Jarvist M Frost

List of Publications by Year in descending order

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47004 110368 12,721 66 47 64 citations h-index g-index papers 72 72 72 14359 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Ionic transport in hybrid lead iodide perovskite solar cells. Nature Communications, 2015, 6, 7497.	12.8	2,154
2	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. Nano Letters, 2014, 14, 2584-2590.	9.1	2,068
3	The dynamics of methylammonium ions in hybrid organic–inorganic perovskite solar cells. Nature Communications, 2015, 6, 7124.	12.8	517
4	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. APL Materials, 2014, 2, .	5.1	481
5	Cubic Perovskite Structure of Black Formamidinium Lead Iodide, α-[HC(NH ₂) ₂]Pbl ₃ , at 298 K. Journal of Physical Chemistry Letters, 2015, 6, 3209-3212.	4.6	457
6	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. Physical Review B, 2015, 92, .	3.2	452
7	What Is Moving in Hybrid Halide Perovskite Solar Cells?. Accounts of Chemical Research, 2016, 49, 528-535.	15.6	385
8	Binary Organic Photovoltaic Blends: A Simple Rationale for Optimum Compositions. Advanced Materials, 2008, 20, 3510-3515.	21.0	364
9	Ferroelectric materials for solar energy conversion: photoferroics revisited. Energy and Environmental Science, 2015, 8, 838-848.	30.8	333
10	Dynamic disorder, phonon lifetimes, and the assignment of modes to the vibrational spectra of methylammonium lead halide perovskites. Physical Chemistry Chemical Physics, 2016, 18, 27051-27066.	2.8	325
11	Real-Time Observation of Organic Cation Reorientation in Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 3663-3669.	4.6	322
12	Indirect to direct bandgap transition in methylammonium lead halide perovskite. Energy and Environmental Science, 2017, 10, 509-515.	30.8	318
13	Modeling Charge Transport in Organic Photovoltaic Materials. Accounts of Chemical Research, 2009, 42, 1768-1778.	15.6	239
14	Band alignment of the hybrid halide perovskites CH ₃ NH ₃ PbCl ₃ , CH ₃ NH ₃ PbBr ₃ and CH ₃ NH ₃ PbBr ₃ . Materials Horizons, 2015, 2, 228-231.	12.2	238
15	Role of microstructure in the electron–hole interaction of hybrid lead halide perovskites. Nature Photonics, 2015, 9, 695-701.	31.4	226
16	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead lodide Perovskite. ACS Energy Letters, 2016, 1, 880-887.	17.4	221
17	Effect of Fluorination on the Properties of a Donor–Acceptor Copolymer for Use in Photovoltaic Cells and Transistors. Chemistry of Materials, 2013, 25, 277-285.	6.7	218
18	Spontaneous Octahedral Tilting in the Cubic Inorganic Cesium Halide Perovskites CsSnX $<$ sub $>$ 3 $<$ /sub $>$ and CsPbX $<$ sub $>$ 3 $<$ /sub $>$ (X = F, Cl, Br, I). Journal of Physical Chemistry Letters, 2017, 8, 4720-4726.	4.6	186

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19	Research Update: Relativistic origin of slow electron-hole recombination in hybrid halide perovskite solar cells. APL Materials, 2016, 4, .	5.1	178
20	Dielectric and ferroic properties of metal halide perovskites. APL Materials, 2019, 7, .	5.1	173
21	Calculating polaron mobility in halide perovskites. Physical Review B, 2017, 96, .	3.2	168
22	Models of charge pair generation in organic solar cells. Physical Chemistry Chemical Physics, 2015, 17, 2311-2325.	2.8	158
23	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano, 2017, 11, 8329-8338.	14.6	136
24	Slow Cooling of Hot Polarons in Halide Perovskite Solar Cells. ACS Energy Letters, 2017, 2, 2647-2652.	17.4	132
25	Phonon anharmonicity, lifetimes, and thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CH</mml:mi><mml: .<="" 2016,="" 94,="" b,="" from="" many-body="" perturbation="" physical="" review="" td="" theory.=""><td>mn3.3<td>ml:#81> </td></td></mml:></mml:msub></mml:mrow></mml:math>	mn 3.3 <td>ml:#81> </td>	ml :#81 >
26	Ultrafast Intraband Spectroscopy of Hot-Carrier Cooling in Lead-Halide Perovskites. ACS Energy Letters, 2018, 3, 2199-2205.	17.4	119
27	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	11.7	115
28	Organic Cation Rotation and Immobilization in Pure and Mixed Methylammonium Lead-Halide Perovskites. Journal of the American Chemical Society, 2017, 139, 4068-4074.	13.7	114
29	Perspective: Theory and simulation of hybrid halide perovskites. Journal of Chemical Physics, 2017, 146, 220901.	3.0	111
30	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	38.1	105
31	Influence of Polymer-Blend Morphology on Charge Transport and Photocurrent Generation in Donorâ° Acceptor Polymer Blends. Nano Letters, 2006, 6, 1674-1681.	9.1	95
32	Synthesis and Exciton Dynamics of Donor-Orthogonal Acceptor Conjugated Polymers: Reducing the Singlet–Triplet Energy Gap. Journal of the American Chemical Society, 2017, 139, 11073-11080.	13.7	95
33	Energetic Disorder in Higher Fullerene Adducts: A Quantum Chemical and Voltammetric Study. Advanced Materials, 2010, 22, 4881-4884.	21.0	87
34	A numerical study of mobility in thin films of fullerene derivatives. Journal of Chemical Physics, 2010, 132, 064904.	3.0	86
35	Controlling Microstructure of Pentacene Derivatives by Solution Processing: Impact of Structural Anisotropy on Optoelectronic Properties. ACS Nano, 2013, 7, 7983-7991.	14.6	86
36	Predictive Study of Charge Transport in Disordered Semiconducting Polymers. Nano Letters, 2007, 7, 1785-1788.	9.1	81

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37	Acoustic phonon lifetimes limit thermal transport in methylammonium lead iodide. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11905-11910.	7.1	81
38	Polaron pair mediated triplet generation in polymer/fullerene blends. Nature Communications, 2015, 6, 6501.	12.8	74
39	The Effect of Morphology on Electron Field-Effect Mobility in Disordered C60 Thin Films. Nano Letters, 2009, 9, 1085-1090.	9.1	72
40	Highly Luminescent Encapsulated Narrow Bandgap Polymers Based on Diketopyrrolopyrrole. Journal of the American Chemical Society, 2018, 140, 1622-1626.	13.7	70
41	Rotational Cation Dynamics in Metal Halide Perovskites: Effect on Phonons and Material Properties. Journal of Physical Chemistry Letters, 2018, 9, 5987-5997.	4.6	68
42	Assessment of dynamic structural instabilities across 24 cubic inorganic halide perovskites. Journal of Chemical Physics, 2020, 152, 024703.	3.0	67
43	Modular design of SPIRO-OMeTAD analogues as hole transport materials in solar cells. Chemical Communications, 2015, 51, 8935-8938.	4.1	64
44	Influence of Chemical Structure on the Charge Transfer State Spectrum of a Polymer:Fullerene Complex. Journal of Physical Chemistry C, 2014, 118, 8253-8261.	3.1	61
45	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. Physical Review B, 2019, 99, .	3.2	60
46	Isostructural, Deeper Highest Occupied Molecular Orbital Analogues of Poly(3-hexylthiophene) for High-Open Circuit Voltage Organic Solar Cells. Chemistry of Materials, 2013, 25, 4239-4249.	6.7	55
47	Influence of Bridging Atom and Side Chains on the Structure and Crystallinity of Cyclopentadithiophene–Benzothiadiazole Polymers. Chemistry of Materials, 2014, 26, 1226-1233.	6.7	50
48	Distinguishing the influence of structural and energetic disorder on electron transport in fullerene multi-adducts. Materials Horizons, 2015, 2, 113-119.	12.2	49
49	Giant Huang–Rhys Factor for Electron Capture by the Iodine Intersitial in Perovskite Solar Cells. Journal of the American Chemical Society, 2021, 143, 9123-9128.	13.7	37
50	Parameter free calculation of the subgap density of states in poly(3-hexylthiophene). Faraday Discussions, 2014, 174, 255-266.	3.2	29
51	Atomistic insights into the order–disorder transition in Cu ₂ ZnSnS ₄ solar cells from Monte Carlo simulations. Journal of Materials Chemistry A, 2019, 7, 312-321.	10.3	23
52	Descriptors for Electron and Hole Charge Carriers in Metal Oxides. Journal of Physical Chemistry Letters, 2020, 11, 438-444.	4.6	22
53	Effect of Molecular Fluctuations on Hole Diffusion within Dye Monolayers. Chemistry of Materials, 2014, 26, 4731-4740.	6.7	21
54	The Role of Longâ€Alkylâ€Group Spacers in Glycolated Copolymers for Highâ€Performance Organic Electrochemical Transistors. Advanced Materials, 2022, 34, e2202574.	21.0	21

#	Article	IF	CITATIONS
55	Soluble fullerene derivatives: The effect of electronic structure on transistor performance and air stability. Journal of Applied Physics, $2011,110,.$	2.5	19
56	Zero-Point Fluctuations in Naphthalene and Their Effect on Charge Transport Parameters. Journal of Physical Chemistry A, 2008, 112, 9113-9117.	2.5	14
57	Influence of Intermolecular Interactions on the Reorganization Energy of Charge Transfer between Surface-Attached Dye Molecules. Journal of Physical Chemistry C, 2015, 119, 24337-24341.	3.1	14
58	Influence of a nearby substrate on the reorganization energy of hole exchange between dye molecules. Physical Chemistry Chemical Physics, 2015, 17, 7345-7354.	2.8	12
59	Molecular Motion and Dynamic Crystal Structures of Hybrid Halide Perovskites. , 2016, , 1-17.		12
60	Relating Chain Conformation to the Density of States and Charge Transport in Conjugated Polymers: The Role of the <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"><mml:mi>β</mml:mi></mml:math> -phase in Poly(9,9-dioctylfluorene). Physical Review X, 2019, 9, .	8.9	11
61	Polaron States in Fullerene Adducts Modeled by Coarse-Grained Molecular Dynamics and Tight Binding. Journal of Physical Chemistry Letters, 2018, 9, 6616-6623.	4.6	10
62	Accelerated Hot-Carrier Cooling in MAPbl ₃ Perovskite by Pressure-Induced Lattice Compression. Journal of Physical Chemistry Letters, 2021, 12, 4118-4124.	4.6	8
63	Multipulse Terahertz Spectroscopy Unveils Hot Polaron Photoconductivity Dynamics in Metal-Halide Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 8732-8739.	4.6	8
64	Fr $ ilde{A}$ ¶hlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands. Physical Review B, 2021, 104, .	3.2	8
65	PolaronMobility.jl: Implementation of the Feynman variational polaron model. Journal of Open Source Software, 2018, 3, 566.	4.6	5
66	High Power Irradiance Dependence of Charge Species Dynamics in Hybrid Perovskites and Kinetic Evidence for Transient Vibrational Stark Effect in Formamidinium. Nanomaterials, 2022, 12, 1616.	4.1	0