

Yoshihiro Asai

List of Publications by Year in descending order

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87
papers

2,099
citations

218677

26
h-index

243625

44
g-index

89
all docs

89
docs citations

89
times ranked

2036
citing authors

#	ARTICLE	IF	CITATIONS
1	Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport. <i>Nature Materials</i> , 2019, 18, 357-363.	27.5	160
2	Heat dissipation and its relation to thermopower in single-molecule junctions. <i>New Journal of Physics</i> , 2014, 16, 015004.	2.9	88
3	The Madelung Energy in Copper-Oxide-Based Ceramics. <i>Journal of the Physical Society of Japan</i> , 1988, 57, 4334-4342.	1.6	85
4	Band structure calculations based on screened Fock exchange method. <i>Chemical Physics Letters</i> , 2008, 466, 91-94.	2.6	82
5	Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules. <i>Nature Communications</i> , 2016, 7, 11294.	12.8	80
6	Novel Mechanism of Photoinduced Reversible Phase Transitions in Molecule-Based Magnets. <i>Physical Review Letters</i> , 2001, 86, 348-351.	7.8	79
7	Inelastic Transport and Low-Bias Rectification in a Single-Molecule Diode. <i>ACS Nano</i> , 2011, 5, 8331-8339.	14.6	78
8	Controlling Formation of Single-Molecule Junctions by Electrochemical Reduction of Diazonium Terminal Groups. <i>Journal of the American Chemical Society</i> , 2013, 135, 3319-3322.	13.7	71
9	Theory of length-dependent conductance in one-dimensional chains. <i>Physical Review B</i> , 2005, 72, .	3.2	65
10	Toward Multiple Conductance Pathways with Heterocycle-Based Oligo(phenyleneethynylene) Derivatives. <i>Journal of the American Chemical Society</i> , 2015, 137, 13818-13826.	13.7	64
11	Long-Range Electron Transport of Ruthenium-Centered Multilayer Films <i>via</i> a Stepping-Stone Mechanism. <i>ACS Nano</i> , 2012, 6, 1988-1999.	14.6	62
12	Nonequilibrium phonon effects on transport properties through atomic and molecular bridge junctions. <i>Physical Review B</i> , 2008, 78, .	3.2	58
13	Adiabatic and nonadiabatic electronâ€“intramolecular-vibration couplings and superconductivity in fullerenes. <i>Physical Review B</i> , 1992, 46, 1265-1268.	3.2	55
14	Theory of Inelastic Electric Current through Single Molecules. <i>Physical Review Letters</i> , 2004, 93, 246102.	7.8	55
15	First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions. <i>Physical Review B</i> , 2015, 91, .	3.2	54
16	First principles band structure calculations based on self-consistent screened Hartreeâ€“Fock exchange potential. <i>Journal of Chemical Physics</i> , 2009, 130, 164702.	3.0	53
17	Ab initio calculations on the mechanism of charge transfer in Co-Fe Prussian-blue compounds. <i>Physical Review B</i> , 1999, 60, 12990-12993.	3.2	52
18	Energy band structure calculations based on screened Hartreeâ€“Fock exchange method: Si, AlP, AlAs, GaP, and GaAs. <i>Journal of Chemical Physics</i> , 2010, 132, 224105.	3.0	48

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19	Switch of Conducting Orbital by Bias-Induced Electronic Contact Asymmetry in a Bipyrimidinyl-biphenyl Diblock Molecule: Mechanism to Achieve a <i>pn</i> Directional Molecular Diode. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19931-19938.	3.1	48
20	Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire. <i>ACS Nano</i> , 2012, 6, 5078-5082.	14.6	42
21	Electronic structure of a linear C60 polymer. <i>Solid State Communications</i> , 1995, 93, 163-165.	1.9	39
22	Resistive switching mechanism of GeTe/Sb ₂ Te ₃ interfacial phase change memory and topological properties of embedded two-dimensional states. <i>Nanoscale</i> , 2017, 9, 9386-9395.	5.6	36
23	The effect of a Ta oxygen scavenger layer on HfO ₂ -based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7502-7510.	2.8	31
24	Theoretical study of the lineshape of inelastic electron tunneling spectroscopy. <i>Physical Review B</i> , 2008, 77, .	3.2	30
25	Theory of Electric Conductance of DNA Molecule. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4647-4652.	2.6	29
26	Single-molecule conductance of a chemically modified, π -extended tetrathiafulvalene and its charge-transfer complex with F ₄ TCNQ. <i>Beilstein Journal of Organic Chemistry</i> , 2015, 11, 1068-1078.	2.2	29
27	Thermoelectric Efficiency of Organometallic Complex Wires via Quantum Resonance Effect and Long-Range Electric Transport Property. <i>Journal of the American Chemical Society</i> , 2013, 135, 16545-16552.	13.7	27
28	Quantum Chemical Calculations of Ground Electronic State of High-TcCopper Oxides. <i>Journal of the Physical Society of Japan</i> , 1989, 58, 3264-3269.	1.6	26
29	Theoretical Rate Constants of Super-Exchange Hole Transfer and Thermally Induced Hopping in DNA. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1295-1303.	2.6	26
30	Orientation dependent magnetic interaction in TDAE-C60, where TDAE is tetrakis(dimethylamino)ethylene. <i>Chemical Physics Letters</i> , 1996, 259, 574-578.	2.6	24
31	Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes. <i>Nanoscale</i> , 2015, 7, 20497-20502.	5.6	24
32	Dynamic coupling of electronic motion and molecular vibration. <i>Chemical Physics Letters</i> , 1984, 106, 36-40.	2.6	22
33	Jahn-Teller mechanism of the half width of the intramolecular vibrational spectrum in dopedC60: Coupling withHg,T1u, andHumodes. <i>Physical Review B</i> , 1994, 49, 4289-4294.	3.2	22
34	Competitive effects of oxygen vacancy formation and interfacial oxidation on an ultra-thin HfO ₂ -based resistive switching memory: beyond filament and charge hopping models. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8820-8826.	2.8	22
35	The Orbital Selection Rule for Molecular Conductance as Manifested in Tetraphenyl-Based Molecular Junctions. <i>Journal of the American Chemical Society</i> , 2017, 139, 2989-2993.	13.7	22
36	How To Probe the Limits of the Wiedemann-Franz Law at Nanoscale. <i>Nano Letters</i> , 2018, 18, 7358-7361.	9.1	20

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37	Dynamic analysis of electron density in the course of the internal motion of molecular system. Journal of Chemical Physics, 1984, 80, 6170-6178.	3.0	19
38	Electronic Structure Calculations under Periodic Boundary Conditions Based on the Gaussian and Fourier Transform (GFT) Method. Journal of Chemical Theory and Computation, 2009, 5, 136-143.	5.3	18
39	Thermal conductance of Teflon and Polyethylene: Insight from an atomistic, single-molecule level. Scientific Reports, 2017, 7, 41898.	3.3	18
40	Deep-Learning Approach to First-Principles Transport Simulations. Physical Review Letters, 2021, 126, 177701.	7.8	18
41	Band structure of orthorhombic Rb1C60. Chemical Physics Letters, 1995, 241, 149-153.	2.6	17
42	A theoretical study of molecular conduction. II. A Hartree-Fock approach to transmission probability. Journal of Chemical Physics, 2005, 123, 164111.	3.0	17
43	Bias voltage dependence on the vibronic electric current. Physical Review B, 2008, 77, .	3.2	14
44	Theory of local heating in single molecular bridge junctions. Physical Review B, 2011, 84, .	3.2	12
45	Morphology of dynamic electron transfer characteristic of chemical reaction dynamics. Journal of Chemical Physics, 1985, 83, 6334-6343.	3.0	11
46	Magnetic interactions in TDAE-C60. Physical Review B, 1996, 53, 4176-4179.	3.2	11
47	Reduced-density-matrix analysis of superconducting correlation in two-dimensional and two-chain Hubbard models. Physical Review B, 1994, 50, 6519-6522.	3.2	10
48	Superconducting, magnetic, and charge correlations in the doped two-chain Hubbard model. Physical Review B, 1995, 52, 10390-10394.	3.2	10
49	The mechanism of the photo-induced magnetic transition in Co ²⁺ Fe cyanide with ab initio calculations. Journal of Luminescence, 2000, 87-89, 658-660.	3.1	10
50	Electron correlation enhancement of the diode property of asymmetric molecules. Physical Review B, 2011, 84, .	3.2	7
51	Length and energy gap dependences of thermoelectricity in nanostructured junctions. Journal of Physics Condensed Matter, 2013, 25, 155305.	1.8	7
52	Dynamic electron current induced by molecular vibration. Computational and Theoretical Chemistry, 1985, 123, 267-285.	1.5	6
53	Theoretical study on carbocation with a triple bond. Computational and Theoretical Chemistry, 1987, 153, 295-305.	1.5	6
54	Superconductivity by suhl-kondo pair transfer interaction in dp+ π model. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1633-1634.	1.2	6

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55	Stable geometry and rotation of the dinitrogen ligand in a nickel complex, dinitrogen dioxygen nickel. <i>Inorganic Chemistry</i> , 1983, 22, 3218-3220.	4.0	5
56	A Cooper Pairing Mechanism Mediated by the Virtual Exchange of the RVB Quanta. <i>Journal of the Physical Society of Japan</i> , 1988, 57, 3491-3498.	1.6	5
57	Electron transport accompanying molecular vibration. <i>Synthetic Metals</i> , 1987, 17, 149-154.	3.9	4
58	Isomorphic electron orbitals for vibronic flexibility in a cyclopropenyl radical molecular device. <i>Theoretica Chimica Acta</i> , 1990, 78, 1-9.	0.8	4
59	Isotope effect in TTF-analog based organic superconductors. <i>Synthetic Metals</i> , 1991, 42, 2231-2234.	3.9	4
60	Coupled-cluster approach to electron correlations in the two-dimensional Hubbard model. <i>Physical Review B</i> , 1999, 60, R13946-R13949.	3.2	4
61	Adaptive sampling approach to the negative-sign problem in the auxiliary-field quantum Monte Carlo method. <i>Physical Review B</i> , 2000, 62, 10674-10679.	3.2	4
62	Symmetry of superconductivity in $\text{NH}_3\text{K}_3\text{C}_6\text{O}$ superconductors: nonadiabatic effects in multiband systems. <i>Physical Review B</i> , 2003, 68, .	3.2	4
63	A new method for partition of interaction energy. Relation between stabilization energy and orbital mixing. <i>Theoretica Chimica Acta</i> , 1984, 66, 77-90.	0.8	3
64	Elementary-spin-excitation spectrum of undoped and doped single-band Hubbard models. <i>Physical Review B</i> , 1994, 49, 10013-10015.	3.2	3
65	Theory of zero-bias anomaly in low-temperature inelastic tunneling spectroscopy. <i>Physical Review B</i> , 2012, 86, .	3.2	3
66	Vibronic spectroscopy using current noise. <i>Physical Review B</i> , 2015, 91, .	3.2	3
67	The ground state of the two-dimensional Hubbard model. <i>Physica B: Condensed Matter</i> , 2000, 281-282, 935-937.	2.7	2
68	Theoretical Study of the Charge Transfer Absorption in Cobalt-Iron Cyanide. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 376, 423-429.	0.9	2
69	On the Hartree-Fock approximation to the electronic structure of molecule in the intense radiation field and the strong vibronic coupling. <i>Theoretica Chimica Acta</i> , 1988, 73, 147-154.	0.8	1
70	Correlation functions and susceptibilities of the dp model. <i>Physica C: Superconductivity and Its Applications</i> , 1991, 185-189, 1497-1498.	1.2	1
71	Adiabatic-antiadiabatic crossover of vibronic couplings in a two-level system as a model of $\text{C}_n \sim 60$. <i>Chemical Physics Letters</i> , 1992, 195, 551-555.	2.6	1
72	Local Electronic Excitation Mechanism for Nanofabrication of Polydiacetylene Molecular Wire. <i>Journal of the Physical Society of Japan</i> , 2003, 72, 3286-3290.	1.6	1

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73	Gaussian and Fourier Transform (GFT) Method and Screened Hartree-Fock Exchange Potential for First-principles Band Structure Calculations. , 2011, , .		1
74	First-Principles Transport Modeling for Metal/Insulator/Metal Structures. , 2014, , .		1
75	Design of ReRAM cell structure by metal buffer and contact engineering via first-principles transport calculations. , 2014, , .		1
76	(Invited) Non-Equilibrium Transport Theory Applied to Nano Electronics Problems. ECS Transactions, 2014, 64, 63-69.	0.5	1
77	Vibronic Mechanisms for Charge Transport and Migration Through DNA and Single Molecules. Nanoscience and Technology, 2007, , 121-138.	1.5	1
78	Effect of vibronic coupling on the long range intermolecular interaction. International Journal of Quantum Chemistry, 1987, 32, 569-572.	2.0	0
79	Quantum Monte Carlo and quantum chemical study of the ground state of the high-Tc copper oxides. Physica B: Condensed Matter, 1990, 165-166, 1017-1018.	2.7	0
80	A quantum chemical study of interchain hopping model of negatively charged solitons in polyacetylene. International Journal of Quantum Chemistry, 1992, 41, 461-474.	2.0	0
81	Spin gap and superconductivity in the ground state of the two-dimensional Hubbard model. Journal of Physics and Chemistry of Solids, 2001, 62, 231-235.	4.0	0
82	Possible change of the superconducting symmetry in the vicinity of the SC \leftrightarrow AF transition in NH ₃ A ₃ C ₆ O. Physica C: Superconductivity and Its Applications, 2003, 388-389, 620-621.	1.2	0
83	Rectification in substituted atomic wires: a theoretical insight. Journal of Physics Condensed Matter, 2012, 24, 164213.	1.8	0
84	First-Principles Modeling for Current-Voltage Characteristics of Resistive Random Access Memories. Materials Research Society Symposia Proceedings, 2013, 1562, 1.	0.1	0
85	Ground State Electronic Structure and Mechanism of High-Tc Copper Oxides. , 1990, , 459-462.		0
86	Superconductivity in Pseudodegenerate Overlapping Bands Systems: Copper Oxides and C ₆₀ Kx. , 1992, , 61-64.		0
87	Thermoelectric Transport from First-Principles \rightarrow Biphenyl-Based Single-Molecule Junctions. , 2016, , 43-51.		0