with chiral dopant. <i>Liquid Crystals</i> , 1998, 25, 95-100.	0.9	2
149	Porphyrin Functionalization of CsPbBr <sub>2</sub> /SiO <sub>2</sub> Core-Shell Nanocrystals Enhances the Stability and Efficiency in Electroluminescent Devices. <i>Advanced Optical Materials</i> , 2022, 10, 2101945.	3.6	2
150	Modeling of organic light emitting diodes: From molecular to device properties. , 2017, , .		1
151	Recollections of Professor Yuriy Reznikov. <i>Journal of Molecular Liquids</i> , 2018, 267, 11-28.	2.3	1
152	Multiscale Concepts in Simulations of Organic Semiconductors. , 2020, , 1431-1442.		1
153	A personal recollection: A tribute to Yuriy Reznikov. <i>Journal of Molecular Liquids</i> , 2017, 340, 108152.	2.3	0
154	Ultrafast Energy Transfer Triggers Ionization Energy Offset Dependence of Quantum Efficiency in Low-bandgap Non-fullerene Acceptor Solar Cells. , 0, , .		0
155	Non-geminate Recombination Limits Fill Factor in Polymer:ITIC Bulk Heterojunction Solar Cells. , 0, , .		0
156	An Energetic Perspective to Improve the Photostability of Non-Fullerene Acceptor based Organic PhotoVoltaics. , 0, , .		0