

Daniele Fazzi

List of Publications by Year in descending order

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88
papers

4,487
citations

81900

39
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106344

65
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92
all docs

92
docs citations

92
times ranked

5806
citing authors

#	ARTICLE	IF	CITATIONS
1	Hot exciton dissociation in polymer solar cells. <i>Nature Materials</i> , 2013, 12, 29-33.	27.5	567
2	Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 515-524.	5.3	249
3	Thermoelectric Properties of Solution-Processed n-Doped Ladder-Type Conducting Polymers. <i>Advanced Materials</i> , 2016, 28, 10764-10771.	21.0	245
4	Transient Absorption Imaging of P3HT:PCBM Photovoltaic Blend: Evidence For Interfacial Charge Transfer State. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1099-1105.	4.6	171
5	Very Low Degree of Energetic Disorder as the Origin of High Mobility in an n-channel Polymer Semiconductor. <i>Advanced Functional Materials</i> , 2011, 21, 3371-3381.	14.9	169
6	A Chemically Doped Naphthalenediimide-Bithiazole Polymer for n-Type Organic Thermoelectrics. <i>Advanced Materials</i> , 2018, 30, e1801898.	21.0	165
7	Biradicaloid and Polyenic Character of Quinoidal Oligothiophenes Revealed by the Presence of a Low-Lying Double-Exciton State. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3334-3339.	4.6	150
8	Spectroscopic Investigation of Oxygen- and Water-Induced Electron Trapping and Charge Transport Instabilities in n-type Polymer Semiconductors. <i>Journal of the American Chemical Society</i> , 2012, 134, 14877-14889.	13.7	138
9	Ground-state electron transfer in all-polymer donor-acceptor heterojunctions. <i>Nature Materials</i> , 2020, 19, 738-744.	27.5	111
10	Structure-Function Relationships of High-Electron Mobility Naphthalene Diimide Copolymers Prepared Via Direct Arylation. <i>Chemistry of Materials</i> , 2014, 26, 6233-6240.	6.7	105
11	Quantum-Chemical Insights into the Prediction of Charge Transport Parameters for a Naphthalenetetracarboxydiimide-Based Copolymer with Enhanced Electron Mobility. <i>Journal of the American Chemical Society</i> , 2011, 133, 19056-19059.	13.7	95
12	Evidence for Solution-State Nonlinearity of sp-Carbon Chains Based on IR and Raman Spectroscopy: Violation of Mutual Exclusion. <i>Journal of the American Chemical Society</i> , 2009, 131, 4239-4244.	13.7	93
13	Resistive Molecular Memories: Influence of Molecular Parameters on the Electrical Bistability. <i>Journal of the American Chemical Society</i> , 2009, 131, 6591-6598.	13.7	86
14	C-H Arylation of Unsubstituted Furan and Thiophene with Acceptor Bromides: Access to Donor-Acceptor-Donor-Type Building Blocks for Organic Electronics. <i>Journal of Organic Chemistry</i> , 2015, 80, 980-987.	3.2	78
15	Neuronal firing modulation by a membrane-targeted photoswitch. <i>Nature Nanotechnology</i> , 2020, 15, 296-306.	31.5	71
16	Low-frequency modes in the Raman spectrum of s^2 carbon. <i>Physical Review B</i> , 2008, 77, .	3.2	69
17	Synthesis, Electronic Structure, and Charge Transport Characteristics of Naphthalenediimide-Based CoPolymers with Different Oligothiophene Donor Units. <i>Advanced Functional Materials</i> , 2014, 24, 1151-1162.	14.9	65
18	Reversible P3HT/Oxygen Charge Transfer Complex Identification in Thin Films Exposed to Direct Contact with Water. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6291-6299.	3.1	64

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19	Molecular Level Investigation of the Film Structure of a High Electron Mobility Copolymer via Vibrational Spectroscopy. <i>Macromolecules</i> , 2013, 46, 2658-2670.	4.8	63
20	On the role of aggregation effects in the performance of perylene-diimide based solar cells. <i>Organic Electronics</i> , 2014, 15, 1347-1361.	2.6	60
21	Toward carbyne: Synthesis and stability of really long polyynes. <i>Pure and Applied Chemistry</i> , 2010, 82, 891-904.	1.9	59
22	Tuning the Quinoid versus Biradicaloid Character of Thiophene-Based Heteroquaterphenoquinones by Means of Functional Groups. <i>Journal of the American Chemical Society</i> , 2012, 134, 19070-19083.	13.7	59
23	Polymerization Inhibition by Triplet State Absorption for Nanoscale Lithography. <i>Advanced Materials</i> , 2013, 25, 904-909.	21.0	59
24	Raman spectroscopy and microscopy of electrochemically and chemically doped high-mobility semiconducting polymers. <i>Journal of Materials Chemistry C</i> , 2017, 5, 6176-6184.	5.5	57
25	Multi-length-scale relationships between the polymer molecular structure and charge transport: the case of poly-naphthalene diimide bithiophene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8573-8590.	2.8	56
26	On the Effect of Prevalent Carbazole Homocoupling Defects on the Photovoltaic Performance of PCDTBT:PC ₇₁ BM Solar Cells. <i>Advanced Energy Materials</i> , 2016, 6, 1601232.	19.5	52
27	The Activation of Carboxylic Acids via Self-Assembly Asymmetric Organocatalysis: A Combined Experimental and Computational Investigation. <i>Journal of the American Chemical Society</i> , 2016, 138, 14740-14749.	13.7	52
28	Structure and chain polarization of long polyynes investigated with infrared and Raman spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2013, 44, 1398-1410.	2.5	50
29	Modeling ultrafast exciton deactivation in oligothiophenes via nonadiabatic dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7787-7799.	2.8	48
30	π-Conjugation and End Group Effects in Long Cumulenes: Raman Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26415-26425.	3.1	46
31	Intramolecular Vibrational Force Fields for Linear Carbon Chains through an Adaptive Linear Scaling Scheme. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11645-11651.	2.5	45
32	Highly Planarized Naphthalene Diimide-Bifuran Copolymers with Unexpected Charge Transport Performance. <i>Chemistry of Materials</i> , 2017, 29, 5473-5483.	6.7	45
33	A computational investigation on singlet and triplet exciton couplings in acene molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18615.	2.8	44
34	Effect of Backbone Regiochemistry on Conductivity, Charge Density, and Polaron Structure of n-Doped Donor-Acceptor Polymers. <i>Chemistry of Materials</i> , 2019, 31, 3395-3406.	6.7	44
35	First-principles calculation of the Peierls distortion in an infinite linear carbon chain: the contribution of Raman spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 164-168.	2.5	43
36	Biradicaloid Character of Thiophene-Based Heterophenoquinones: The Role of Electron-Phonon Coupling. <i>ChemPhysChem</i> , 2010, 11, 3685-3695.	2.1	43

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37	Ultrafast internal conversion in a low band gap polymer for photovoltaics: experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6367.	2.8	43
38	Electron transport in crystalline PCBM-like fullerene derivatives: a comparative computational study. <i>Journal of Materials Chemistry C</i> , 2014, 2, 7313-7325.	5.5	41
39	Unveiling the Role of <i>Hot</i> Charge-Transfer States in Molecular Aggregates via Nonadiabatic Dynamics. <i>Journal of the American Chemical Society</i> , 2016, 138, 4502-4511.	13.7	41
40	sp Carbon chain interaction with silver nanoparticles probed by Surface Enhanced Raman Scattering. <i>Chemical Physics Letters</i> , 2009, 478, 45-50.	2.6	40
41	Ultrafast Energy Transfer in Ultrathin Organic Donor/Acceptor Blend. <i>Scientific Reports</i> , 2013, 3, 2073.	3.3	39
42	Highly Fluorescent Metal-Organic-Framework Nanocomposites for Photonic Applications. <i>Nano Letters</i> , 2018, 18, 528-534.	9.1	37
43	Mapping Orientational Order of Charge-Probed Domains in a Semiconducting Polymer. <i>ACS Nano</i> , 2014, 8, 5968-5978.	14.6	36
44	Hot and Cold Charge-Transfer Mechanisms in Organic Photovoltaics: Insights into the Excited States of Donor/Acceptor Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4727-4734.	4.6	36
45	Absolute Raman intensity measurements and determination of the vibrational second hyperpolarizability of adamantyl endcapped polyynes. <i>Journal of Raman Spectroscopy</i> , 2012, 43, 1293-1298.	2.5	30
46	Nature of Charge Carriers in a High Electron Mobility Naphthalenediimide Based Semiconducting Copolymer. <i>Advanced Functional Materials</i> , 2014, 24, 5584-5593.	14.9	30
47	Microstructural control suppresses thermal activation of electron transport at room temperature in polymer transistors. <i>Nature Communications</i> , 2019, 10, 3365.	12.8	30
48	Membrane Environment Enables Ultrafast Isomerization of Amphiphilic Azobenzene. <i>Advanced Science</i> , 2020, 7, 1903241.	11.2	28
49	Bent polyynes: ring geometry studied by Raman and IR spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2012, 43, 95-101.	2.5	27
50	First-Principles Study of the Nuclear Dynamics of Doped Conjugated Polymers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1994-2001.	3.1	25
51	Polarons in Narrow Band Gap Polymers Probed over the Entire Infrared Range: A Joint Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4438-4444.	4.6	24
52	Photogenerated cumulenonic structure of adamantyl endcapped linear carbon chains: An experimental and computational investigation based on infrared spectroscopy. <i>Journal of Chemical Physics</i> , 2011, 134, 124512.	3.0	22
53	Atomistic Simulations of P(NDI2OD-T2) Morphologies: From Single Chain to Condensed Phases. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12556-12565.	2.6	22
54	Polarons in π -conjugated ladder-type polymers: a broken symmetry density functional description. <i>Journal of Materials Chemistry C</i> , 2019, 7, 12876-12885.	5.5	21

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55	Modeling phonons of carbon nanowires. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 2570-2576.	2.7	19
56	Structural Characterization of Highly Oriented Naphthalene-Diimide-Bithiophene Copolymer Films via Vibrational Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2062-2073.	2.6	19
57	The critical role of interfacial dynamics in the stability of organic photovoltaic devices. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8294-8300.	2.8	18
58	On the Origin of Seebeck Coefficient Inversion in Highly Doped Conducting Polymers. <i>Advanced Functional Materials</i> , 2022, 32, .	14.9	18
59	Resistive memories based on Rose Bengal and related xanthene derivatives: insights from modeling charge transport properties. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1600.	2.8	16
60	Reply to 'Measuring internal quantum efficiency to demonstrate hot exciton dissociation'. <i>Nature Materials</i> , 2013, 12, 594-595.	27.5	15
61	Ultrafast spectroscopy of linear carbon chains: the case of dinaphthylpolyynes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9384.	2.8	15
62	Photochromic Torsional Switch (PTS): a light-driven actuator for the dynamic tuning of π -conjugation extension. <i>Chemical Science</i> , 2017, 8, 361-365.	7.4	15
63	Size-selected polyynes synthesised by submerged arc discharge in water. <i>Chemical Physics Letters</i> , 2020, 740, 137054.	2.6	13
64	Radical Anion Yield, Stability, and Electrical Conductivity of Naphthalene Diimide Copolymers n -Doped with Tertiary Amines. <i>ACS Applied Polymer Materials</i> , 2020, 2, 1954-1963.	4.4	12
65	Stable and Solution-Processable Cumulenic π -Carbon Wires: A New Paradigm for Organic Electronics. <i>Advanced Materials</i> , 2022, 34, e2110468.	21.0	12
66	A density matrix based approach for studying excitons in organic crystals. <i>Chemical Physics Letters</i> , 2010, 496, 284-290.	2.6	11
67	Guiding Charge Transport in Semiconducting Carbon Nanotube Networks by Local Optical Switching. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 28392-28403.	8.0	11
68	Effective hamiltonian for π electrons in linear carbon chains. <i>Chemical Physics Letters</i> , 2007, 450, 86-90.	2.6	10
69	Enhancing the light driven modulation of the refractive index in organic photochromic materials: A quantum chemical strategy. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010, 214, 61-68.	3.9	10
70	Optical Modulation of Amplified Emission in a Polyfluorene-Diarylethene Blend. <i>ChemPhysChem</i> , 2011, 12, 3619-3623.	2.1	10
71	Probing Exciton Delocalization in Organic Semiconductors: Insight from Time-Resolved Electron Paramagnetic Resonance and Magnetophotoselection Experiments. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 7026-7031.	4.6	9
72	Addressing the Elusive Polaronic Nature of Multiple Redox States in a π -Conjugated Ladder-Type Polymer. <i>Advanced Electronic Materials</i> , 2021, 7, 2000786.	5.1	9

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73	Understanding the structural and charge transport property relationships for a variety of merocyanine single-crystals: a bottom up computational investigation. Journal of Materials Chemistry C, 2021, 9, 10851-10864.	5.5	9
74	Structure and Electrical Bistability of a New Class of Diphenyl-bithiophenes: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2008, 112, 18628-18637.	3.1	7
75	Effects of Polymer Packing Structure on Photoinduced Triplet Generation and Dynamics. Journal of Physical Chemistry C, 2012, 116, 11298-11305.	3.1	7
76	Effect of the iodine atom position on the phosphorescence of BODIPY derivatives: a combined computational and experimental study. Photochemical and Photobiological Sciences, 2022, 21, 777-786.	2.9	7
77	Raman spectroscopic characterization of a thiophene-based active material for resistive organic nonvolatile memories. Journal of Raman Spectroscopy, 2010, 41, 406-413.	2.5	6
78	Impact of Fluoroalkylation on the n-Type Charge Transport of Two Naphthodithiophene Diimide Derivatives. Molecules, 2021, 26, 4119.	3.8	6
79	Modulation of the electronic structure of polyconjugated organic molecules by geometry relaxation: A discussion based on local Raman parameters. Journal of Molecular Structure, 2011, 993, 26-37.	3.6	5
80	Impact of the Interfacial Molecular Structure Organization on the Charge Transfer State Formation and Exciton Delocalization in Merocyanine:PC ₆₁ BM Blends. Journal of Physical Chemistry C, 2020, 124, 21978-21984.	3.1	5
81	Ultrafast exciton dissociation at donor/acceptor interfaces. , 2013, , .		1
82	Ultrafast Charge Separation in Low Band-Gap Polymer Blend for Photovoltaics. EPJ Web of Conferences, 2013, 41, 04010.	0.3	1
83	Linear Carbon Chains. , 2016, , 27-48.		1
84	Hot Exciton Dissociation at Organic Interfaces. Materials Research Society Symposia Proceedings, 2013, 1537, 1.	0.1	0
85	Ultrafast hot exciton dissociation at organic interfaces. , 2013, , .		0
86	Ultrafast spectroscopy of dinaphthylpolyynes. , 2013, , .		0
87	Ultrafast spectroscopy of linear carbon chains: the case of dinaphthylpolyynes. EPJ Web of Conferences, 2013, 41, 05026.	0.3	0
88	Time-domain spectroscopy of methane excited by resonant high-energy mid-IR pulses. JPhys Photonics, 2021, 3, 034020.	4.6	0