

Yukihiro Shimoi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

102
papers

1,473
citations

22
h-index

34
g-index

105
ext. papers

1,577
ext. citations

3.1
avg, IF

4.41
L-index

#	Paper	IF	Citations
102	Microscopic observation of efficient intergrain charge transport processes in organic transistors of semicrystalline poly(3-hexylthiophene). <i>Applied Physics Express</i> , 2022 , 15, 041004	2.4	
101	Theoretical Study of the Mechanism for the Reaction of Trimethylaluminum with Ozone. <i>ACS Omega</i> , 2021 , 6, 26282-26292	3.9	0
100	Simulation Study of the Effects of Interfacial Bonds on Adhesion and Fracture Behavior of Epoxy Resin Layers. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 11044-11057	3.4	0
99	Architecting layered molecular packing in substituted benzobisbenzothiophene (BBBT) semiconductor crystals. <i>CrystEngComm</i> , 2020 , 22, 3618-3626	3.3	8
98	Structure dependency of the reactivity of aromatic hydrocarbons involving the formation of oxygenated polycyclic aromatic hydrocarbons (OPAHs). <i>Chemical Physics Letters</i> , 2020 , 754, 137652	2.5	2
97	Spatial extent of wave functions of charge carriers in a thienothiophene-based high-mobility molecular semiconductor. <i>Applied Physics Express</i> , 2020 , 13, 041004	2.4	1
96	Thermoelectric properties of a semicrystalline polymer doped beyond the insulator-to-metal transition by electrolyte gating. <i>Science Advances</i> , 2020 , 6, eaay8065	14.3	40
95	Highly Efficient Microscopic Charge Transport within Crystalline Domains in a Furan-Flanked Diketopyrrolopyrrole-Based Conjugated Copolymer. <i>Advanced Functional Materials</i> , 2020 , 30, 2000389	15.6	5
94	Crystal Structures and Fluorescence Spectroscopic Properties of a Series of π -Di(4-pyridyl)polyenes: Effect of Aggregation-Induced Emission. <i>ChemPlusChem</i> , 2020 , 85, 1968-1980	2.8	1
93	Simulation Study of the Effects of Nanoporous Structures on Mechanical Properties at Polymer-Metal Interfaces. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 1161-1170	3.4	6
92	Microscopic observation of efficient charge transport processes across domain boundaries in donor-acceptor-type conjugated polymers. <i>Communications Physics</i> , 2019 , 2,	5.4	17
91	Vibrational entropy as an indicator of temperature coefficient of redox potential in conjugated polymers. <i>Japanese Journal of Applied Physics</i> , 2019 , 58, 097004	1.4	2
90	Temperature-Dependent Evolution of Raman Spectra of Methylammonium Lead Halide Perovskites, $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X = I, Br). <i>Molecules</i> , 2019 , 24,	4.8	38
89	Structures and Fluorescence Properties for the Crystals, Powders, and Thin Films of Dithienylhexatrienes: Effects of Positional Isomerism. <i>Crystal Growth and Design</i> , 2018 , 18, 6477-6487	3.5	4
88	Enhanced Layered-Herringbone Packing due to Long Alkyl Chain Substitution in Solution-Processable Organic Semiconductors. <i>Chemistry of Materials</i> , 2017 , 29, 1245-1254	9.6	80
87	Activation of N ₂ by isolated small tungsten clusters at room temperature. <i>Chemical Physics Letters</i> , 2017 , 667, 267-271	2.5	5
86	Investigation of the electrochromic properties of tri-block polyaniline-polythiophene-polyaniline under visible light. <i>Synthetic Metals</i> , 2017 , 226, 80-88	3.6	25

85	Halogenated (F, Cl, Br, or I) Diphenylhexatrienes: Crystal Structures, Fluorescence Spectroscopic Properties, and Quantum Chemical Calculations. <i>Crystal Growth and Design</i> , 2016 , 16, 4060-4071	3.5	13
84	Spectroscopic Investigations on Degradative Processes of cis-Bis(isothiocyanato)bis(2,2'-bipyridyl-4,4'-dicarboxylato) Ruthenium(II) Anchored on Anatase TiO ₂ Surface. <i>Molecular Crystals and Liquid Crystals</i> , 2015 , 622, 158-163	0.5	
83	Effects of pn Doping in Thiophene/Phenylene Co-oligomers Thin Films. <i>Molecular Crystals and Liquid Crystals</i> , 2015 , 620, 153-158	0.5	5
82	Photo-Fries rearrangement of phenyl salicylate studied by two-dimensional infrared spectroscopy. <i>Vibrational Spectroscopy</i> , 2015 , 81, 131-135	2.1	4
81	Direct observation of spins at bathocuproine (BCP) interfaces: An electron spin resonance study on BCP/metal (Al or Au) thin films. <i>Chemical Physics Letters</i> , 2014 , 607, 29-33	2.5	8
80	Low-temperature carrier dynamics in high-mobility organic transistors of alkylated dinaphtho-thienothiophene as investigated by electron spin resonance. <i>Applied Physics Letters</i> , 2014 , 105, 033301	3.4	13
79	Theoretical prediction of crystal structures of rubrene. <i>Japanese Journal of Applied Physics</i> , 2014 , 53, 01AD02	1.4	12
78	Characterization of P3HT:PCBM Thin Film Interfaces by Doubly Resonant Sum-Frequency Generation Spectroscopy. <i>Molecular Crystals and Liquid Crystals</i> , 2014 , 597, 33-36	0.5	2
77	Preferable Molecular Orientation of Poly(3-hexylthiophene) on Self-Assembled Monolayers: Molecular Dynamics Simulation. <i>Molecular Crystals and Liquid Crystals</i> , 2013 , 578, 33-36	0.5	1
76	Fluorescence properties of (E,E,E)-1,6-di(n-naphthyl)-1,3,5-hexatriene (n = 1, 2): effects of internal rotation. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 566-78	2.8	12
75	Control of molecular orientations of poly(3-hexylthiophene) on self-assembled monolayers: molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 9265-70	3.6	27
74	Direct Observation of Charge Carriers in Highly Magnesium-Doped Tris(8-hydroxyquinoline) Aluminum Thin Film by Electron Spin Resonance. <i>Japanese Journal of Applied Physics</i> , 2013 , 52, 05DB07	1.4	4
73	Electronic states of thiophene/phenylene co-oligomers: Extreme-ultra violet excited photoelectron spectroscopy observations and density functional theory calculations. <i>Journal of Applied Physics</i> , 2013 , 113, 083710	2.5	13
72	Electron Spin Resonance of Thin Films of N,N'-Di(1-naphthyl)-N,N'-diphenylbenzidine (NPB) Doped by Iodine Vapor. <i>Chemistry Letters</i> , 2012 , 41, 191-193	1.7	8
71	Electron spin resonance of thin films of organic light-emitting material tris(8-hydroxyquinoline) aluminum doped by magnesium. <i>Synthetic Metals</i> , 2012 , 162, 2451-2454	3.6	16
70	Molecular Arrangements of Regioregular and Regiorandom Poly(3-hexylthiophene): Molecular Dynamics Simulations. <i>Transactions of the Materials Research Society of Japan</i> , 2012 , 37, 311-314	0.2	1
69	Tight-Binding Study of Polarons in Two-Dimensional Systems: Implications for Organic Field-Effect Transistor Materials. <i>Journal of the Physical Society of Japan</i> , 2011 , 80, 034702	1.5	6
68	Electron Spin Resonance Study of Interface Trap States and Charge Carrier Concentration in Rubrene Single-Crystal Field-Effect Transistors. <i>Applied Physics Express</i> , 2011 , 4, 085702	2.4	10

67	Intermolecular CH ₂ O hydrogen bonds in formyl-substituted diphenylhexatriene, a [2+2] photoreactive organic solid: Crystal structure and IR, NMR spectroscopic evidence. <i>Journal of Molecular Structure</i> , 2011 , 1006, 366-374	3.4	10
66	Direct determination of interfacial molecular orientations in field-effect devices of P3HT/PCBM composites by electron spin resonance. <i>Organic Electronics</i> , 2011 , 12, 716-723	3.5	23
65	Microscopic mechanisms behind the high mobility in rubrene single-crystal transistors as revealed by field-induced electron spin resonance. <i>Physical Review B</i> , 2011 , 83,	3.3	62
64	Observation of field-induced charge carriers in high-mobility organic transistors of a thienothiophene-based small molecule: Electron spin resonance measurements. <i>Physical Review B</i> , 2011 , 84,	3.3	24
63	Strong Electron Correlation in the High-Temperature Phase of (EDO-TTF)2PF6 as a Quasi-One-Dimensional Molecular Conductor. <i>Journal of the Physical Society of Japan</i> , 2010 , 79, 103705	1.5	4
62	Nickel(II) complexes bearing a pincer ligand containing thioamide units: Comparison between SNS- and SCS-pincer ligands. <i>Inorganica Chimica Acta</i> , 2010 , 363, 2474-2480	2.7	35
61	Charge ordering in EDO-TTF salts and their optical spectra: toward the first-principles understanding of photoinduced phase transition. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2009 , 6, 120-123		3
60	Highly fluorescent oligomers with donor and acceptor groups: DFT calculations and experiments. <i>Synthetic Metals</i> , 2009 , 159, 2211-2214	3.6	3
59	DFT calculations for the high-temperature structure of (EDO-TTF)2PF6: Identification of an electronic molecular dimer. <i>Journal of Physics: Conference Series</i> , 2009 , 148, 012010	0.3	2
58	Photophysical properties of oligophenylene ethynyls modified by donor and/or acceptor groups. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 5074-84	2.8	19
57	Spectral evidence and DFT calculations on the formation of Bis(2,2'Biipyridine)platinum(II)-N-base adducts. <i>Inorganic Chemistry</i> , 2008 , 47, 3477-9	5.1	7
56	Large electric-potential bias in an EDO-TTF tetramer as a major mechanism of charge ordering observed in its PF6 salt: A density functional theory study. <i>Physical Review B</i> , 2008 , 77,	3.3	20
55	Optical selection rule for the lower Davydov excitons in co-oligomer single crystals. <i>Physical Review B</i> , 2008 , 77,	3.3	42
54	Electron-nuclear double-resonance observation of spatial extent of polarons in polythiophene and poly(3-alkylthiophene). <i>Chemical Physics Letters</i> , 2007 , 435, 273-277	2.5	22
53	Density Functional Theory of Chlorine-Bridged Platinum Complexes: Monomer, Chain, and Two-Leg Ladders. <i>Journal of the Physical Society of Japan</i> , 2007 , 76, 063708	1.5	16
52	Surface potential switching by metal ion complexation/decomplexation using bipyridinethiolate monolayers on gold. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 9195-203	3.4	13
51	Optical and electronic control of spin-alignment in molecular magnets. <i>Synthetic Metals</i> , 2005 , 152, 469-472	3.2	3
50	Electron Spin Resonance of Field-Induced Polarons in Regioregular Poly(3-alkylthiophene) Using Metal Insulator Semiconductor Diode Structures. <i>Journal of the Physical Society of Japan</i> , 2005 , 74, 3066-3076	1.5	67

49	Theory of photoinduced high-spin states in organic molecules. <i>Physical Review B</i> , 2005 , 72,	3.3	7
48	Charge-induced spin alignment in diradical donor molecules: numerical calculations of correlated many-electron-spin systems. <i>Journal of Chemical Physics</i> , 2005 , 122, 244324	3.9	1
47	Theoretical study on novel electronic properties in nanographite materials. <i>Journal of Physics and Chemistry of Solids</i> , 2004 , 65, 123-126	3.9	7
46	Novel electronic states in graphene ribbons—competing spin and charge orders. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2004 , 22, 688-691	3	22
45	A density functional study of backbone structures of polydiacetylene: destabilization of butatriene structure. <i>Chemical Physics</i> , 2004 , 306, 191-200	2.3	7
44	Theoretical study of spin-alignment control in molecular magnets. <i>Current Applied Physics</i> , 2004 , 4, 539-548	2.4	4
43	Magnetic and charge orders in zigzag nanographene ribbons. <i>Current Applied Physics</i> , 2004 , 4, 587-590	2.6	2
42	Theory on carrier dynamics in branching conjugated molecular wires. <i>Current Applied Physics</i> , 2004 , 4, 570-572	2.6	
41	Stability of the staging structure of charge-transfer complexes showing a neutral-ionic transition. <i>Physical Review B</i> , 2004 , 70,	3.3	9
40	Theory of Doping Induced High-Spin in a Model of Polyene-based Molecular Magnets. <i>Journal of the Physical Society of Japan</i> , 2004 , 73, 3149-3157	1.5	2
39	Spin- and charge-polarized states in nanographene ribbons with zigzag edges. <i>Physical Review B</i> , 2003 , 68,	3.3	130
38	Theory of spin alignment in π -conjugated molecular magnets. <i>Synthetic Metals</i> , 2003 , 137, 1255-1256	3.6	6
37	Electronic control of spin alignment in π -conjugated molecular magnets. <i>Physical Review Letters</i> , 2003 , 90, 207203	7.4	15
36	ESR Observation of Optically-Generated Polarons in Conjugated Electroluminescent Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 2001 , 371, 159-162		4
35	A THEORETICAL STUDY OF BISTABILITY OF POLYDIACETYLENE: TCDU(poly(5,7-dodecadiyne-1,12-diyl-bis-phenylurethane). <i>International Journal of Modern Physics B</i> , 2001 , 15, 3821-3824	1.1	
34	Crucial effects of intramolecular charge distribution on the neutral-ionic transition of tetrathiafulvalene π -chloranil. <i>Physical Review B</i> , 2001 , 64,	3.3	15
33	Highly doped nondegenerate conjugated polymers— theory using the DMRG method. <i>Synthetic Metals</i> , 2001 , 119, 213-214	3.6	6
32	A tight-binding model of phenylene molecules with meta-connections— implications for phenylacetylene dendrimers. <i>Chemical Physics</i> , 1999 , 250, 13-22	2.3	9

31	Polarons and bipolarons in conjugated polymers: a density matrix renormalization group study. <i>Synthetic Metals</i> , 1999 , 101, 395-396	3.6	2
30	Flat-band ferromagnetism induced by off-site repulsions. <i>Physical Review B</i> , 1998 , 57, 10609-10612	3.3	8
29	Theory on Photoinduced Absorption from Singlet Excited States in Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 1998 , 314, 77-82		
28	Polaron versus Bipolaron in Conducting Polymers: a Density Matrix Renormalization Group Study. <i>Journal of the Physical Society of Japan</i> , 1998 , 67, 1521-1524	1.5	19
27	Electron-Nuclear Double-Resonance Spectra of Polarons in Poly(Paraphenylene Vinylene). <i>Journal of the Physical Society of Japan</i> , 1998 , 67, 3936-3944	1.5	11
26	Theory on electroabsorption in poly(p-phenylene vinylene). <i>Synthetic Metals</i> , 1997 , 91, 363-365	3.6	5
25	Electron Spin Resonance Spectra of Photogenerated Polarons in Poly(Paraphenylene Vinylene). <i>Journal of the Physical Society of Japan</i> , 1996 , 65, 3743-3746	1.5	16
24	Electronic and optical properties of neutral and charged poly (p-phenylene vinylene). <i>Synthetic Metals</i> , 1996 , 78, 219-226	3.6	48
23	EXACT RESULTS IN STRONGLY CORRELATED ELECTRONS SPIN-REFLECTION POSITIVITY AND THE PERRON-FROBENIUS THEOREM. <i>International Journal of Modern Physics B</i> , 1996 , 10, 3383-3450	1.1	31
22	Exciton Effects and Nonlinear Optical Response in Soliton Lattice States of Doped Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 1996 , 283, 271-276		2
21	Polarons and their ENDOR spectra in poly(p-phenylene vinylene). <i>Solid State Communications</i> , 1995 , 95, 137-141	1.6	38
20	Superconducting phase of a two-chain Hubbard model. <i>Physical Review B</i> , 1995 , 52, R3860-R3863	3.3	30
19	Ground state of the Kondo-Hubbard model at half filling. <i>Physical Review Letters</i> , 1995 , 74, 4939-4942	7.4	29
18	Theory of Optical Absorption in Doped Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 1995 , 267, 329-334		16
17	Superconductivity due to the two-band mechanism in the two-chain and two-dimensional hubbard models. <i>Synthetic Metals</i> , 1995 , 70, 1017-1018	3.6	3
16	Coulomb effects on bipolarons and polarons in non-degenerate conjugated polymers. <i>Synthetic Metals</i> , 1995 , 69, 687-688	3.6	7
15	Competition between polarons and bipolarons in nondegenerate conjugated polymers. <i>Physical Review B</i> , 1994 , 50, 14781-14784	3.3	63
14	Theory of triplet exciton polarons and photoinduced absorption in conjugated polymers. <i>Physical Review B</i> , 1994 , 49, 14113-14121	3.3	35

13	Two-band mechanism of superconductivity in dimeric hubbard models. <i>Journal of Superconductivity and Novel Magnetism</i> , 1994 , 7, 589-591		3
12	Itinerant ferromagnetism of the multiband Hubbard model. <i>Physica B: Condensed Matter</i> , 1994 , 194-196, 329-330	2.8	
11	Two-band mechanism of superconductivity in the two-dimensional Hubbard model. <i>Physica B: Condensed Matter</i> , 1994 , 194-196, 1399-1400	2.8	3
10	Superconducting transition of the two-chain Hubbard model indicated by diagonalization calculations. <i>Physica C: Superconductivity and Its Applications</i> , 1994 , 222, 349-360	1.3	61
9	Exact diagonalization study of the two-dimensional Hubbard model [Superconductivity due to the two-band mechanism] <i>Physica C: Superconductivity and Its Applications</i> , 1994 , 235-240, 2211-2212	1.3	
8	Lattice relaxation of photoexcited states in conjugated polymers. <i>Journal of Luminescence</i> , 1994 , 58, 134-137	3.8	1
7	Itinerant ferromagnetism in strongly correlated electron systems. <i>Physical Review B</i> , 1993 , 48, 6104-6110	0.3	12
6	A 5 kDa protein (SCS23) from the 30 S subunit of the spinach chloroplast ribosome. <i>FEBS Letters</i> , 1993 , 319, 115-8	3.8	6
5	Superconducting State of the Two-Chain Hubbard Model Indicated by the Diagonalization Calculation 1993 , 41-44		2
4	Coulomb repulsion dependences of SDW solitons and polarons in the one dimensional Hubbard model [Lifting of degeneracies in solitons and polarons in the strong correlation regime] <i>Solid State Communications</i> , 1992 , 82, 407-411	1.6	8
3	Solitonic Generation of Valence Alternation Pairs in As ₂ S ₃ . <i>Journal of the Physical Society of Japan</i> , 1990 , 59, 2790-2803	1.5	1
2	Degeneracy in the Crystal Structure of As ₂ S ₃ . <i>Journal of the Physical Society of Japan</i> , 1990 , 59, 1264-1276	1.5	3
1	Vector charge density wave model of metallic Te and Se. <i>Journal of Non-Crystalline Solids</i> , 1990 , 117-118, 332-335	3.9	