Yoshihiro Asai

List of Publications by Year
in descending order

87	2,099	218677	243625
papers	citations	26 h-index	44 g-index

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

#	Article	IF	Citations
1	Deep-Learning Approach to First-Principles Transport Simulations. Physical Review Letters, 2021, 126, 177701.	7.8	18
2	Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport. Nature Materials, 2019, 18, 357-363.	27.5	160
3	How To Probe the Limits of the Wiedemannâ€“Franz Law at Nanoscale. Nano Letters, 2018, 18, 7358-7361.	9.1	20
4	The Orbital Selection Rule for Molecular Conductance as Manifested in Tetraphenyl-Based Molecular Junctions. Journal of the American Chemical Society, 2017, 139, 2989-2993.	13.7	22
5	Thermal conductance of Teflon and Polyethylene: Insight from an atomistic, single-molecule level. Scientific Reports, 2017, 7, 41898.	3.3	18
6	Resistive switching mechanism of GeTeâ€“Sb₂Te₃ interfacial phase change memory and topological properties of embedded two-dimensional states. Nanoscale, 2017, 9, 9386-9395.	5.6	36
7	Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules. Nature Communications, 2016, 7, 11294.	12.8	80
8	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.	2.8	31
9	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.	2.8	22
10	Thermoelectric Transport from First-Principlesâ€”Biphenyl-Based Single-Molecule Junctions. , 2016, , 43-51.		0
11	Vibronic spectroscopy using current noise. Physical Review B, 2015, 91, .	3.2	3
12	First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions. Physical Review B, 2015, 91, .	3.2	54
13	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.	2.2	29
14	Toward Multiple Conductance Pathways with Heterocycle-Based Oligo(phenyleneethynylene) Derivatives. Journal of the American Chemical Society, 2015, 137, 13818-13826.	13.7	64
15	Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes. Nanoscale, 2015, 7, 20497-20502.	5.6	24
16	First-Principles Transport Modeling for Metal/Insulator/Metal Structures. , 2014, , .		1
17	Design of ReRAM cell structure by metal buffer and contact engineering via first-principles transport calculations. , 2014, , .		1
18	Heat dissipation and its relation to thermopower in single-molecule junctions. New Journal of Physics, 2014, 16, 015004.	2.9	88

#	Article	IF	Citations
19	(Invited) Non-Equilibrium Transport Theory Applied to Nano Electronics Problems. ECS Transactions, 2014, 64, 63-69.	0.5	1
20	Controlling Formation of Single-Molecule Junctions by Electrochemical Reduction of Diazonium Terminal Groups. Journal of the American Chemical Society, 2013, 135, 3319-3322.	13.7	71
21	Length and energy gap dependences of thermoelectricity in nanostructured junctions. Journal of Physics Condensed Matter, 2013, 25, 155305.	1.8	7
22	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.	13.7	27
23	First-Principles Modeling for Current-Voltage Characteristics of Resistive Random Access Memories. Materials Research Society Symposia Proceedings, 2013, 1562, 1.	0.1	0
24	Rectification in substituted atomic wires: a theoretical insight. Journal of Physics Condensed Matter, 2012, 24, 164213.	1.8	0
25	Theory of zero-bias anomaly in low-temperature inelastic tunneling spectroscopy. Physical Review B, 2012, 86, .	3.2	3
26	Long-Range Electron Transport of Ruthenium-Centered Multilayer Films via a Stepping-Stone Mechanism. ACS Nano, 2012, 6, 1988-1999.	14.6	62
27	Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire. ACS Nano, 2012, 6, 5078-5082.	14.6	42
28	Inelastic Transport and Low-Bias Rectification in a Single-Molecule Diode. ACS Nano, 2011, 5, 8331-8339.	14.6	78
29	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.	3.1	48
30	Electron correlation enhancement of the diode property of asymmetric molecules. Physical Review B, 2011, 84, .	3.2	7
31	Gaussian and Fourier Transform (GFT) Method and Screened Hartree-Fock Exchange Potential for First-principles Band Structure Calculations. , 2011, , .		1
32	Theory of local heating in single molecular bridge junctions. Physical Review B, 2011, 84, .	3.2	12
33	Energy band structure calculations based on screened Hartreeâ€“Fock exchange method: Si, AlP, AlAs, GaP, and GaAs. Journal of Chemical Physics, 2010, 132, 224105.	3.0	48
34	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
35	First principles band structure calculations based on self-consistent screened Hartreeâ€“Fock exchange potential. Journal of Chemical Physics, 2009, 130, 164702.	3.0	53
36	Band structure calculations based on screened Fock exchange method. Chemical Physics Letters, 2008, 466, 91-94.	2.6	82

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37	Nonequilibrium phonon effects on transport properties through atomic and molecular bridge junctions. Physical Review B, 2008, 78, .	3.2	58
38	Theoretical study of the lineshape of inelastic electron tunneling spectroscopy. Physical Review B, 2008, 77, .	3.2	30
39	Bias voltage dependence on the vibronic electric current. Physical Review B, 2008, 77, .	3.2	14
40	Vibronic Mechanisms for Charge Transport and Migration Through DNA and Single Molecules. Nanoscience and Technology, 2007, , 121-138.	1.5	1
41	A theoretical study of molecular conduction. II. A Hartree-Fock approach to transmission probability. Journal of Chemical Physics, 2005, 123, 164111.	3.0	17
42	Theory of length-dependent conductance in one-dimensional chains. Physical Review B, 2005, 72, .	3.2	65
43	Theoretical Rate Constants of Super-Exchange Hole Transfer and Thermally Induced Hopping in DNA. Journal of Physical Chemistry B, 2005, 109, 1295-1303.	2.6	26
44	Theory of Inelastic Electric Current through Single Molecules. Physical Review Letters, 2004, 93, 246102.	7.8	55
45	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.	1.2	0
46	Local Electronic Excitation Mechanism for Nanofabrication of Polydiacetylene Molecular Wire. Journal of the Physical Society of Japan, 2003, 72, 3286-3290.	1.6	1
47	Theory of Electric Conductance of DNA Molecule. Journal of Physical Chemistry B, 2003, 107, 4647-4652.	2.6	29
48	Symmetry of superconductivity inNH3K3C60superconductors: nonadiabatic effects in multiband systems. Physical Review B, 2003, 68, .	3.2	4
49	Theoretical Study of the Charge Transfer Absorption in Cobalt-Iron Cyanide. Molecular Crystals and Liquid Crystals, 2002, 376, 423-429.	0.9	2
50	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
51	Novel Mechanism of Photoinduced Reversible Phase Transitions in Molecule-Based Magnets. Physical Review Letters, 2001, 86, 348-351.	7.8	79
52	The ground state of the two-dimensional Hubbard model. Physica B: Condensed Matter, 2000, 281-282, 935-937.	2.7	2
53	The mechanism of the photo-induced magnetic transition in Coâ€“Fe cyanide with ab initio calculations. Journal of Luminescence, 2000, 87-89, 658-660.	3.1	10
54	Adaptive sampling approach to the negative-sign problem in the auxiliary-field quantum Monte Carlo method. Physical Review B, 2000, 62, 10674-10679.	3.2	4

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55	Coupled-cluster approach to electron correlations in the two-dimensional Hubbard model. Physical Review B, 1999, 60, R13946-R13949.	3.2	4
56	Ab initiocalculations on the mechanism of charge transfer in Co-Fe Prussian-blue compounds. Physical Review B, 1999, 60, 12990-12993.	3.2	52
57	Orientation dependent magnetic interaction in TDAE-C60, where TDAE is tetrakis(dimethylamino)ethylene. Chemical Physics Letters, 1996, 259, 574-578.	2.6	24
58	Magnetic interactions in TDAE-C60. Physical Review B, 1996, 53, 4176-4179.	3.2	11
59	Band structure of orthorhombic Rb1C60. Chemical Physics Letters, 1995, 241, 149-153.	2.6	17
60	Electronic structure of a linear C60 polymer. Solid State Communications, 1995, 93, 163-165.	1.9	39
61	Superconducting, magnetic, and charge correlations in the doped two-chain Hubbard model. Physical Review B, 1995, 52, 10390-10394.	3.2	10
62	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.	3.2	22
63	Elementary-spin-excitation spectrum of undoped and doped single-band Hubbard models. Physical Review B, 1994, 49, 10013-10015.	3.2	3
64	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
65	Adiabatic and nonadiabatic electronâ€“intramolecular-vibration couplings and superconductivity in fullerenes. Physical Review B, 1992, 46, 1265-1268.	3.2	55
66	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
67	Adiabaticâ€”antiadiabatic crossover of vibronic couplings in a two-level system as a model of Cnâ¯60. Chemical Physics Letters, 1992, 195, 551-555.	2.6	1
68	Superconductivity in Pseudodegenerate Overlapping Bands Systems: Copper Oxides and C60Kx. , 1992, , 61-64.		0
69	Isotope effect in TTF-analog based organic superconductors. Synthetic Metals, 1991, 42, 2231-2234.	3.9	4
70	Correlation functions and susceptibilities of the dp model. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1497-1498.	1.2	1
71	Superconductivity by suhl-kondo pair transfer interaction in dp+Ï€ model. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1633-1634.	1.2	6
72	Isomorphic electron orbitals for vibronic flexibility in a cyclopropenyl radical molecular device. Theoretica Chimica Acta, 1990, 78, 1-9.	0.8	4

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73	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
74	Ground State Electronic Structure and Mechanism of High-Tc Copper Oxides. , 1990, , 459-462.		0
75	Quantum Chemical Calculations of Ground Electronic State of High-TcCopper Oxides. Journal of the Physical Society of Japan, 1989, 58, 3264-3269.	1.6	26
76	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.	0.8	1
77	The Madelung Energy in Copper-Oxide-Based Ceramics. Journal of the Physical Society of Japan, 1988, 57, 4334-4342.	1.6	85
78	A Cooper Pairing Mechanism Mediated by the Virtual Exchange of the RVB Quanta. Journal of the Physical Society of Japan, 1988, 57, 3491-3498.	1.6	5
79	Theoretical study on carbocation with a triple bond. Computational and Theoretical Chemistry, 1987, 153, 295-305.	1.5	6
80	Electron transport accompanying molecular vibration. Synthetic Metals, 1987, 17, 149-154.	3.9	4
81	Effect of vibronic coupling on the long range intermolecular interaction. International Journal of Quantum Chemistry, 1987, 32, 569-572.	2.0	0
82	Morphology of dynamic electron transfer characteristic of chemical reaction dynamics. Journal of Chemical Physics, 1985, 83, 6334-6343.	3.0	11
83	Dynamic electron current induced by molecular vibration. Computational and Theoretical Chemistry, 1985, 123, 267-285.	1.5	6
84	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
85	Dynamic coupling of electronic motion and molecular vibration. Chemical Physics Letters, 1984, 106, 36-40.	2.6	22
86	A new method for partition of interaction energy. Relation between stabilization energy and orbital mixing. Theoretica Chimica Acta, 1984, 66, 77-90.	0.8	3
87	Stable geometry and rotation of the dinitrogen ligand in a nickel complex, dinitrogendioxygennickel. Inorganic Chemistry, 1983, 22, 3218-3220.	4.0	5