

# Nobuhiko Kobayashi

## List of Publications by Year in descending order

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117  
papers

1,851  
citations

279798

23  
h-index

302126

39  
g-index

117  
all docs

117  
docs citations

117  
times ranked

1855  
citing authors

#	ARTICLE	IF	CITATIONS
1	Conduction channels at finite bias in single-atom gold contacts. Physical Review B, 1999, 60, 17064-17070.	3.2	143
2	Conductance Quantization and Magnetoresistance in Magnetic Point Contacts. Physical Review Letters, 2000, 84, 1003-1006.	7.8	116
3	First-principles study of electron transport through monatomic Al and Na wires. Physical Review B, 2000, 62, 8430-8437.	3.2	113
4	Magnetism-mediated thermoelectric performance of the Cr-doped bismuth telluride tetradymite. Materials Today Physics, 2019, 9, 100090.	6.0	112
5	Theoretical investigation on electron transport through an organic molecule: Effect of the contact structure. Journal of Chemical Physics, 2004, 121, 6485-6492.	3.0	59
6	Thermoelectric properties of a magnetic semiconductor CuFeS <sub>2</sub> . Materials Today Physics, 2017, 3, 85-92.	6.0	59
7	Conduction channels of Al wires at finite bias. Physical Review B, 2001, 64, .	3.2	58
8	Inelastic Transport in Vibrating Disordered Carbon Nanotubes: Scattering Times and Temperature-Dependent Decoherence Effects. Physical Review Letters, 2010, 104, 116801.	7.8	55
9	Wave-packet approach to transport properties of carrier coupled with intermolecular and intramolecular vibrations of organic semiconductors. Physical Review B, 2012, 85, .	3.2	48
10	Charge transport in carbon nanotubes based materials: a Kubo "Greenwood computational approach. Comptes Rendus Physique, 2009, 10, 283-296.	0.9	46
11	Ab initio calculations for quantum transport through atomic bridges by the recursion transfer-matrix method. Physical Review B, 2004, 69, 041407.	3.2	44
12	Quasifree Neutron Knockout Reaction Reveals a Small $s$ -Orbital Component in the Borromean Nucleus	7.8	42
13	Resonance in $B$ $\rightarrow$ $Li$ $\beta$ -Decay	7.8	41
14	Transmission channels through Na and Al atom wire. Surface Science, 1999, 433-435, 854-857.	1.9	39
15	Surface Localization of the Dineutron in $Li$ $\beta$ -Decay	7.8	36
16	Conductance through Atoms: Dot or Channel?. Japanese Journal of Applied Physics, 1999, 38, 336-338.	1.5	35
17	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, .	3.2	34
18	First-principles calculations of Seebeck coefficients in a magnetic semiconductor CuFeS <sub>2</sub> . Applied Physics Letters, 2017, 110, .	3.3	34

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19	Theory of Quantum Conductance of Atomic and Molecular Bridges. Journal of the Physical Society of Japan, 2005, 74, 1079-1092.	1.6	32
20	Roles of intramolecular and intermolecular electron-phonon coupling on the formation and transport of large polarons in organic semiconductors. Physical Review B, 2012, 86, .	3.2	27
21	Strong anisotropy of momentum-relaxation time induced by intermolecular vibrations of single-crystal organic semiconductors. Physical Review B, 2013, 88, .	3.2	27
22	Effective Insulating Properties of Autooxidized Monolayers Using Organic Ditellurides. Journal of the American Chemical Society, 2002, 124, 12642-12643.	13.7	25
23	Theoretical investigation of contact effects in conductance of single organic molecule. Thin Solid Films, 2003, 438-439, 221-224.	1.8	23
24	Alkyl Chain Conformation and the Electronic Structure of Octyl Heavy Chalcogenolate Monolayers Adsorbed on Au(111). Langmuir, 2005, 21, 5026-5033.	3.5	23
25	Anisotropic Free-Electron-Like Dispersions and Standing Waves Realized in Self-Assembled Monolayers of Glycine on Cu(100). Journal of the American Chemical Society, 2007, 129, 740-741.	13.7	23
26	Operando Direct Observation of Charge Accumulation and the Correlation with Performance Deterioration in PTB7 Polymer Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 26434-26442.	8.0	23
27	Quantum Transport Calculations for Nanosystems. , 0, , .		23
28	Adsorption States of Dialkyl Ditelluride Autooxidized Monolayers on Au(111). Langmuir, 2005, 21, 3344-3353.	3.5	22
29	Numerical Method for Local Density of States and Current Density Decomposed into Eigenchannels in Multichannel System. Japanese Journal of Applied Physics, 1999, 38, 3805-3808.	1.5	21
30	Time-Dependent Wave-Packet Diffusion Method for Quantum Transport Calculation: From Diffusive to Ballistic Regimes. Applied Physics Express, 0, 1, 123002.	2.4	20
31	High-field ESR study of kagome-like substance $\text{Cu}_3\text{V}_2\text{O}_7(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ . Physica B: Condensed Matter, 2001, 294-295, 75-78.	2.7	19
32	The emergence of charge coherence in soft molecular organic semiconductors via the suppression of thermal fluctuations. NPG Asia Materials, 2016, 8, e252-e252.	7.9	19
33	Theoretical Study of Current and Barrier Height between Aluminum Tip and Silicon Surface in Scanning Tunneling Microscopy. Japanese Journal of Applied Physics, 1996, 35, 3710-3713.	1.5	18
34	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.	2.7	17
35	First-principles calculations of thermoelectric properties of TiN/MgO superlattices: The route for an enhancement of thermoelectric effects in artificial nanostructures. Journal of Applied Physics, 2016, 119, .	2.5	16
36	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, .	3.2	16

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37	Physics of artificial nano-structures on surfaces. Progress in Surface Science, 2000, 64, 139-155.	8.3	14
38	Quantum transport properties of carbon nanotube field-effect transistors with electron-phonon coupling. Physical Review B, 2007, 76, .	3.2	14
39	Correlation between thermal fluctuation effects and phase coherence factor in carrier transport of single-crystal organic semiconductors. Applied Physics Letters, 2015, 106, .	3.3	14
40	Quantitative mobility evaluation of organic semiconductors using quantum dynamics based on density functional theory. Physical Review B, 2018, 98, .	3.2	14
41	Effects of Vacancy Defects on Thermal Conduction of Silicon Nanowire: Nonequilibrium Green's Function Approach. Applied Physics Express, 2011, 4, 085001.	2.4	13
42	Integrin $\alpha 7$ and Extracellular Matrix Laminin 211 Interaction Promotes Proliferation of Acute Myeloid Leukemia Cells and Is Associated with Granulocytic Sarcoma. Cancers, 2020, 12, 363.	3.7	13
43	Charge mobility calculation of organic semiconductors without use of experimental single-crystal data. Scientific Reports, 2020, 10, 2524.	3.3	13
44	First-principles study of Na atom transfer induced by the tip of a STM. Surface Science, 1996, 348, 299-304.	1.9	12
45	Calculation of Single-Particle Strength around the Doubly Magic Nucleus $^{132}\text{Sn}$ and the Position of the $\alpha$ -Particle	7.8	12
46	Structural stability and electronic states of gold nanowires. Surface Science, 2001, 482-485, 1266-1271.	1.9	11
47	Structural phase transitions at clean and metal-covered Si(111) surfaces investigated by RHEED spot analysis. Phase Transitions, 1995, 53, 87-114.	1.3	10
48	Theoretical Study of Silicon Adatom Transfer from the Silicon Surface in Scanning Tunneling Microscopy. Japanese Journal of Applied Physics, 1997, 36, 3791-3795.	1.5	10
49	Edge-Phonon Scattering Effects on Electron Transport of Graphene Nanoribbons. Applied Physics Express, 2010, 3, 095102.	2.4	10
50	Sub-molecular structural relaxation at a physisorbed interface with monolayer organic single-crystal semiconductors. Communications Physics, 2020, 3, .	5.3	10
51	Hall conductivity calculations by the time-dependent wave-packet diffusion method. Physical Review B, 2011, 83, .	3.2	9
52	Large-scale conductivity-tensor calculations for Hall effects in time-dependent wave-packet diffusion method. Physical Review B, 2014, 90, .	3.2	9
53	Confinement of the Pt(111) Surface State in Graphene Nanoislands. Journal of Physical Chemistry C, 2016, 120, 345-349.	3.1	9
54	Second highest occupied molecular orbital effects on the valence band structure of organic semiconductors. Japanese Journal of Applied Physics, 2019, 58, S11B27.	1.5	9

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55	First-Principles Calculations of Quantum Transport in Single Molecule. Japanese Journal of Applied Physics, 2006, 45, 2151-2153.	1.5	8
56	Effect of the quantum domain wall on conductance quantization and magnetoresistance in magnetic point contacts. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2001, 84, 107-113.	3.5	7
57	Quantum transport properties of zigzag graphene nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 711-713.	2.7	7
58	First-Principles Study of TiN/MgO Interfaces. E-Journal of Surface Science and Nanotechnology, 2014, 12, 230-237.	0.4	7
59	Theory of electron transmission through atom bridges. Progress in Surface Science, 1998, 59, 245-254.	8.3	6
60	Contact and phonon scattering effects on quantum transport properties of carbon-nanotube field-effect transistors. Applied Surface Science, 2008, 254, 7600-7603.	6.1	6
61	Efficient Ab-Initio Electron Transport Calculations for Heterostructures by the Nonequilibrium Green's Function Method. Journal of Nanomaterials, 2014, 2014, 1-5.	2.7	6
62	Enhancement of Thermoelectric Properties in Surface Nanostructures. Journal of Electronic Materials, 2017, 46, 5593-5598.	2.2	6
63	Carrier transport calculations of organic semiconductors with static and dynamic disorder. Japanese Journal of Applied Physics, 2019, 58, 110501.	1.5	6
64	First-principles calculations of contact effect on quantum transport in carbon nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 29, 551-554.	2.7	5
65	Effect of crystalline electrodes on the transport properties of Al monatomic wires at finite biases. Physical Review B, 2005, 72, .	3.2	5
66	Influence of strong electron-phonon coupling and dynamic lattice disorder on the Hall effect in organic crystals. Physical Review B, 2013, 87, .	3.2	5
67	Surface Structure of Organic Semiconductor [ <i>n</i> ]Phenacene Single Crystals. Journal of the American Chemical Society, 2018, 140, 14046-14049.	13.7	5
68	First-principles calculation of field emission from adsorbed atom on metallic electrode. Applied Surface Science, 2004, 237, 572-575.	6.1	4
69	Ab initio RTM/NEGF study on electron transport through single molecules. Physica E: Low-Dimensional Systems and Nanostructures, 2007, 40, 237-240.	2.7	4
70	Quantum electron transport through carbon nanotubes with electron-phonon coupling. Journal of Vacuum Science & Technology B, 2009, 27, 882.	1.3	4
71	Electric and Thermal Transport Calculations through Interface and Applications to Thermoelectric Energy Conversion. E-Journal of Surface Science and Nanotechnology, 2014, 12, 115-118.	0.4	4
72	Ab initio calculation of contact effects on electron transport through single molecules by the RTM/NEGF method. Journal of Physics: Conference Series, 2006, 38, 65-68.	0.4	3

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73	Effects of atomic-scale contacts on transport properties through single molecules – ab initio study. <i>Surface Science</i> , 2007, 601, 4113-4116.	1.9	3
74	First-principles study of electron transport in Si atom wires under finite bias voltage. <i>Applied Surface Science</i> , 2012, 258, 1985-1990.	6.1	3
75	On the Phononic Bandgap of Carbon Nanotubes. <i>Journal of Nanomaterials</i> , 2013, 2013, 1-4.	2.7	3
76	Electronic band structure of TiN/MgO nanostructures. <i>Japanese Journal of Applied Physics</i> , 2017, 56, 04CK06.	1.5	3
77	Seebeck coefficients in CuFeS <sub>2</sub> thin films by first-principles calculations. <i>Japanese Journal of Applied Physics</i> , 2019, 58, S1B01.	1.5	3
78	SAKE: first-principles electron transport calculation code. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 325901.	1.8	3
79	Time-dependent wave-packet approach to the quantum transport of carbon nanotubes with vacancies. <i>Surface Science</i> , 2007, 601, 5266-5269.	1.9	2
80	The Edge Current on Zigzag Graphene Nanoribbons. <i>Japanese Journal of Applied Physics</i> , 2010, 49, 08LB04.	1.5	2
81	Thermal conductance calculations of silicon nanowires: comparison with diamond nanowires. <i>Nanoscale Research Letters</i> , 2013, 8, 256.	5.7	2
82	Electronic Band Structure of Various TiN/MgO Superlattices. , 2015, , .		2
83	Computational Study on Atomic Structures, Electronic Properties, and Chemical Reactions at Surfaces and Interfaces and in Biomaterials. <i>Journal of the Physical Society of Japan</i> , 2018, 87, 061013.	1.6	2
84	Ab initio calculations of quantum transport through Al atomic wire mixed with various atoms. <i>Thin Solid Films</i> , 2004, 464-465, 255-259.	1.8	1
85	Theory for electron hopping through nanometer-scale contacts: From tunneling regime to ballistic regime. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2005, 29, 515-519.	2.7	1
86	Ï€ Channel Effects in Transport Properties of Al Nanowires at Finite Biases. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 6317-6320.	1.5	1
87	Theoretical bases of nano-scale devices. , 0, , .		1
88	First-Principles Study of Atomic-Scale Contact Effects on the Anomalous Electric Transport Through Molecules. <i>Journal of Physics: Conference Series</i> , 2007, 61, 420-424.	0.4	1
89	Length dependence of effect of electrode contact on transport properties of semiconducting carbon nanotubes. <i>Surface Science</i> , 2007, 601, 4131-4133.	1.9	1
90	Wave Packet Dynamical Calculations for Charge Transport of Organic Semiconductors: Role of Molecular Vibrations and Trap Potentials. <i>Molecular Crystals and Liquid Crystals</i> , 2015, 620, 2-9.	0.9	1

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91	Electronic band structure of TiN/MgO-4 Å– 4 and 5 Å– 5 nanostructures. Japanese Journal of Applied Physics, 2019, 58, SBBH06.	1.5	1
92	Electronic and lattice properties of nanostructured TiN/MgO and ScN/MgO superlattices. Japanese Journal of Applied Physics, 2021, 60, SE1006.	1.5	1
93	Theoretical Studies on Surface Electronics States. Atom Manipulation and Atomic Contact.. Hyomen Kagaku, 1998, 19, 161-166.	0.0	1
94	First principles study of Fe <sub>2</sub> Al and Fe <sub>2</sub> Al/Si thin films and their magnetic properties. Japanese Journal of Applied Physics, 0, , .	1.5	1
95	Two-dimensional angular correlation study of delocalized positronium in alkali halides. Journal of Physics Condensed Matter, 1997, 9, 11239-11246.	1.8	0
96	Ab initio calculations of transport properties of atomic bridges by the recursion-transfer-matrix method. Superlattices and Microstructures, 2003, 34, 443-449.	3.1	0
97	First-principles calculation of spin transport in magnetic nanowire using Green's function method with localized basis set. Journal of Physics: Conference Series, 2006, 38, 95-98.	0.4	0
98	Effects of Electrode Contact on Transport Properties of Carbon Nanotubes. , 0, , .		0
99	Effects of Electrode Contact on Transport Properties of Carbon Nanotubes. , 2006, , .		0
100	Ab initio Calculation of Electron Transport Through Single Molecules by the RTM/NEGF Method. Materials Research Society Symposia Proceedings, 2006, 938, 1.	0.1	0
101	CONTACT EFFECTS ON TRANSPORT PROPERTIES OF SEMICONDUCTING CARBON NANOTUBES CONNECTED TO METALLIC ELECTRODES. Surface Review and Letters, 2006, 13, 309-311.	1.1	0
102	NONLINEAR BEHAVIOR OF QUANTUM TRANSPORT THROUGH NANOCONTACTS – AB INITIO CALCULATION STUDY. Surface Review and Letters, 2006, 13, 179-183.	1.1	0
103	Effects of contacts to electrodes and phonon scattering on transport of carbon-nanotube devices. Journal of Physics: Conference Series, 2008, 100, 052062.	0.4	0
104	First-principles calculation of electron transport in Si atom wire. Journal of Vacuum Science & Technology B, 2009, 27, 810-812.	1.3	0
105	Theoretical Study of Moiré Pattern in Scanning Tunneling Microscopy Images of Carbon Nanotubes on Metallic Substrate. Japanese Journal of Applied Physics, 2010, 49, 08LB02.	1.5	0
106	Bias drop and phonon emission in molecular wires. Applied Surface Science, 2012, 258, 2121-2123.	6.1	0
107	Field emission from vertically-aligned graphene edges on graphitized pencil lead. , 2018, , .		0
108	Origin of the FEM pattern from C <sub>60</sub> molecules adsorbed on tungsten tips. , 2018, , .		0

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109	Theory of electron transport at the atomistic level. Japanese Journal of Applied Physics, 2018, 57, 08NA01.	1.5	0
110	Theory of Electronic and Atomic Processes in Scanning Probe Microscopy. , 2001, , 147-179.		0
111	Transport Properties through Single Molecules on the Semiconductor Electrodes " Ab initio Calculation Study. AIP Conference Proceedings, 2007, , .	0.4	0
112	DFT Analysis of Quantum Transport in Si Atom Wire under Finite Bias Voltage. E-Journal of Surface Science and Nanotechnology, 2009, 7, 17-20.	0.4	0
113	Multi-Scale Quantum Transport Simulations from Atomistic Levels. Journal of the Vacuum Society of Japan, 2011, 54, 501-506.	0.3	0
114	Thermal Conduction Calculation of Nanowire by Non-equilibrium Green's Function. Hyomen Kagaku, 2011, 32, 410-415.	0.0	0
115	Atomistic Calculations of Heat Transport in a Silicon Crystal. E-Journal of Surface Science and Nanotechnology, 2014, 12, 154-156.	0.4	0
116	Ab Initio Calculations of the Transport Through Single Molecules and Carbon Nanotubes. , 2007, , 429-432.		0
117	Gate induced modulation of electronic states in monolayer organic field-effect transistor. Applied Physics Letters, 2021, 119, 223301.	3.3	0