Yoshihiro Asai

List of Publications by Year
in descending order

87	2,099	218592	243529
papers	citations	26 h-index	44 g-index

89	89	89	2036
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport. Nature Materials, 2019, 18, 357-363.	13.3	160
2	Heat dissipation and its relation to thermopower in single-molecule junctions. New Journal of Physics, 2014, 16, 015004.	1.2	88
3	The Madelung Energy in Copper-Oxide-Based Ceramics. Journal of the Physical Society of Japan, 1988, 57, 4334-4342.	0.7	85
4	Band structure calculations based on screened Fock exchange method. Chemical Physics Letters, 2008, 466, 91-94.	1.2	82
5	Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules. Nature Communications, 2016, 7, 11294.	5.8	80
6	Novel Mechanism of Photoinduced Reversible Phase Transitions in Molecule-Based Magnets. Physical Review Letters, 2001, 86, 348-351.	2.9	79
7	Inelastic Transport and Low-Bias Rectification in a Single-Molecule Diode. ACS Nano, 2011, 5, 8331-8339.	7.3	78
8	Controlling Formation of Single-Molecule Junctions by Electrochemical Reduction of Diazonium Terminal Groups. Journal of the American Chemical Society, 2013, 135, 3319-3322.	6.6	71
9	Theory of length-dependent conductance in one-dimensional chains. Physical Review B, 2005, 72, .	1.1	65
10	Toward Multiple Conductance Pathways with Heterocycle-Based Oligo(phenyleneethynylene) Derivatives. Journal of the American Chemical Society, 2015, 137, 13818-13826.	6.6	64
11	Long-Range Electron Transport of Ruthenium-Centered Multilayer Films via a Stepping-Stone Mechanism. ACS Nano, 2012, 6, 1988-1999.	7.3	62
12	Nonequilibrium phonon effects on transport properties through atomic and molecular bridge junctions. Physical Review B, 2008, 78, .	1.1	58
13	Adiabatic and nonadiabatic electronâ€“intramolecular-vibration couplings and superconductivity in fullerenes. Physical Review B, 1992, 46, 1265-1268.	1.1	55
14	Theory of Inelastic Electric Current through Single Molecules. Physical Review Letters, 2004, 93, 246102.	2.9	55
15	First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions. Physical Review B, 2015, 91, .	1.1	54
16	First principles band structure calculations based on self-consistent screened Hartreeâ€“Fock exchange potential. Journal of Chemical Physics, 2009, 130, 164702.	1.2	53
17	Ab initiocalculations on the mechanism of charge transfer in Co-Fe Prussian-blue compounds. Physical Review B, 1999, 60, 12990-12993.	1.1	52
18	Energy band structure calculations based on screened Hartreeâ€“Fock exchange method: Si, AlP, AlAs, GaP, and GaAs. Journal of Chemical Physics, 2010, 132, 224105.	1.2	48

#	Article	IF	Citations
19	Switch of Conducting Orbital by Bias-Induced Electronic Contact Asymmetry in a Bipyrimidinyl-biphenyl Diblock Molecule: Mechanism to Achieve a pn Directional Molecular Diode. Journal of Physical Chemistry C, 2011, 115, 19931-19938.	1.5	48
20	Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire. ACS Nano, 2012, 6, 5078-5082.	7.3	42
21	Electronic structure of a linear C60 polymer. Solid State Communications, 1995, 93, 163-165.	0.9	39
22	Resistive switching mechanism of GeTeâ€“Sb₂Te₃ interfacial phase change memory and topological properties of embedded two-dimensional states. Nanoscale, 2017, 9, 9386-9395.	2.8	36
23	The effect of a Ta oxygen scavenger layer on HfO₂-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport. Physical Chemistry Chemical Physics, 2016, 18, 7502-7510.	1.3	31
24	Theoretical study of the lineshape of inelastic electron tunneling spectroscopy. Physical Review B, 2008, 77, .	1.1	30
25	Theory of Electric Conductance of DNA Molecule. Journal of Physical Chemistry B, 2003, 107, 4647-4652.	1.2	29
26	Single-molecule conductance of a chemically modified, Ï€-extended tetrathiafulvalene and its charge-transfer complex with F₄TCNQ. Beilstein Journal of Organic Chemistry, 2015, 11, 1068-1078.	1.3	29
27	Thermoelectric Efficiency of Organometallic Complex Wires via Quantum Resonance Effect and Long-Range Electric Transport Property. Journal of the American Chemical Society, 2013, 135, 16545-16552.	6.6	27
28	Quantum Chemical Calculations of Ground Electronic State of High-TcCopper Oxides. Journal of the Physical Society of Japan, 1989, 58, 3264-3269.	0.7	26
29	Theoretical Rate Constants of Super-Exchange Hole Transfer and Thermally Induced Hopping in DNA. Journal of Physical Chemistry B, 2005, 109, 1295-1303.	1.2	26
30	Orientation dependent magnetic interaction in TDAE-C60, where TDAE is tetrakis(dimethylamino)ethylene. Chemical Physics Letters, 1996, 259, 574-578.	1.2	24
31	Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes. Nanoscale, 2015, 7, 20497-20502.	2.8	24
32	Dynamic coupling of electronic motion and molecular vibration. Chemical Physics Letters, 1984, 106, 36-40.	1.2	22
33	Jahn-Teller mechanism of the half width of the intramolecular vibrational spectrum in dopedC60: Coupling withHg,T1u, andHumodes. Physical Review B, 1994, 49, 4289-4294.	1.1	22
34	Competitive effects of oxygen vacancy formation and interfacial oxidation on an ultra-thin HfO₂-based resistive switching memory: beyond filament and charge hopping models. Physical Chemistry Chemical Physics, 2016, 18, 8820-8826.	1.3	22
35	The Orbital Selection Rule for Molecular Conductance as Manifested in Tetraphenyl-Based Molecular Junctions. Journal of the American Chemical Society, 2017, 139, 2989-2993.	6.6	22
36	How To Probe the Limits of the Wiedemannâ€“Franz Law at Nanoscale. Nano Letters, 2018, 18, 7358-7361.	4.5	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.	1.2	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.	2.3	18
39	Thermal conductance of Teflon and Polyethylene: Insight from an atomistic, single-molecule level. Scientific Reports, 2017, 7, 41898.	1.6	18
40	Deep-Learning Approach to First-Principles Transport Simulations. Physical Review Letters, 2021, 126, 177701.	2.9	18
41	Band structure of orthorhombic Rb1C60. Chemical Physics Letters, 1995, 241, 149-153.	1.2	17
42	A theoretical study of molecular conduction. II. A Hartree-Fock approach to transmission probability. Journal of Chemical Physics, 2005, 123, 164111.	1.2	17
43	Bias voltage dependence on the vibronic electric current. Physical Review B, 2008, 77, .	1.1	14
44	Theory of local heating in single molecular bridge junctions. Physical Review B, 2011, 84, .	1.1	12
45	Morphology of dynamic electron transfer characteristic of chemical reaction dynamics. Journal of Chemical Physics, 1985, 83, 6334-6343.	1.2	11
46	Magnetic interactions in TDAE-C60. Physical Review B, 1996, 53, 4176-4179.	1.1	11
47	Reduced-density-matrix analysis of superconducting correlation in two-dimensional and two-chain Hubbard models. Physical Review B, 1994, 50, 6519-6522.	1.1	10
48	Superconducting, magnetic, and charge correlations in the doped two-chain Hubbard model. Physical Review B, 1995, 52, 10390-10394.	1.1	10
49	The mechanism of the photo-induced magnetic transition in Coâ€“Fe cyanide with ab initio calculations. Journal of Luminescence, 2000, 87-89, 658-660.	1.5	10
50	Electron correlation enhancement of the diode property of asymmetric molecules. Physical Review B, 2011, 84, .	1.1	7
51	Length and energy gap dependences of thermoelectricity in nanostructured junctions. Journal of Physics Condensed Matter, 2013, 25, 155305.	0.7	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+Ï€ model. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1633-1634.	0.6	6

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55	Stable geometry and rotation of the dinitrogen ligand in a nickel complex, dinitrogendioxygennickel. Inorganic Chemistry, 1983, 22, 3218-3220.	1.9	5
56	A Cooper Pairing Mechanism Mediated by the Virtual Exchange of the RVB Quanta. Journal of the Physical Society of Japan, 1988, 57, 3491-3498.	0.7	5
57	Electron transport accompanying molecular vibration. Synthetic Metals, 1987, 17, 149-154.	2.1	4
58	Isomorphic electron orbitals for vibronic flexibility in a cyclopropenyl radical molecular device. Theoretica Chimica Acta, 1990, 78, 1-9.	0.9	4
59	Isotope effect in TTF-analog based organic superconductors. Synthetic Metals, 1991, 42, 2231-2234.	2.1	4
60	Coupled-cluster approach to electron correlations in the two-dimensional Hubbard model. Physical Review B, 1999, 60, R13946-R13949.	1.1	4
61	Adaptive sampling approach to the negative-sign problem in the auxiliary-field quantum Monte Carlo method. Physical Review B, 2000, 62, 10674-10679.	1.1	4
62	Symmetry of superconductivity inNH3K3C60superconductors: nonadiabatic effects in multiband systems. Physical Review B, 2003, 68, .	1.1	4
63	A new method for partition of interaction energy. Relation between stabilization energy and orbital mixing. Theoretica Chimica Acta, 1984, 66, 77-90.	0.9	3
64	Elementary-spin-excitation spectrum of undoped and doped single-band Hubbard models. Physical Review B, 1994, 49, 10013-10015.	1.1	3
65	Theory of zero-bias anomaly in low-temperature inelastic tunneling spectroscopy. Physical Review B, 2012, 86, .	1.1	3
66	Vibronic spectroscopy using current noise. Physical Review B, 2015, 91, .	1.1	3
67	The ground state of the two-dimensional Hubbard model. Physica B: Condensed Matter, 2000, 281-282, 935-937.	1.3	2
68	Theoretical Study of the Charge Transfer Absorption in Cobalt-Iron Cyanide. Molecular Crystals and Liquid Crystals, 2002, 376, 423-429.	0.4	2
69	On the Hartree-Fock approximation to the electronic structure of molecule in the intense radiation field and the strong vibronic coupling. Theoretica Chimica Acta, 1988, 73, 147-154.	0.9	1
70	Correlation functions and susceptibilities of the dp model. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1497-1498.	0.6	1
71	Adiabaticâ€”antiadiabatic crossover of vibronic couplings in a two-level system as a model of Cnâ¯60. Chemical Physics Letters, 1992, 195, 551-555.	1.2	1
72	Local Electronic Excitation Mechanism for Nanofabrication of Polydiacetylene Molecular Wire. Journal of the Physical Society of Japan, 2003, 72, 3286-3290.	0.7	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.	0.3	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.	1.0	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.	1.3	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.	1.0	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.	1.9	0
82	Possible change of the superconducting symmetry in the vicinity of the SCâ€“AF transition in NH3A3C60. Physica C: Superconductivity and Its Applications, 2003, 388-389, 620-621.	0.6	0
83	Rectification in substituted atomic wires: a theoretical insight. Journal of Physics Condensed Matter, 2012, 24, 164213.	0.7	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 C60Kx. , 1992, , 61-64.		0
87	Thermoelectric Transport from First-Principlesâ€”Biphenyl-Based Single-Molecule Junctions. , 2016, , 43-51.		0