

Yukihiro Shimoï

List of Publications by Year in descending order

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| # | ARTICLE | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Spin- and charge-polarized states in nanographene ribbons with zigzag edges. <i>Physical Review B</i> , 2003, 68, . | 3.2 | 139 |
| 2 | Enhanced Layered-Herringbone Packing due to Long Alkyl Chain Substitution in Solution-Processable Organic Semiconductors. <i>Chemistry of Materials</i> , 2017, 29, 1245-1254. | 6.7 | 117 |
| 3 | Temperature-Dependent Evolution of Raman Spectra of Methylammonium Lead Halide Perovskites, CH ₃ NH ₃ PbX ₃ (X = I, Br). <i>Molecules</i> , 2019, 24, 626. | 3.8 | 74 |
| 4 | 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. | 1.6 | 67 |
| 5 | Competition between polarons and bipolarons in nondegenerate conjugated polymers. <i>Physical Review B</i> , 1994, 50, 14781-14784. | 3.2 | 66 |
| 6 | 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, . | 3.2 | 64 |
| 7 | Superconducting transition of the two-chain Hubbard model indicated by diagonalization calculations. <i>Physica C: Superconductivity and Its Applications</i> , 1994, 222, 349-360. | 1.2 | 63 |
| 8 | Thermoelectric properties of a semicrystalline polymer doped beyond the insulator-to-metal transition by electrolyte gating. <i>Science Advances</i> , 2020, 6, eaay8065. | 10.3 | 59 |
| 9 | Electronic and optical properties of neutral and charged poly (p-phenylene vinylene). <i>Synthetic Metals</i> , 1996, 78, 219-226. | 3.9 | 49 |
| 10 | Optical selection rule for the lower Davydov excitons in co-oligomer single crystals. <i>Physical Review B</i> , 2008, 77, . | 3.2 | 44 |
| 11 | Polarons and their ENDOR spectra in poly(p-phenylene vinylene). <i>Solid State Communications</i> , 1995, 95, 137-141. | 1.9 | 39 |
| 12 | 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. | 2.4 | 38 |
| 13 | Theory of triplet exciton polarons and photoinduced absorption in conjugated polymers. <i>Physical Review B</i> , 1994, 49, 14113-14121. | 3.2 | 35 |
| 14 | 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. | 2.0 | 32 |
| 15 | Control of molecular orientations of poly(3-hexylthiophene) on self-assembled monolayers: molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9265. | 2.8 | 32 |
| 16 | Ground State of the Kondo-Hubbard Model at Half Filling. <i>Physical Review Letters</i> , 1995, 74, 4939-4942. | 7.8 | 31 |
| 17 | Superconducting phase of a two-chain Hubbard model. <i>Physical Review B</i> , 1995, 52, R3860-R3863. | 3.2 | 30 |
| 18 | Investigation of the electrochromic properties of tri-block polyaniline-polythiophene-polyaniline under visible light. <i>Synthetic Metals</i> , 2017, 226, 80-88. | 3.9 | 29 |

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|----|--|-----|-----------|
| 19 | 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. | 2.6 | 25 |
| 20 | 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, . | 3.2 | 25 |
| 21 | 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. | 2.6 | 24 |
| 22 | Microscopic observation of efficient charge transport processes across domain boundaries in donor-acceptor-type conjugated polymers. <i>Communications Physics</i> , 2019, 2, . | 5.3 | 24 |
| 23 | Novel electronic states in graphene ribbonsâ€”competing spin and charge orders. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2004, 22, 688-691. | 2.7 | 23 |
| 24 | Photophysical Properties of Oligophenylene Ethynyls Modified by Donor and/or Acceptor Groups. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5074-5084. | 2.5 | 21 |
| 25 | Large electric-potential bias in an EDO-TTF tetramer as a major mechanism of charge ordering observed in its $P _{F > 6}$ salt: A density functional theory study. <i>Physical Review B</i> , 2008, 77, . | 3.2 | 21 |
| 26 | 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. | 1.6 | 20 |
| 27 | 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. | 3.9 | 18 |
| 28 | 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. | 3.0 | 18 |
| 29 | Architecting layered molecular packing in substituted benzobisbenzothiophene (BBBT) semiconductor crystals. <i>CrystEngComm</i> , 2020, 22, 3618-3626. | 2.6 | 18 |
| 30 | Theory of Optical Absorption in Doped Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 1995, 267, 329-334. | 0.3 | 16 |
| 31 | Electron Spin Resonance Spectra of Photogenerated Polarons in Poly(Paraphenylene Vinylene). <i>Journal of the Physical Society of Japan</i> , 1996, 65, 3743-3746. | 1.6 | 16 |
| 32 | Electronic Control of Spin Alignment in π -Conjugated Molecular Magnets. <i>Physical Review Letters</i> , 2003, 90, 207203. | 7.8 | 16 |
| 33 | 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. | 1.6 | 16 |
| 34 | Crucial effects of intramolecular charge distribution on the neutral-ionic transition of tetrathiafulvaleneâ€”p-chloranil. <i>Physical Review B</i> , 2001, 64, . | 3.2 | 15 |
| 35 | Theoretical prediction of crystal structures of rubrene. <i>Japanese Journal of Applied Physics</i> , 2014, 53, 01AD02. | 1.5 | 15 |
| 36 | Surface Potential Switching by Metal Ion Complexation/Decomplexation Using Bipyridinethiolate Monolayers on Gold. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9195-9203. | 2.6 | 14 |

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|----|--|------|-----------|
| 37 | 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 | 14 |
| 38 | 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, . | 3.3 | 14 |
| 39 | Fluorescence Properties of (<i>E</i> , <i>E</i> , <i>E</i>)-1,6-Di(<i>n</i> -naphthyl)-1,3,5-hexatriene (<i>n</i> = 1, 2): Effects of Internal Rotation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 566-578. | 2.5 | 13 |
| 40 | Itinerant ferromagnetism in strongly correlated electron systems. <i>Physical Review B</i> , 1993, 48, 6104-6110. | 3.2 | 12 |
| 41 | Intermolecular CH \cdots 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. | 3.6 | 12 |
| 42 | Flat-band ferromagnetism induced by off-site repulsions. <i>Physical Review B</i> , 1998, 57, 10609-10612. | 3.2 | 11 |
| 43 | Electron-Nuclear Double-Resonance Spectra of Polarons in Poly(Paraphenylene Vinylene). <i>Journal of the Physical Society of Japan</i> , 1998, 67, 3936-3944. | 1.6 | 11 |
| 44 | 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 | 11 |
| 45 | Highly Efficient Microscopic Charge Transport within Crystalline Domains in a Furan-Flanked Diketopyrrolopyrrole-Based Conjugated Copolymer. <i>Advanced Functional Materials</i> , 2020, 30, 2000389. | 14.9 | 11 |
| 46 | A 5 kDa protein (SCS23) from the 30 S subunit of the spinach chloroplast ribosome. <i>FEBS Letters</i> , 1993, 319, 115-118. | 2.8 | 10 |
| 47 | Stability of the staging structure of charge-transfer complexes showing a neutral \rightarrow ionic transition. <i>Physical Review B</i> , 2004, 70, . | 3.2 | 10 |
| 48 | 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. | 2.6 | 10 |
| 49 | A tight-binding model of phenylene molecules with meta-connections $\hat{=}$ implications for phenylacetylene dendrimers. <i>Chemical Physics</i> , 1999, 250, 13-22. | 1.9 | 9 |
| 50 | Simulation Study of the Effects of Nanoporous Structures on Mechanical Properties at Polymer $\hat{=}$ Metal Interfaces. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1161-1170. | 2.6 | 9 |
| 51 | Coulomb repulsion dependences of SDW solitons and polarons in the one dimensional Hubbard model $\hat{=}$ Lifting of degeneracies in solitons and polarons in the strong correlation regime $\hat{=}$. <i>Solid State Communications</i> , 1992, 82, 407-411. | 1.9 | 8 |
| 52 | Electron Spin Resonance of Thin Films of <i>N,N'</i> -Di(1-naphthyl)- <i>N,N'</i> -diphenylbenzidine (NPB) Doped by Iodine Vapor. <i>Chemistry Letters</i> , 2012, 41, 191-193. | 1.3 | 8 |
| 53 | Vector Charge Density Wave Model of Metallic and Trigonal Te. <i>Progress of Theoretical Physics</i> , 1992, 87, 307-329. | 2.0 | 8 |
| 54 | Coulomb effects on bipolarons and polarons in non-degenerate conjugated polymers. <i>Synthetic Metals</i> , 1995, 69, 687-688. | 3.9 | 7 |

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| 55 | Theoretical study on novel electronic properties in nanographite materials. <i>Journal of Physics and Chemistry of Solids</i> , 2004, 65, 123-126. | 4.0 | 7 |
| 56 | A density functional study of backbone structures of polydiacetylene: destabilization of butatriene structure. <i>Chemical Physics</i> , 2004, 306, 191-200. | 1.9 | 7 |
| 57 | Theory of photoinduced high-spin states in organic molecules. <i>Physical Review B</i> , 2005, 72, . | 3.2 | 7 |
| 58 | Spectral Evidence and DFT Calculations on the Formation of Bis(2,2'-bipyridine)platinum(II)-N-Base Adducts. <i>Inorganic Chemistry</i> , 2008, 47, 3477-3479. | 4.0 | 7 |
| 59 | Highly doped nondegenerate conjugated polymers – a theory using the DMRG method. <i>Synthetic Metals</i> , 2001, 119, 213-214. | 3.9 | 6 |
| 60 | Theory of spin alignment in π -conjugated molecular magnets. <i>Synthetic Metals</i> , 2003, 137, 1255-1256. | 3.9 | 6 |
| 61 | 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. | 1.6 | 6 |
| 62 | 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. | 2.6 | 6 |
| 63 | Theory on electroabsorption in poly(p-phenylene vinylene). <i>Synthetic Metals</i> , 1997, 91, 363-365. | 3.9 | 5 |
| 64 | 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. | 1.5 | 5 |
| 65 | Effects of pn Doping in Thiophene/Phenylene Co-oligomers Thin Films. <i>Molecular Crystals and Liquid Crystals</i> , 2015, 620, 153-158. | 0.9 | 5 |
| 66 | Activation of N ₂ by isolated small tungsten clusters at room temperature. <i>Chemical Physics Letters</i> , 2017, 667, 267-271. | 2.6 | 5 |
| 67 | 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. | 3.0 | 5 |
| 68 | Theoretical Study of the Mechanism for the Reaction of Trimethylaluminum with Ozone. <i>ACS Omega</i> , 2021, 6, 26282-26292. | 3.5 | 5 |
| 69 | ESR Observation of Optically-Generated Polarons in Conjugated Electroluminescent Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 2001, 371, 159-162. | 0.3 | 4 |
| 70 | Theoretical study of spin-alignment control in molecular magnets. <i>Current Applied Physics</i> , 2004, 4, 539-542. | 2.4 | 4 |
| 71 | Strong Electron Correlation in the High-Temperature Phase of (EDO-TTF) ₂ PF ₆ as a Quasi-One-Dimensional Molecular Conductor. <i>Journal of the Physical Society of Japan</i> , 2010, 79, 103705. | 1.6 | 4 |
| 72 | Photo-Fries rearrangement of phenyl salicylate studied by two-dimensional infrared spectroscopy. <i>Vibrational Spectroscopy</i> , 2015, 81, 131-135. | 2.2 | 4 |

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|----|---|-----|-----------|
| 73 | 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. | 2.6 | 4 |
| 74 | Degeneracy in the Crystal Structure of As ₂ S ₃ . <i>Journal of the Physical Society of Japan</i> , 1990, 59, 1264-1276. | 1.6 | 3 |
| 75 | Two-band mechanism of superconductivity in dimeric hubbard models. <i>Journal of Superconductivity and Novel Magnetism</i> , 1994, 7, 589-591. | 0.5 | 3 |
| 76 | Two-band mechanism of superconductivity in the two-dimensional Hubbard model. <i>Physica B: Condensed Matter</i> , 1994, 194-196, 1399-1400. | 2.7 | 3 |
| 77 | Superconductivity due to the two-band mechanism in the two-chain and two-dimensional hubbard models. <i>Synthetic Metals</i> , 1995, 70, 1017-1018. | 3.9 | 3 |
| 78 | Optical and electronic control of spin-alignment in molecular magnets. <i>Synthetic Metals</i> , 2005, 152, 469-472. | 3.9 | 3 |
| 79 | 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. | 0.8 | 3 |
| 80 | Highly fluorescent oligomers with donor and acceptor groups: DFT calculations and experiments. <i>Synthetic Metals</i> , 2009, 159, 2211-2214. | 3.9 | 3 |
| 81 | DFT calculations for the high-temperature structure of (EDO-TTF) ₂ PF ₆ : Identification of an electronic molecular dimer. <i>Journal of Physics: Conference Series</i> , 2009, 148, 012010. | 0.4 | 3 |
| 82 | 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 | 3 |
| 83 | Crystal Structures and Fluorescence Spectroscopic Properties of a Series of \hat{I}_{\pm} (4-pyridyl)polyenes: Effect of Aggregation-Induced Emission. <i>ChemPlusChem</i> , 2020, 85, 1968-1980. | 2.8 | 3 |
| 84 | Competing ferroelectric polarization: hydroxyl flip-flop versus proton-transfer mechanisms. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10099-10105. | 5.5 | 3 |
| 85 | 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. | 0.3 | 2 |
| 86 | Polarons and bipolarons in conjugated polymers: a density matrix renormalization group study. <i>Synthetic Metals</i> , 1999, 101, 395-396. | 3.9 | 2 |
| 87 | Magnetic and charge orders in zigzag nanographene ribbons. <i>Current Applied Physics</i> , 2004, 4, 587-590. | 2.4 | 2 |
| 88 | 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. | 1.6 | 2 |
| 89 | 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. | 0.9 | 2 |
| 90 | Vibrational entropy as an indicator of temperature coefficient of redox potential in conjugated polymers. <i>Japanese Journal of Applied Physics</i> , 2019, 58, 097004. | 1.5 | 2 |

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| 91 | Superconducting State of the Two-Chain Hubbard Model Indicated by the Diagonalization Calculation. , 1993, , 41-44. | | 2 |
| 92 | Solitonic Generation of Valence Alternation Pairs in As ₂ S ₃ . Journal of the Physical Society of Japan, 1990, 59, 2790-2803. | 1.6 | 1 |
| 93 | Lattice relaxation of photoexcited states in conjugated polymers. Journal of Luminescence, 1994, 58, 134-137. | 3.1 | 1 |
| 94 | Charge-induced spin alignment in diradical donor molecules: Numerical calculations of correlated many-electron-spin systems. Journal of Chemical Physics, 2005, 122, 244324. | 3.0 | 1 |
| 95 | Preferable Molecular Orientation of Poly(3-hexylthiophene) on Self-Assembled Monolayers: Molecular Dynamics Simulation. Molecular Crystals and Liquid Crystals, 2013, 578, 33-36. | 0.9 | 1 |
| 96 | Spatial extent of wave functions of charge carriers in a thienothiophene-based high-mobility molecular semiconductor. Applied Physics Express, 2020, 13, 041004. | 2.4 | 1 |
| 97 | Vector charge density wave model of metallic Te and Se. Journal of Non-Crystalline Solids, 1990, 117-118, 332-335. | 3.1 | 0 |
| 98 | Itinerant ferromagnetism of the multiband Hubbard model. Physica B: Condensed Matter, 1994, 194-196, 329-330. | 2.7 | 0 |
| 99 | Exact diagonalization study of the two-dimensional Hubbard model "superconductivity due to the two-band mechanism". Physica C: Superconductivity and Its Applications, 1994, 235-240, 2211-2212. | 1.2 | 0 |
| 100 | Theory on Photoinduced Absorption from Singlet Excited States in Conjugated Polymers. Molecular Crystals and Liquid Crystals, 1998, 314, 77-82. | 0.3 | 0 |
| 101 | A THEORETICAL STUDY OF BISTABILITY OF POLYDIACETYLENE: | | |