# Daniele Fazzi

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6470456/publications.pdf

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|---|---|---|---|
| 88 papers | 4,487 citations | 81900 39 h-index | 106344 65 g-index |
| 92 all docs | 92 docs citations | 92 times ranked | 5806 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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 |
| 2 | On the Origin of Seebeck Coefficient Inversion in Highly Doped Conducting Polymers. Advanced Functional Materials, 2022, 32, . | 14.9 | 18 |
| 3 | Stable and Solutionâ€Processable Cumulenic spâ€Carbon Wires: A New Paradigm for Organic Electronics. Advanced Materials, 2022, 34, e2110468. | 21.0 | 12 |
| 4 | Addressing the Elusive Polaronic Nature of Multiple Redox States in a Ïâ€Conjugated Ladderâ€Type Polymer. Advanced Electronic Materials, 2021, 7, 2000786. | 5.1 | 9 |
| 5 | Impact of Fluoroalkylation on the n-Type Charge Transport of Two Naphthodithiophene Diimide Derivatives. Molecules, 2021, 26, 4119. | 3.8 | 6 |
| 6 | Time-domain spectroscopy of methane excited by resonant high-energy mid-IR pulses. JPhys Photonics, 2021, 3, 034020. | 4.6 | 0 |
| 7 | 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 |
| 8 | Size-selected polyynes synthesised by submerged arc discharge in water. Chemical Physics Letters, 2020, 740, 137054. | 2.6 | 13 |
| 9 | Impact of the Interfacial Molecular Structure Organization on the Charge Transfer State Formation and Exciton Delocalization in Merocyanine:PC<sub>61</sub>BM Blends. Journal of Physical Chemistry C, 2020, 124, 21978-21984. | 3.1 | 5 |
| 10 | Guiding Charge Transport in Semiconducting Carbon Nanotube Networks by Local Optical Switching. ACS Applied Materials & Interfaces, 2020, 12, 28392-28403. | 8.0 | 11 |
| 11 | Membrane Environment Enables Ultrafast Isomerization of Amphiphilic Azobenzene. Advanced Science, 2020, 7, 1903241. | 11.2 | 28 |
| 12 | Ground-state electron transfer in all-polymer donorâ€“acceptor heterojunctions. Nature Materials, 2020, 19, 738-744. | 27.5 | 111 |
| 13 | Radical Anion Yield, Stability, and Electrical Conductivity of Naphthalene Diimide Copolymers n-Doped with Tertiary Amines. ACS Applied Polymer Materials, 2020, 2, 1954-1963. | 4.4 | 12 |
| 14 | Neuronal firing modulation by a membrane-targeted photoswitch. Nature Nanotechnology, 2020, 15, 296-306. | 31.5 | 71 |
| 15 | Polarons in Ï€-conjugated ladder-type polymers: a broken symmetry density functional description. Journal of Materials Chemistry C, 2019, 7, 12876-12885. | 5.5 | 21 |
| 16 | Microstructural control suppresses thermal activation of electron transport at room temperature in polymer transistors. Nature Communications, 2019, 10, 3365. | 12.8 | 30 |
| 17 | Effect of Backbone Regiochemistry on Conductivity, Charge Density, and Polaron Structure of n-Doped Donorâ€“Acceptor Polymers. Chemistry of Materials, 2019, 31, 3395-3406. | 6.7 | 44 |
| 18 | Highly Fluorescent Metalâ€“Organic-Framework Nanocomposites for Photonic Applications. Nano Letters, 2018, 18, 528-534. | 9.1 | 37 |

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|---|---|---|---|
| 19 | Probing Exciton Delocalization in Organic Semiconductors: Insight from Time-Resolved Electron Paramagnetic Resonance and Magnetophotoselection Experiments. Journal of Physical Chemistry Letters, 2018, 9, 7026-7031. | 4.6 | 9 |
| 20 | A Chemically Doped Naphthalenediimideâ€Bithiazole Polymer for nâ€Type Organic Thermoelectrics. Advanced Materials, 2018, 30, e1801898. | 21.0 | 165 |
| 21 | Raman spectroscopy and microscopy of electrochemically and chemically doped high-mobility semiconducting polymers. Journal of Materials Chemistry C, 2017, 5, 6176-6184. | 5.5 | 57 |
| 22 | Highly Planarized Naphthalene Diimideâ€“Bifuran Copolymers with Unexpected Charge Transport Performance. Chemistry of Materials, 2017, 29, 5473-5483. | 6.7 | 45 |
| 23 | Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods. Journal of Chemical Theory and Computation, 2017, 13, 515-524. | 5.3 | 249 |
| 24 | Hot and Cold Charge-Transfer Mechanisms in Organic Photovoltaics: Insights into the Excited States of Donor/Acceptor Interfaces. Journal of Physical Chemistry Letters, 2017, 8, 4727-4734. | 4.6 | 36 |
| 25 | Photochromic Torsional Switch (PTS): a light-driven actuator for the dynamic tuning of Ï€-conjugation extension. Chemical Science, 2017, 8, 361-365. | 7.4 | 15 |
| 26 | On the Effect of Prevalent Carbazole Homocoupling Defects on the Photovoltaic Performance of PCDTBT:PC<sub>71</sub>BM Solar Cells. Advanced Energy Materials, 2016, 6, 1601232. | 19.5 | 52 |
| 27 | Linear Carbon Chains. , 2016, , 27-48. | | 1 |
| 28 | The Activation of Carboxylic Acids via Self-Assembly Asymmetric Organocatalysis: A Combined Experimental and Computational Investigation. Journal of the American Chemical Society, 2016, 138, 14740-14749. | 13.7 | 52 |
| 29 | Thermoelectric Properties of Solutionâ€Processed nâ€Doped Ladderâ€Type Conducting Polymers. Advanced Materials, 2016, 28, 10764-10771. | 21.0 | 245 |
| 30 | Polarons in Narrow Band Gap Polymers Probed over the Entire Infrared Range: A Joint Experimental and Theoretical Investigation. Journal of Physical Chemistry Letters, 2016, 7, 4438-4444. | 4.6 | 24 |
| 31 | First-Principles Study of the Nuclear Dynamics of Doped Conjugated Polymers. Journal of Physical Chemistry C, 2016, 120, 1994-2001. | 3.1 | 25 |
| 32 | Unveiling the Role of Hot Charge-Transfer States in Molecular Aggregates via Nonadiabatic Dynamics. Journal of the American Chemical Society, 2016, 138, 4502-4511. | 13.7 | 41 |
| 33 | Modeling ultrafast exciton deactivation in oligothiophenes via nonadiabatic dynamics. Physical Chemistry Chemical Physics, 2015, 17, 7787-7799. | 2.8 | 48 |
| 34 | Câ€“H Arylation of Unsubstituted Furan and Thiophene with Acceptor Bromides: Access to Donorâ€“Acceptorâ€“Donor-Type Building Blocks for Organic Electronics. Journal of Organic Chemistry, 2015, 80, 980-987. | 3.2 | 78 |
| 35 | Structural Characterization of Highly Oriented Naphthalene-Diimide-Bithiophene Copolymer Films via Vibrational Spectroscopy. Journal of Physical Chemistry B, 2015, 119, 2062-2073. | 2.6 | 19 |
| 36 | Multi-length-scale relationships between the polymer molecular structure and charge transport: the case of poly-naphthalene diimide bithiophene. Physical Chemistry Chemical Physics, 2015, 17, 8573-8590. | 2.8 | 56 |

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|---|---|---|---|
| 37 | On the role of aggregation effects in the performance of perylene-diimide based solar cells. Organic Electronics, 2014, 15, 1347-1361. | 2.6 | 60 |
| 38 | Mapping Orientational Order of Charge-Probed Domains in a Semiconducting Polymer. ACS Nano, 2014, 8, 5968-5978. | 14.6 | 36 |
| 39 | Ï€-Conjugation and End Group Effects in Long Cumulenes: Raman Spectroscopy and DFT Calculations. Journal of Physical Chemistry C, 2014, 118, 26415-26425. | 3.1 | 46 |
| 40 | The critical role of interfacial dynamics in the stability of organic photovoltaic devices. Physical Chemistry Chemical Physics, 2014, 16, 8294-8300. | 2.8 | 18 |
| 41 | Atomistic Simulations of P(NDI2OD-T2) Morphologies: From Single Chain to Condensed Phases. Journal of Physical Chemistry B, 2014, 118, 12556-12565. | 2.6 | 22 |
| 42 | Electron transport in crystalline PCBM-like fullerene derivatives: a comparative computational study. Journal of Materials Chemistry C, 2014, 2, 7313-7325. | 5.5 | 41 |
| 43 | Nature of Charge Carriers in a High Electron Mobility Naphthalenediimide Based Semiconducting Copolymer. Advanced Functional Materials, 2014, 24, 5584-5593. | 14.9 | 30 |
| 44 | Structureâ€“Function Relationships of High-Electron Mobility Naphthalene Diimide Copolymers Prepared Via Direct Arylation. Chemistry of Materials, 2014, 26, 6233-6240. | 6.7 | 105 |
| 45 | Reversible P3HT/Oxygen Charge Transfer Complex Identification in Thin Films Exposed to Direct Contact with Water. Journal of Physical Chemistry C, 2014, 118, 6291-6299. | 3.1 | 64 |
| 46 | Synthesis, Electronic Structure, and Charge Transport Characteristics of Naphthalenediimideâ€Based Coâ€Polymers with Different Oligothiophene Donor Units. Advanced Functional Materials, 2014, 24, 1151-1162. | 14.9 | 65 |
| 47 | Reply to 'Measuring internal quantum efficiency to demonstrate hot exciton dissociation'. Nature Materials, 2013, 12, 594-595. | 27.5 | 15 |
| 48 | Hot exciton dissociation in polymer solar cells. Nature Materials, 2013, 12, 29-33. | 27.5 | 567 |
| 49 | Polymerization Inhibition by Triplet State Absorption for Nanoscale Lithography. Advanced Materials, 2013, 25, 904-909. | 21.0 | 59 |
| 50 | Structure and chain polarization of long polyynes investigated with infrared and Raman spectroscopy. Journal of Raman Spectroscopy, 2013, 44, 1398-1410. | 2.5 | 50 |
| 51 | Molecular Level Investigation of the Film Structure of a High Electron Mobility Copolymer via Vibrational Spectroscopy. Macromolecules, 2013, 46, 2658-2670. | 4.8 | 63 |
| 52 | Ultrafast spectroscopy of linear carbon chains: the case of dinaphthylpolyynes. Physical Chemistry Chemical Physics, 2013, 15, 9384. | 2.8 | 15 |
| 53 | Ultrafast Energy Transfer in Ultrathin Organic Donor/Acceptor Blend. Scientific Reports, 2013, 3, 2073. | 3.3 | 39 |
| 54 | Ultrafast exciton dissociation at donor/acceptor interfaces. , 2013, , . | | 1 |

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|---|---|---|---|
| 55 | Hot Exciton Dissociation at Organic Interfaces. Materials Research Society Symposia Proceedings, 2013, 1537, 1. | 0.1 | 0 |
| 56 | Ultrafast hot exciton dissociation at organic interfaces. , 2013, , . | | 0 |
| 57 | Ultrafast spectroscopy of dinaphthylpolyynes. , 2013, , . | | 0 |
| 58 | Ultrafast spectroscopy of linear carbon chains: the case of dinaphthylpolyynes. EPJ Web of Conferences, 2013, 41, 05026. | 0.3 | 0 |
| 59 | Ultrafast Charge Separation in Low Band-Gap Polymer Blend for Photovoltaics. EPJ Web of Conferences, 2013, 41, 04010. | 0.3 | 1 |
| 60 | Spectroscopic Investigation of Oxygen- and Water-Induced Electron Trapping and Charge Transport Instabilities in n-type Polymer Semiconductors. Journal of the American Chemical Society, 2012, 134, 14877-14889. | 13.7 | 138 |
| 61 | Effects of Polymer Packing Structure on Photoinduced Triplet Generation and Dynamics. Journal of Physical Chemistry C, 2012, 116, 11298-11305. | 3.1 | 7 |
| 62 | Ultrafast internal conversion in a low band gap polymer for photovoltaics: experimental and theoretical study. Physical Chemistry Chemical Physics, 2012, 14, 6367. | 2.8 | 43 |
| 63 | Tuning the Quinoid versus Biradicaloid Character of Thiophene-Based Heteroquaterphenoquinones by Means of Functional Groups. Journal of the American Chemical Society, 2012, 134, 19070-19083. | 13.7 | 59 |
| 64 | Absolute Raman intensity measurements and determination of the vibrational second hyperpolarizability of adamantyl endcapped polyynes. Journal of Raman Spectroscopy, 2012, 43, 1293-1298. | 2.5 | 30 |
| 65 | Bent polyynes: ring geometry studied by Raman and IR spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 95-101. | 2.5 | 27 |
| 66 | Transient Absorption Imaging of P3HT:PCBM Photovoltaic Blend: Evidence For Interfacial Charge Transfer State. Journal of Physical Chemistry Letters, 2011, 2, 1099-1105. | 4.6 | 171 |
| 67 | A computational investigation on singlet and triplet exciton couplings in acene molecular crystals. Physical Chemistry Chemical Physics, 2011, 13, 18615. | 2.8 | 44 |
| 68 | Quantum-Chemical Insights into the Prediction of Charge Transport Parameters for a Naphthalenetetracarboxydiimide-Based Copolymer with Enhanced Electron Mobility. Journal of the American Chemical Society, 2011, 133, 19056-19059. | 13.7 | 95 |
| 69 | 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 |
| 70 | Very Low Degree of Energetic Disorder as the Origin of High Mobility in an nâ€channel Polymer Semiconductor. Advanced Functional Materials, 2011, 21, 3371-3381. | 14.9 | 169 |
| 71 | Optical Modulation of Amplified Emission in a Polyfluoreneâ€“Diarylethene Blend. ChemPhysChem, 2011, 12, 3619-3623. | 2.1 | 10 |
| 72 | Photogenerated cumulenic structure of adamantyl endcapped linear carbon chains: An experimental and computational investigation based on infrared spectroscopy. Journal of Chemical Physics, 2011, 134, 124512. | 3.0 | 22 |

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|---|---|---|---|
| 73 | Biradicaloid Character of Thiopheneâ€Based Heterophenoquinones: The Role of Electronâ€“Phonon Coupling. ChemPhysChem, 2010, 11, 3685-3695. | 2.1 | 43 |
| 74 | Raman spectroscopic characterization of a thiopheneâ€based active material for resistive organic nonvolatile memories. Journal of Raman Spectroscopy, 2010, 41, 406-413. | 2.5 | 6 |
| 75 | Enhancing the light driven modulation of the refractive index in organic photochromic materials: A quantum chemical strategy. Journal of Photochemistry and Photobiology A: Chemistry, 2010, 214, 61-68. | 3.9 | 10 |
| 76 | A density matrix based approach for studying excitons in organic crystals. Chemical Physics Letters, 2010, 496, 284-290. | 2.6 | 11 |
| 77 | Toward carbyne: Synthesis and stability of really long polyynes. Pure and Applied Chemistry, 2010, 82, 891-904. | 1.9 | 59 |
| 78 | Biradicaloid and Polyenic Character of Quinoidal Oligothiophenes Revealed by the Presence of a Low-Lying Double-Exciton State. Journal of Physical Chemistry Letters, 2010, 1, 3334-3339. | 4.6 | 150 |
| 79 | Resistive memories based on Rose Bengal and related xanthene derivatives: insights from modeling charge transport properties. Physical Chemistry Chemical Physics, 2010, 12, 1600. | 2.8 | 16 |
| 80 | sp Carbon chain interaction with silver nanoparticles probed by Surface Enhanced Raman Scattering. Chemical Physics Letters, 2009, 478, 45-50. | 2.6 | 40 |
| 81 | Resistive Molecular Memories: Influence of Molecular Parameters on the Electrical Bistability. Journal of the American Chemical Society, 2009, 131, 6591-6598. | 13.7 | 86 |
| 82 | Evidence for Solution-State Nonlinearity of sp-Carbon Chains Based on IR and Raman Spectroscopy: Violation of Mutual Exclusion. Journal of the American Chemical Society, 2009, 131, 4239-4244. | 13.7 | 93 |
| 83 | Firstâ€principles calculation of the Peierls distortion in an infinite linear carbon chain: the contribution of Raman spectroscopy. Journal of Raman Spectroscopy, 2008, 39, 164-168. | 2.5 | 43 |
| 84 | Modeling phonons of carbon nanowires. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 2570-2576. | 2.7 | 19 |
| 85 | Low-frequency modes in the Raman spectrum of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:mi>p</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>s</mml:mi><mml:mi> carbon. Physical Review B, 2008, 77, . | 3.2 | 69 |
| 86 | 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 |
| 87 | Intramolecular Vibrational Force Fields for Linear Carbon Chains through an Adaptative Linear Scaling Scheme. Journal of Physical Chemistry A, 2007, 111, 11645-11651. | 2.5 | 45 |
| 88 | Effective hamiltonian for Ï€ electrons in linear carbon chains. Chemical Physics Letters, 2007, 450, 86-90. | 2.6 | 10 |