Adam J Moulé

List of Publications by Year in descending order

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95 papers 6,095 citations

39 h-index 69250 77 g-index

96 all docs 96
docs citations

96 times ranked 7127 citing authors

#	Article	IF	Citations
1	Quantifying Polaron Mole Fractions and Interpreting Spectral Changes in Molecularly Doped Conjugated Polymers. Advanced Electronic Materials, 2022, 8, .	5.1	7
2	Quantitative Hole Mobility Simulation and Validation in Substituted Acenes. Journal of Physical Chemistry Letters, 2022, 13, 5530-5537.	4.6	7
3	Super-Resolution Photothermal Patterning in Conductive Polymers Enabled by Thermally Activated Solubility. ACS Nano, 2021, 15, 7006-7020.	14.6	3
4	Computing inelastic neutron scattering spectra from molecular dynamics trajectories. Scientific Reports, 2021, 11, 7938.	3.3	7
5	Davis Computational Spectroscopy Workflow—From Structure to Spectra. Journal of Chemical Information and Modeling, 2021, 61, 4486-4496.	5.4	4
6	Anion Exchange Doping: Tuning Equilibrium to Increase Doping Efficiency in Semiconducting Polymers. Journal of Physical Chemistry Letters, 2021, 12, 1284-1289.	4.6	24
7	Comparing the Expense and Accuracy of Methods to Simulate Atomic Vibrations in Rubrene. Journal of Chemical Theory and Computation, 2021, , .	5. 3	3
8	Investigation of Hierarchical Structure Formation in Merocyanine Photovoltaics. Journal of Physical Chemistry C, 2020, 124, 19457-19466.	3.1	4
9	Reversible Doping and Photo Patterning of Polymer Nanowires. Advanced Electronic Materials, 2020, 6, 2000469.	5.1	4
10	Structural characterization of a polycrystalline epitaxially-fused colloidal quantum dot superlattice by electron tomography. Journal of Materials Chemistry A, 2020, 8, 18254-18265.	10.3	7
11	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. Journal of Chemical Theory and Computation, 2020, 16, 3494-3503.	5.3	12
12	Toward Fast Screening of Organic Solar Cell Blends. Advanced Science, 2020, 7, 2000960.	11.2	15
13	Understanding charge transport in donor/acceptor blends from large-scale device simulations based on experimental film morphologies. Energy and Environmental Science, 2020, 13, 601-615.	30.8	14
14	High-Speed Photothermal Patterning of Doped Polymer Films. ACS Applied Materials & Samp; Interfaces, 2019, 11, 41717-41725.	8.0	9
15	Effect of processing conditions on additive DISC patterning of P3HT films. Journal of Materials Chemistry C, 2019, 7, 302-313.	5.5	10
16	Additive solution deposition of multi-layered semiconducting polymer films for design of sophisticated device architectures. Journal of Materials Chemistry C, 2019, 7, 953-960.	5 . 5	10
17	Direct probe of the nuclear modes limiting charge mobility in molecular semiconductors. Materials Horizons, 2019, 6, 182-191.	12.2	53
18	Electronic structure basis for enhanced overall water splitting photocatalysis with aluminum doped SrTiO ₃ in natural sunlight. Energy and Environmental Science, 2019, 12, 1385-1395.	30.8	134

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19	A Freely Soluble, High Electron Affinity Molecular Dopant for Solution Processing of Organic Semiconductors. Chemistry of Materials, 2019, 31, 1500-1506.	6.7	33
20	Double doping of conjugated polymers with monomer molecular dopants. Nature Materials, 2019, 18, 149-155.	27.5	225
21	Put Your Backbone into It: Excited-State Structural Relaxation of PffBT4T-2DT Conducting Polymer in Solution. Journal of Physical Chemistry C, 2018, 122, 7020-7026.	3.1	7
22	Morphological consequences of ligand exchange in quantum dot - Polymer solar cells. Organic Electronics, 2018, 54, 119-125.	2.6	11
23	Polymorphism controls the degree of charge transfer in a molecularly doped semiconducting polymer. Materials Horizons, 2018, 5, 655-660.	12.2	92
24	Photoinduced degradation from trace 1,8-diiodooctane in organic photovoltaics. Journal of Materials Chemistry C, 2018, 6, 219-225.	5.5	30
25	Side chain length affects backbone dynamics in poly(3â€alkylthiophene)s. Journal of Polymer Science, Part B: Polymer Physics, 2018, 56, 1193-1202.	2.1	31
26	Optical Patterning: Directâ€Write Optical Patterning of P3HT Films Beyond the Diffraction Limit (Adv.) Tj ETQq0	0 <u>9 1</u> gBT /	Overlock 10
27	Modeling organic electronic materials: bridging length and time scales. Molecular Simulation, 2017, 43, 730-742.	2.0	8
28	Identifying Atomic Scale Structure in Undoped/Doped Semicrystalline P3HT Using Inelastic Neutron Scattering. Macromolecules, 2017, 50, 2424-2435.	4.8	52
29	Quantitative Dedoping of Conductive Polymers. Chemistry of Materials, 2017, 29, 832-841.	6.7	35
30	Controlling Molecular Doping in Organic Semiconductors. Advanced Materials, 2017, 29, 1703063.	21.0	394
31	Nanoscale Morphology of Doctor Bladed versus Spinâ€Coated Organic Photovoltaic Films. Advanced Energy Materials, 2017, 7, 1701269.	19.5	24
32	Quantitative Measurements of the Temperature-Dependent Microscopic and Macroscopic Dynamics of a Molecular Dopant in a Conjugated Polymer. Macromolecules, 2017, 50, 5476-5489.	4.8	44
33	Directâ€Write Optical Patterning of P3HT Films Beyond the Diffraction Limit. Advanced Materials, 2017, 29, 1603221.	21.0	40
34	Solution aging and degradation of a transparent conducting polymer dispersion. Organic Electronics, 2016, 34, 172-178.	2.6	4
35	Optical Dedoping Mechanism for P3HT:F4TCNQ Mixtures. Journal of Physical Chemistry Letters, 2016, 7, 4297-4303.	4.6	37
36	Nanoscale Morphology of PTB7 Based Organic Photovoltaics as a Function of Fullerene Size. Scientific Reports, 2016, 6, 30915.	3.3	25

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37	Comparison of solution-mixed and sequentially processed P3HT:F4TCNQ films: effect of doping-induced aggregation on film morphology. Journal of Materials Chemistry C, 2016, 4, 3454-3466.	5.5	256
38	The effect of thermal annealing on dopant site choice in conjugated polymers. Organic Electronics, 2016, 33, 23-31.	2.6	54
39	Measurement of Small Molecular Dopant F4TCNQ and C ₆₀ F ₃₆ Diffusion in Organic Bilayer Architectures. ACS Applied Materials & Samp; Interfaces, 2015, 7, 28420-28428.	8.0	82
40	High-resolution patterning electronic polymers using dopant induced solubility control (Presentation Recording). Proceedings of SPIE, 2015, , .	0.8	0
41	Reversible Optical Control of Conjugated Polymer Solubility with Sub-micrometer Resolution. ACS Nano, 2015, 9, 1905-1912.	14.6	52
42	Mixed interlayers at the interface between PEDOT:PSS and conjugated polymers provide charge transport control. Journal of Materials Chemistry C, 2015, 3, 2664-2676.	5.5	26
43	Introducing Solubility Control for Improved Organic P-Type Dopants. Chemistry of Materials, 2015, 27, 5765-5774.	6.7	86
44	Material profile influences in bulk-heterojunctions. Journal of Polymer Science, Part B: Polymer Physics, 2014, 52, 1291-1300.	2.1	9
45	P3HT-Based Solar Cells: Structural Properties and Photovoltaic Performance. Advances in Polymer Science, 2014, , 181-232.	0.8	11
46	High work-function hole transport layers by self-assembly using a fluorinated additive. Journal of Materials Chemistry C, 2014, 2, 115-123.	5.5	21
47	Effect of fractal silver electrodes on charge collection and light distribution in semiconducting organic polymer films. Journal of Materials Chemistry A, 2014, 2, 16608-16616.	10.3	13
48	Molecular Dynamics Study of the Local Structure of Photovoltaic Polymer PCDTBT. Journal of Chemical & Engineering Data, 2014, 59, 2982-2986.	1.9	4
49	P3HT:PCBM Bulk-Heterojunctions: Observing Interfacial and Charge Transfer States with Surface Photovoltage Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 14723-14731.	3.1	44
50	The effect of 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane charge transfer dopants on the conformation and aggregation of poly(3-hexylthiophene). Journal of Materials Chemistry C, 2013, 1, 5638.	5.5	108
51	Quantifying organic solar cell morphology: a computational study of three-dimensional maps. Energy and Environmental Science, 2013, 6, 3060.	30.8	44
52	Photochemical Charge Separation in Poly(3-hexylthiophene) (P3HT) Films Observed with Surface Photovoltage Spectroscopy. Journal of Physical Chemistry C, 2013, 117, 26905-26913.	3.1	41
53	Selfâ€Assembly of Selective Interfaces in Organic Photovoltaics. Advanced Functional Materials, 2013, 23, 1935-1946.	14.9	50
54	Packing Dependent Electronic Coupling in Single Poly(3-hexylthiophene) H- and J-Aggregate Nanofibers. Journal of Physical Chemistry B, 2013, 117, 4478-4487.	2.6	73

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55	Correlating dilute solvent interactions to morphology and OPV device performance. Organic Electronics, 2013, 14, 2431-2443.	2.6	31
56	Threeâ€Dimensional Concentration Mapping of Organic Blends. Advanced Functional Materials, 2013, 23, 2115-2122.	14.9	64
57	J-Aggregate Behavior in Poly-3-hexylthiophene Nanofibers. Journal of Physical Chemistry Letters, 2012, 3, 259-263.	4.6	258
58	Calcium niobate nanosheets as a novel electron transport material for solution-processed multi-junction polymer solar cells. Journal of Materials Chemistry, 2012, 22, 20443.	6.7	19
59	Investigating the Morphology of Polymer/Fullerene Layers Coated Using Orthogonal Solvents. Journal of Physical Chemistry C, 2012, 116, 7287-7292.	3.1	61
60	Hybrid solar cells: basic principles and the role of ligands. Journal of Materials Chemistry, 2012, 22, 2351-2368.	6.7	127
61	Directional dependence of electron blocking in PEDOT:PSS. Organic Electronics, 2012, 13, 2747-2756.	2.6	35
62	Controlling microstructure in poly(3-hexylthiophene) nanofibers. Journal of Materials Chemistry, 2012, 22, 2498-2506.	6.7	136
63	Excited-State Self-Trapping and Ground-State Relaxation Dynamics in Poly(3-hexylthiophene) Resolved with Broadband Pump–Dump–Probe Spectroscopy. Journal of Physical Chemistry Letters, 2011, 2, 2764-2769.	4.6	86
64	Characterization of new transparent organic electrode materials. Organic Electronics, 2011, 12, 1948-1956.	2.6	28
65	Acceptor dependent polaron recombination dynamics in poly 3-hexyl thiophene: Fullerene composite films. Chemical Physics Letters, 2011, 513, 77-83.	2.6	7
66	The Consequences of Interface Mixing on Organic Photovoltaic Device Characteristics. Advanced Functional Materials, 2011, 21, 1657-1665.	14.9	76
67	Effect of Trace Solvent on the Morphology of P3HT:PCBM Bulk Heterojunction Solar Cells. Advanced Functional Materials, 2011, 21, 1779-1787.	14.9	183
68	Characterization of polymerâ€"fullerene mixtures for organic photovoltaics by systematically coarse-grained molecular simulations. Fluid Phase Equilibria, 2011, 302, 21-25.	2.5	51
69	A comparative MD study of the local structure of polymer semiconductors P3HT and PBTTT. Physical Chemistry Chemical Physics, 2010, 12, 14735.	2.8	69
70	Coarse-Grained Computer Simulations of Polymer/Fullerene Bulk Heterojunctions for Organic Photovoltaic Applications. Journal of Chemical Theory and Computation, 2010, 6, 526-537.	5.3	166
71	Power from plastic. Current Opinion in Solid State and Materials Science, 2010, 14, 123-130.	11.5	32
72	Morphology Control in Solutionâ€Processed Bulkâ€Heterojunction Solar Cell Mixtures. Advanced Functional Materials, 2009, 19, 3028-3036.	14.9	252

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73	Optical description of solid-state dye-sensitized solar cells. I. Measurement of layer optical properties. Journal of Applied Physics, 2009, 106, .	2.5	39
74	Optical description of solid-state dye-sensitized solar cells. II. Device optical modeling with implications for improving efficiency. Journal of Applied Physics, 2009, 106, .	2.5	15
75	An optical spacer is no panacea for light collection in organic solar cells. Applied Physics Letters, 2009, 94, .	3.3	73
76	Intensity-dependent photocurrent generation at the anode in bulk-heterojunction solar cells. Applied Physics B: Lasers and Optics, 2008, 92, 209-218.	2.2	63
77	Controlling Morphology in Polymer–Fullerene Mixtures. Advanced Materials, 2008, 20, 240-245.	21.0	495
78	Two Novel Cyclopentadithiophene-Based Alternating Copolymers as Potential Donor Components for High-Efficiency Bulk-Heterojunction-Type Solar Cells. Chemistry of Materials, 2008, 20, 4045-4050.	6.7	179
79	Effect of Polymer Nanoparticle Formation on the Efficiency of Polythiophene Based "Bulk-Heterojunction―Solar Cells. Journal of Physical Chemistry C, 2008, 112, 12583-12589.	3.1	60
80	Controlling organic polymer structure. SPIE Newsroom, 2008, , .	0.1	0
81	Efficiency Enhancements in Solid-State Hybrid Solar Cells via Reduced Charge Recombination and Increased Light Capture. Nano Letters, 2007, 7, 3372-3376.	9.1	363
82	Interference method for the determination of the complex refractive index of thin polymer layers. Applied Physics Letters, 2007, 91, .	3.3	37
83	Minimizing optical losses in bulk heterojunction polymer solar cells. Applied Physics B: Lasers and Optics, 2007, 86, 721-727.	2.2	87
84	The effect of active layer thickness and composition on the performance of bulk-heterojunction solar cells. Journal of Applied Physics, 2006, 100, 094503.	2.5	249
85	Detailed study of the decay mechanism in polymeric OLEDs. , 2005, , .		5
86	The effect of active layer thickness on the efficiency of polymer solar cells. , 2005, , .		3
87	High-resolution NMR of static samples by rotation of the magnetic field. Journal of Magnetic Resonance, 2004, 169, 13-18.	2.1	22
88	Amplification of xenon NMR and MRI by remote detection. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 9122-9127.	7.1	98
89	Two-Dimensional High-Resolution NMR Spectra in Matched BO and B1 Field Gradients. Journal of Magnetic Resonance, 2002, 156, 146-151.	2.1	22
90	Laser-polarized 129Xe NMR and MRI at Ultralow Magnetic Fields. Journal of Magnetic Resonance, 2002, 157, 235-241.	2.1	31

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91	Variable rotation composite pulses for high resolution nuclear magnetic resonance using inhomogeneous magnetic and radiofrequency fields. Chemical Physics Letters, 2002, 363, 25-33.	2.6	18
92	Approach to High-Resolution ex Situ NMR Spectroscopy. Science, 2001, 293, 82-85.	12.6	147
93	Resolution of 129Xe Chemical Shifts at Ultralow Magnetic Field. Journal of the American Chemical Society, 2001, 123, 8133-8134.	13.7	8
94	Synthesis and characterization of solution processable, high electron affinity molecular dopants. Journal of Materials Chemistry C, 0, , .	5 . 5	7
95	Approaching Rapid, Highâ€Resolution, Largeâ€Area Patterning of Semiconducting Polymers Using Projection Photothermal Lithography. Advanced Materials Technologies, 0, , 2100812.	5.8	0