

# Yukihiro Shimoi

## List of Publications by Citations

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102  
papers

1,473  
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22  
h-index

34  
g-index

105  
ext. papers

1,577  
ext. citations

3.1  
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4.41  
L-index

#	Paper	IF	Citations
102	Spin- and charge-polarized states in nanographene ribbons with zigzag edges. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	130
101	Enhanced Layered-Herringbone Packing due to Long Alkyl Chain Substitution in Solution-Processable Organic Semiconductors. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 1245-1254	9.6	80
100	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> , <b>2005</b> , 74, 3066-3076	1.5	67
99	Competition between polarons and bipolarons in nondegenerate conjugated polymers. <i>Physical Review B</i> , <b>1994</b> , 50, 14781-14784	3.3	63
98	Microscopic mechanisms behind the high mobility in rubrene single-crystal transistors as revealed by field-induced electron spin resonance. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	62
97	Superconducting transition of the two-chain Hubbard model indicated by diagonalization calculations. <i>Physica C: Superconductivity and Its Applications</i> , <b>1994</b> , 222, 349-360	1.3	61
96	Electronic and optical properties of neutral and charged poly (p-phenylene vinylene ). <i>Synthetic Metals</i> , <b>1996</b> , 78, 219-226	3.6	48
95	Optical selection rule for the lower Davydov excitons in co-oligomer single crystals. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	42
94	Thermoelectric properties of a semicrystalline polymer doped beyond the insulator-to-metal transition by electrolyte gating. <i>Science Advances</i> , <b>2020</b> , 6, eaay8065	14.3	40
93	Polarons and their ENDOR spectra in poly(p-phenylene vinylene). <i>Solid State Communications</i> , <b>1995</b> , 95, 137-141	1.6	38
92	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> , <b>2019</b> , 24,	4.8	38
91	Nickel(II) complexes bearing a pincer ligand containing thioamide units: Comparison between SNS- and SCS-pincer ligands. <i>Inorganica Chimica Acta</i> , <b>2010</b> , 363, 2474-2480	2.7	35
90	Theory of triplet exciton polarons and photoinduced absorption in conjugated polymers. <i>Physical Review B</i> , <b>1994</b> , 49, 14113-14121	3.3	35
89	EXACT RESULTS IN STRONGLY CORRELATED ELECTRONS: SPIN-REFLECTION POSITIVITY AND THE PERRON-FROBENIUS THEOREM. <i>International Journal of Modern Physics B</i> , <b>1996</b> , 10, 3383-3450	1.1	31
88	Superconducting phase of a two-chain Hubbard model. <i>Physical Review B</i> , <b>1995</b> , 52, R3860-R3863	3.3	30
87	Ground state of the Kondo-Hubbard model at half filling. <i>Physical Review Letters</i> , <b>1995</b> , 74, 4939-4942	7.4	29
86	Control of molecular orientations of poly(3-hexylthiophene) on self-assembled monolayers: molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 9265-70	3.6	27

85	Investigation of the electrochromic properties of tri-block polyaniline-polythiophene-polyaniline under visible light. <i>Synthetic Metals</i> , <b>2017</b> , 226, 80-88	3.6	25
84	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> , <b>2011</b> , 84,	3.3	24
83	Direct determination of interfacial molecular orientations in field-effect devices of P3HT/PCBM composites by electron spin resonance. <i>Organic Electronics</i> , <b>2011</b> , 12, 716-723	3.5	23
82	Electron-nuclear double-resonance observation of spatial extent of polarons in polythiophene and poly(3-alkylthiophene). <i>Chemical Physics Letters</i> , <b>2007</b> , 435, 273-277	2.5	22
81	Novel electronic states in graphene ribbons—competing spin and charge orders. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2004</b> , 22, 688-691	3	22
80	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> , <b>2008</b> , 77,	3.3	20
79	Photophysical properties of oligophenylene ethynyls modified by donor and/or acceptor groups. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 5074-84	2.8	19
78	Polaron versus Bipolaron in Conducting Polymers: a Density Matrix Renormalization Group Study. <i>Journal of the Physical Society of Japan</i> , <b>1998</b> , 67, 1521-1524	1.5	19
77	Microscopic observation of efficient charge transport processes across domain boundaries in donor-acceptor-type conjugated polymers. <i>Communications Physics</i> , <b>2019</b> , 2,	5.4	17
76	Electron spin resonance of thin films of organic light-emitting material tris(8-hydroxyquinoline) aluminum doped by magnesium. <i>Synthetic Metals</i> , <b>2012</b> , 162, 2451-2454	3.6	16
75	Electron Spin Resonance Spectra of Photogenerated Polarons in Poly(Paraphenylene Vinylene). <i>Journal of the Physical Society of Japan</i> , <b>1996</b> , 65, 3743-3746	1.5	16
74	Density Functional Theory of Chlorine-Bridged Platinum Complexes: Monomer, Chain, and Two-Leg Ladders. <i>Journal of the Physical Society of Japan</i> , <b>2007</b> , 76, 063708	1.5	16
73	Theory of Optical Absorption in Doped Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , <b>1995</b> , 267, 329-334		16
72	Electronic control of spin alignment in pi-conjugated molecular magnets. <i>Physical Review Letters</i> , <b>2003</b> , 90, 207203	7.4	15
71	Crucial effects of intramolecular charge distribution on the neutral-ionic transition of tetrathiafulvalene $\beta$ -chloranil. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	15
70	Halogenated (F, Cl, Br, or I) Diphenylhexatrienes: Crystal Structures, Fluorescence Spectroscopic Properties, and Quantum Chemical Calculations. <i>Crystal Growth and Design</i> , <b>2016</b> , 16, 4060-4071	3.5	13
69	Low-temperature carrier dynamics in high-mobility organic transistors of alkylated dinaphtho-thienothiophene as investigated by electron spin resonance. <i>Applied Physics Letters</i> , <b>2014</b> , 105, 033301	3.4	13
68	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> , <b>2013</b> , 113, 083710	2.5	13

67	Surface potential switching by metal ion complexation/decomplexation using bipyridinethiolate monolayers on gold. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 9195-203	3.4	13
66	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> , <b>2013</b> , 117, 566-78	2.8	12
65	Theoretical prediction of crystal structures of rubrene. <i>Japanese Journal of Applied Physics</i> , <b>2014</b> , 53, 01AD02	1.4	12
64	Itinerant ferromagnetism in strongly correlated electron systems. <i>Physical Review B</i> , <b>1993</b> , 48, 6104-6110	3.3	12
63	Electron-Nuclear Double-Resonance Spectra of Polarons in Poly(Paraphenylene Vinylene). <i>Journal of the Physical Society of Japan</i> , <b>1998</b> , 67, 3936-3944	1.5	11
62	Electron Spin Resonance Study of Interface Trap States and Charge Carrier Concentration in Rubrene Single-Crystal Field-Effect Transistors. <i>Applied Physics Express</i> , <b>2011</b> , 4, 085702	2.4	10
61	Intermolecular CH <sub>2</sub> 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> , <b>2011</b> , 1006, 366-374	3.4	10
60	Stability of the staging structure of charge-transfer complexes showing a neutral $\pi$ - $\pi$ transition. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	9
59	A tight-binding model of phenylene molecules with meta-connections – implications for phenylacetylene dendrimers. <i>Chemical Physics</i> , <b>1999</b> , 250, 13-22	2.3	9
58	Architecting layered molecular packing in substituted benzobisbenzothiophene (BBBT) semiconductor crystals. <i>CrystEngComm</i> , <b>2020</b> , 22, 3618-3626	3.3	8
57	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> , <b>2014</b> , 607, 29-33	2.5	8
56	Electron Spin Resonance of Thin Films of N,N'-Di(1-naphthyl)-N,N'-diphenylbenzidine (NPB) Doped by Iodine Vapor. <i>Chemistry Letters</i> , <b>2012</b> , 41, 191-193	1.7	8
55	Flat-band ferromagnetism induced by off-site repulsions. <i>Physical Review B</i> , <b>1998</b> , 57, 10609-10612	3.3	8
54	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> , <b>1992</b> , 82, 407-411	1.6	8
53	Spectral evidence and DFT calculations on the formation of Bis(2,2Rbipyridine)platinum(II)-N-base adducts. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 3477-9	5.1	7
52	Theoretical study on novel electronic properties in nanographite materials. <i>Journal of Physics and Chemistry of Solids</i> , <b>2004</b> , 65, 123-126	3.9	7
51	A density functional study of backbone structures of polydiacetylene: destabilization of butatriene structure. <i>Chemical Physics</i> , <b>2004</b> , 306, 191-200	2.3	7
50	Theory of photoinduced high-spin states in organic molecules. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	7

49	Coulomb effects on bipolarons and polarons in non-degenerate conjugated polymers. <i>Synthetic Metals</i> , <b>1995</b> , 69, 687-688	3.6	7
48	Simulation Study of the Effects of Nanoporous Structures on Mechanical Properties at Polymer-Metal Interfaces. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 1161-1170	3.4	6
47	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> , <b>2011</b> , 80, 034702	1.5	6
46	Theory of spin alignment in $\pi$ -conjugated molecular magnets. <i>Synthetic Metals</i> , <b>2003</b> , 137, 1255-1256	3.6	6
45	Highly doped nondegenerate conjugated polymers – theory using the DMRG method. <i>Synthetic Metals</i> , <b>2001</b> , 119, 213-214	3.6	6
44	A 5 kDa protein (SCS23) from the 30 S subunit of the spinach chloroplast ribosome. <i>FEBS Letters</i> , <b>1993</b> , 319, 115-8	3.8	6
43	Activation of N <sub>2</sub> by isolated small tungsten clusters at room temperature. <i>Chemical Physics Letters</i> , <b>2017</b> , 667, 267-271	2.5	5
42	Highly Efficient Microscopic Charge Transport within Crystalline Domains in a Furan-Flanked Diketopyrrolopyrrole-Based Conjugated Copolymer. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2000389	15.6	5
41	Effects of pn Doping in Thiophene/Phenylene Co-oligomers Thin Films. <i>Molecular Crystals and Liquid Crystals</i> , <b>2015</b> , 620, 153-158	0.5	5
40	Theory on electroabsorption in poly(p-phenylene vinylene). <i>Synthetic Metals</i> , <b>1997</b> , 91, 363-365	3.6	5
39	Photo-Fries rearrangement of phenyl salicylate studied by two-dimensional infrared spectroscopy. <i>Vibrational Spectroscopy</i> , <b>2015</b> , 81, 131-135	2.1	4
38	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> , <b>2013</b> , 52, 05DB07	1.4	4
37	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> , <b>2010</b> , 79, 103705	1.5	4
36	Theoretical study of spin-alignment control in molecular magnets. <i>Current Applied Physics</i> , <b>2004</b> , 4, 539-542	3.4	4
35	ESR Observation of Optically-Generated Polarons in Conjugated Electroluminescent Polymers. <i>Molecular Crystals and Liquid Crystals</i> , <b>2001</b> , 371, 159-162		4
34	Structures and Fluorescence Properties for the Crystals, Powders, and Thin Films of Dithienylhexatrienes: Effects of Positional Isomerism. <i>Crystal Growth and Design</i> , <b>2018</b> , 18, 6477-6487	3.5	4
33	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> , <b>2009</b> , 6, 120-123		3
32	Highly fluorescent oligomers with donor and acceptor groups: DFT calculations and experiments. <i>Synthetic Metals</i> , <b>2009</b> , 159, 2211-2214	3.6	3

31	Optical and electronic control of spin-alignment in molecular magnets. <i>Synthetic Metals</i> , <b>2005</b> , 152, 469-472	3
30	Superconductivity due to the two-band mechanism in the two-chain and two-dimensional hubbard models. <i>Synthetic Metals</i> , <b>1995</b> , 70, 1017-1018	3.6 3
29	Two-band mechanism of superconductivity in dimeric hubbard models. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>1994</b> , 7, 589-591	3
28	Two-band mechanism of superconductivity in the two-dimensional Hubbard model. <i>Physica B: Condensed Matter</i> , <b>1994</b> , 194-196, 1399-1400	2.8 3
27	Degeneracy in the Crystal Structure of As <sub>2</sub> S <sub>3</sub> . <i>Journal of the Physical Society of Japan</i> , <b>1990</b> , 59, 1264-1276	3
26	Structure dependency of the reactivity of aromatic hydrocarbons involving the formation of oxygenated polycyclic aromatic hydrocarbons (OPAHs). <i>Chemical Physics Letters</i> , <b>2020</b> , 754, 137652	2.5 2
25	Vibrational entropy as an indicator of temperature coefficient of redox potential in conjugated polymers. <i>Japanese Journal of Applied Physics</i> , <b>2019</b> , 58, 097004	1.4 2
24	Characterization of P3HT:PCBM Thin Film Interfaces by Doubly Resonant Sum-Frequency Generation Spectroscopy. <i>Molecular Crystals and Liquid Crystals</i> , <b>2014</b> , 597, 33-36	0.5 2
23	DFT calculations for the high-temperature structure of (EDO-TTF)2PF6: Identification of an electronic molecular dimer. <i>Journal of Physics: Conference Series</i> , <b>2009</b> , 148, 012010	0.3 2
22	Magnetic and charge orders in zigzag nanographene ribbons. <i>Current Applied Physics</i> , <b>2004</b> , 4, 587-590	2.6 2
21	Theory of Doping Induced High-Spin in a Model of Polyene-based Molecular Magnets. <i>Journal of the Physical Society of Japan</i> , <b>2004</b> , 73, 3149-3157	1.5 2
20	Polarons and bipolarons in conjugated polymers: a density matrix renormalization group study. <i>Synthetic Metals</i> , <b>1999</b> , 101, 395-396	3.6 2
19	Exciton Effects and Nonlinear Optical Response in Soliton Lattice States of Doped Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , <b>1996</b> , 283, 271-276	2
18	Superconducting State of the Two-Chain Hubbard Model Indicated by the Diagonalization Calculation <b>1993</b> , 41-44	2
17	Spatial extent of wave functions of charge carriers in a thienothiophene-based high-mobility molecular semiconductor. <i>Applied Physics Express</i> , <b>2020</b> , 13, 041004	2.4 1
16	Preferable Molecular Orientation of Poly(3-hexylthiophene) on Self-Assembled Monolayers: Molecular Dynamics Simulation. <i>Molecular Crystals and Liquid Crystals</i> , <b>2013</b> , 578, 33-36	0.5 1
15	Molecular Arrangements of Regioregular and Regiorandom Poly(3-hexylthiophene): Molecular Dynamics Simulations. <i>Transactions of the Materials Research Society of Japan</i> , <b>2012</b> , 37, 311-314	0.2 1
14	Charge-induced spin alignment in diradical donor molecules: numerical calculations of correlated many-electron-spin systems. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 244324	3.9 1

13	Lattice relaxation of photoexcited states in conjugated polymers. <i>Journal of Luminescence</i> , <b>1994</b> , 58, 134-137	3.8	1
12	Solitonic Generation of Valence Alternation Pairs in As <sub>2</sub> S <sub>3</sub> . <i>Journal of the Physical Society of Japan</i> , <b>1990</b> , 59, 2790-2803	1.5	1
11	Crystal Structures and Fluorescence Spectroscopic Properties of a Series of $\pi$ -Di(4-pyridyl)polyenes: Effect of Aggregation-Induced Emission. <i>ChemPlusChem</i> , <b>2020</b> , 85, 1968-1980	2.8	1
10	Theoretical Study of the Mechanism for the Reaction of Trimethylaluminum with Ozone. <i>ACS Omega</i> , <b>2021</b> , 6, 26282-26292	3.9	0
9	Simulation Study of the Effects of Interfacial Bonds on Adhesion and Fracture Behavior of Epoxy Resin Layers. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 11044-11057	3.4	0
8	Spectroscopic Investigations on Degradative Processes of cis-Bis(isothiocyanato)bis(2,2'-bipyridyl-4,4'-dicarboxylato) Ruthenium(II) Anchored on Anatase TiO <sub>2</sub> Surface. <i>Molecular Crystals and Liquid Crystals</i> , <b>2015</b> , 622, 158-163	0.5	
7	Theory on carrier dynamics in branching conjugated molecular wires. <i>Current Applied Physics</i> , <b>2004</b> , 4, 570-572	2.6	
6	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> , <b>2001</b> , 15, 3821-3824	1.1	
5	Theory on Photoinduced Absorption from Singlet Excited States in Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , <b>1998</b> , 314, 77-82		
4	Itinerant ferromagnetism of the multiband Hubbard model. <i>Physica B: Condensed Matter</i> , <b>1994</b> , 194-196, 329-330	2.8	
3	Exact diagonalization study of the two-dimensional Hubbard model $\square$ Superconductivity due to the two-band mechanism $\square$ <i>Physica C: Superconductivity and Its Applications</i> , <b>1994</b> , 235-240, 2211-2212	1.3	
2	Vector charge density wave model of metallic Te and Se. <i>Journal of Non-Crystalline Solids</i> , <b>1990</b> , 117-118, 332-335	3.9	
1	Microscopic observation of efficient intergrain charge transport processes in organic transistors of semicrystalline poly(3-hexylthiophene). <i>Applied Physics Express</i> , <b>2022</b> , 15, 041004	2.4	