

# Hiroyuki Ishii

## List of Publications by Year in descending order

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75  
papers

1,221  
citations

471061

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433756

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docs citations

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times ranked

1306  
citing authors

#	ARTICLE	IF	CITATIONS
1	Photoemission Tomography of a One-Dimensional Row Structure of a Flat-Lying Picene Multilayer on Ag(110). <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1512-1518.	2.1	5
2	Nitrogen-Containing Perylene Diimides: Molecular Design, Robust Aggregated Structures, and Advances in n-Type Organic Semiconductors. <i>Accounts of Chemical Research</i> , 2022, 55, 660-672.	7.6	38
3	Mixed-Orbital Charge Transport in N-Shaped Benzene- and Pyrazine-Fused Organic Semiconductors. <i>Journal of the American Chemical Society</i> , 2022, 144, 11159-11167.	6.6	14
4	Conduction band structure of high-mobility organic semiconductors and partially dressed polaron formation. <i>Nature Materials</i> , 2022, 21, 910-916.	13.3	17
5	Role of Perfluorophenyl Group in the Side Chain of Small-Molecule n-Type Organic Semiconductors in Stress Stability of Single-Crystal Transistors. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2095-2101.	2.1	10
6	Chrysenodithiophene-Based Conjugated Polymer: An Elongated Fused $\pi$ -Electronic Backbone with a Unique Orbital Structure Toward Efficient Intermolecular Carrier Transport. <i>Macromolecules</i> , 2021, 54, 2113-2123.	2.2	2
7	Extended $\pi$ -Electron Delocalization in Quinoid-Based Conjugated Polymers Boosts Intrachain Charge Carrier Transport. <i>Chemistry of Materials</i> , 2021, 33, 8183-8193.	3.2	17
8	Gate induced modulation of electronic states in monolayer organic field-effect transistor. <i>Applied Physics Letters</i> , 2021, 119, 223301.	1.5	0
9	Approaching isotropic charge transport of n-type organic semiconductors with bulky substituents. <i>Communications Chemistry</i> , 2021, 4, .	2.0	10
10	Cooperative Aggregations of Nitrogen-Containing Perylene Diimides Driven by Rigid and Flexible Functional Groups. <i>Chemistry of Materials</i> , 2020, 32, 9115-9125.	3.2	14
11	Effect of Electronically Distinct Aromatic Substituents on the Molecular Assembly and Hole Transport of V-Shaped Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17503-17511.	1.5	1
12	Coherent Electron Transport in Air-Stable, Printed Single-Crystal Organic Semiconductor and Application to Megahertz Transistors. <i>Advanced Materials</i> , 2020, 32, e2003245.	11.1	19
13	Band-like transporting and thermally durable V-shaped organic semiconductors with a phenyl key block. <i>Journal of Materials Chemistry C</i> , 2020, 8, 14172-14179.	2.7	7
14	Alkyl-Substituted Selenium-Bridged V-Shaped Organic Semiconductors Exhibiting High Hole Mobility and Unusual Aggregation Behavior. <i>Journal of the American Chemical Society</i> , 2020, 142, 14974-14984.	6.6	25
15	Robust, high-performance n-type organic semiconductors. <i>Science Advances</i> , 2020, 6, eaaz0632.	4.7	135
16	Charge mobility calculation of organic semiconductors without use of experimental single-crystal data. <i>Scientific Reports</i> , 2020, 10, 2524.	1.6	13
17	Sub-molecular structural relaxation at a physisorbed interface with monolayer organic single-crystal semiconductors. <i>Communications Physics</i> , 2020, 3, .	2.0	10
18	Bent-Shaped <i>p</i> -Type Small-Molecule Organic Semiconductors: A Molecular Design Strategy for Next-Generation Practical Applications. <i>Journal of the American Chemical Society</i> , 2020, 142, 9083-9096.	6.6	108

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19	Second highest occupied molecular orbital effects on the valence band structure of organic semiconductors. Japanese Journal of Applied Physics, 2019, 58, S11B27.	0.8	9
20	Air-Stable Benzo[ <i>c</i> ]thiophene Diimide <i>n</i> -Type $\pi$ -Electron Core. Organic Letters, 2019, 21, 4448-4453.	2.4	23
21	Fabrication of Highly Oriented Multilayer Films of Picene and DNTT on Their Bulklike Monolayer. ACS Omega, 2019, 4, 8669-8673.	1.6	6
22	Carrier transport calculations of organic semiconductors with static and dynamic disorder. Japanese Journal of Applied Physics, 2019, 58, 110501.	0.8	6
23	Disorder and localization dynamics in polymorphs of the molecular semiconductor pentacene probed by <i>in situ</i> micro-Raman spectroscopy and molecular dynamics simulations. Physical Review Materials, 2019, 3, .	0.9	11
24	Organic Semiconductors: Zigzag-Elongated Fused $\pi$ -Electronic Core: A Molecular Design Strategy to Maximize Charge-Carrier Mobility (Adv. Sci. 1/2018). Advanced Science, 2018, 5, 1870005.	5.6	2
25	Zigzag-Elongated Fused $\pi$ -Electronic Core: A Molecular Design Strategy to Maximize Charge-Carrier Mobility. Advanced Science, 2018, 5, 1700317.	5.6	43
26	Quantitative mobility evaluation of organic semiconductors using quantum dynamics based on density functional theory. Physical Review B, 2018, 98, .	1.1	14
27	Surface Structure of Organic Semiconductor [ <i>n</i> ]Phenacene Single Crystals. Journal of the American Chemical Society, 2018, 140, 14046-14049.	6.6	5
28	End-Capping $\pi$ -Conjugated Systems with Medium-Sized Sulfur-Containing Rings: A Route Towards Solution-Processable Air-Stable Semiconductors. Chemistry - A European Journal, 2018, 24, 11503-11510.	1.7	5
29	Theory of electron transport at the atomistic level. Japanese Journal of Applied Physics, 2018, 57, 08NA01.	0.8	0
30	Oxygen- and Sulfur-Bridged L-shaped $\pi$ -Conjugated Molecules: Synthesis, Aggregated Structures, and Charge Transporting Behavior. Asian Journal of Organic Chemistry, 2018, 7, 2309-2314.	1.3	6
31	High-Performance Simulation for Quantum Charge Transport in Large Scale Materials -Application to Carbon Nanotubes and Organic Semiconductors-. ECS Meeting Abstracts, 2018, , .	0.0	0
32	High performance solution-crystallized thin-film transistors based on V-shaped thieno[3,2- <i>f</i> :4,5- <i>f'</i> ]bis[1]benzothiophene semiconductors. Journal of Materials Chemistry C, 2017, 5, 1903-1909.	2.7	22
33	Oxygen- and Sulfur-Bridged Bianthracene V-Shaped Organic Semiconductors. Bulletin of the Chemical Society of Japan, 2017, 90, 931-938.	2.0	28
34	Charge transport calculations by a wave-packet dynamical approach using maximally localized Wannier functions based on density functional theory: Application to high-mobility organic semiconductors. Physical Review B, 2017, 95, .	1.1	16
35	Boron-Stabilized Planar Neutral $\pi$ -Radicals with Well-Balanced Ambipolar Charge-Transport Properties. Journal of the American Chemical Society, 2017, 139, 14336-14339.	6.6	97
36	The emergence of charge coherence in soft molecular organic semiconductors via the suppression of thermal fluctuations. NPG Asia Materials, 2016, 8, e252-e252.	3.8	19

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37	Charge Transport Theory of Organic Semiconductors. Journal of the Institute of Electrical Engineers of Japan, 2016, 136, 434-437.	0.0	2
38	Wave Packet Dynamical Calculations for Charge Transport of Organic Semiconductors: Role of Molecular Vibrations and Trap Potentials. Molecular Crystals and Liquid Crystals, 2015, 620, 2-9.	0.4	1
39	Numerical Approach to Charge Transport Problems on Organic Molecular Crystals. Springer Series in Materials Science, 2015, , 319-347.	0.4	1
40	Correlation between thermal fluctuation effects and phase coherence factor in carrier transport of single-crystal organic semiconductors. Applied Physics Letters, 2015, 106, .	1.5	14
41	Evidence for Charge Trapping Inducing Polymorphic Structural Phase Transition in Pentacene. Advanced Materials, 2015, 27, 122-129.	11.1	22
42	Large-scale conductivity-tensor calculations for Hall effects in time-dependent wave-packet diffusion method. Physical Review B, 2014, 90, .	1.1	9
43	Electric and Thermal Transport Calculations through Interface and Applications to Thermoelectric Energy Conversion. E-Journal of Surface Science and Nanotechnology, 2014, 12, 115-118.	0.1	4
44	Atomistic Calculations of Heat Transport in a Silicon Crystal. E-Journal of Surface Science and Nanotechnology, 2014, 12, 154-156.	0.1	0
45	Thermal conductance calculations of silicon nanowires: comparison with diamond nanowires. Nanoscale Research Letters, 2013, 8, 256.	3.1	2
46	Influence of strong electron-phonon coupling and dynamic lattice disorder on the Hall effect in organic crystals. Physical Review B, 2013, 87, .	1.1	5
47	On the Phononic Bandgap of Carbon Nanotubes. Journal of Nanomaterials, 2013, 2013, 1-4.	1.5	3
48	Strong anisotropy of momentum-relaxation time induced by intermolecular vibrations of single-crystal organic semiconductors. Physical Review B, 2013, 88, .	1.1	27
49	Crossover to Quantized Thermal Conductance in Nanotubes and Nanowires. Open Journal of Composite Materials, 2013, 03, 48-54.	0.4	0
50	Wave-packet approach to transport properties of carrier coupled with intermolecular and intramolecular vibrations of organic semiconductors. Physical Review B, 2012, 85, .	1.1	48
51	Roles of intramolecular and intermolecular electron-phonon coupling on the formation and transport of large polarons in organic semiconductors. Physical Review B, 2012, 86, .	1.1	27
52	Bias drop and phonon emission in molecular wires. Applied Surface Science, 2012, 258, 2121-2123.	3.1	0
53	Hall conductivity calculations by the time-dependent wave-packet diffusion method. Physical Review B, 2011, 83, .	1.1	9
54	Effects of Vacancy Defects on Thermal Conduction of Silicon Nanowire: Nonequilibrium Green's Function Approach. Applied Physics Express, 2011, 4, 085001.	1.1	13

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55	Multi-Scale Quantum Transport Simulations from Atomistic Levels. Journal of the Vacuum Society of Japan, 2011, 54, 501-506.	0.3	0
56	Thermal Conduction Calculation of Nanowire by Non-equilibrium Green's Function. Hyomen Kagaku, 2011, 32, 410-415.	0.0	0
57	Inelastic Transport in Vibrating Disordered Carbon Nanotubes: Scattering Times and Temperature-Dependent Decoherence Effects. Physical Review Letters, 2010, 104, 116801.	2.9	55
58	Order-Nelectron transport calculations from ballistic to diffusive regimes by a time-dependent wave-packet diffusion method: Application to transport properties of carbon nanotubes. Physical Review B, 2010, 82, .	1.1	34
59	Edge-Phonon Scattering Effects on Electron Transport of Graphene Nanoribbons. Applied Physics Express, 2010, 3, 095102.	1.1	10
60	Quantum electron transport through carbon nanotubes with electron-phonon coupling. Journal of Vacuum Science & Technology B, 2009, 27, 882.	1.3	4
61	Charge transport in carbon nanotubes based materials: a Kubo's "Greenwood computational approach. Comptes Rendus Physique, 2009, 10, 283-296.	0.3	46
62	Transient Current Behavior through Molecular Bridge Systems; Effects of Intra-Molecule Current on Quantum Relaxation and Oscillation. E-Journal of Surface Science and Nanotechnology, 2009, 7, 606-616.	0.1	13
63	Contact and phonon scattering effects on quantum transport properties of carbon-nanotube field-effect transistors. Applied Surface Science, 2008, 254, 7600-7603.	3.1	6
64	Relaxation Process of Transient Current Through Nanoscale Systems; Density Matrix Calculations. E-Journal of Surface Science and Nanotechnology, 2008, 6, 213-221.	0.1	12
65	Quantum transport properties of carbon nanotube field-effect transistors with electron-phonon coupling. Physical Review B, 2007, 76, .	1.1	14
66	Time-dependent wave-packet approach to the quantum transport of carbon nanotubes with vacancies. Surface Science, 2007, 601, 5266-5269.	0.8	2
67	Electron-phonon coupling effect on quantum transport in carbon nanotubes using time-dependent wave-packet approach. Physica E: Low-Dimensional Systems and Nanostructures, 2007, 40, 249-252.	1.3	17
68	Relaxation processes of transient current in nano-contact system: effects of electrode. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 481-484.	0.8	8
69	Ab Initio Calculations of the Transport Through Single Molecules and Carbon Nanotubes. , 2007, , 429-432.		0
70	Quantum electron transport in kagomÃ©-lattice-chain systems with electric fields. Physical Review B, 2006, 73, .	1.1	11
71	Symmetry Breaking and Electron Transport in Kagome-Chain Systems. E-Journal of Surface Science and Nanotechnology, 2005, 3, 399-404.	0.1	0
72	Quantum Electron Transport in Finite-size Flat-band Kagome Lattice Systems. AIP Conference Proceedings, 2005, , .	0.3	1

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73	Flat-band exciton in two-dimensional KagomÃ© quantum wire systems. Physical Review B, 2004, 69, .	1.1	12
74	Photoemission study of the skutterudite compounds CoSb <sub>3</sub> and RhSb <sub>3</sub> . Journal of the Physical Society of Japan, 2002, 71, 2271-2275.	0.7	12
75	Time-Dependent Wave-Packet Diffusion Method for Quantum Transport Calculation: From Diffusive to Ballistic Regimes. Applied Physics Express, 0, 1, 123002.	1.1	20