Tomofumi Tada

List of Publications by Year
in descending order

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117 papers	4,658 citations	94381 37 h-index	106281 65 g-index
125 all docs	125 docs citations	125 times ranked	4603 citing authors

#	Article	IF	Citations
1	Vacancy-enabled N2 activation for ammonia synthesis on an Ni-loaded catalyst. Nature, 2020, 583, 391-395.	13.7	309
2	Orbital Views of the Electron Transport in Molecular Devices. Journal of the American Chemical Society, 2008, 130, 9406-9413.	6.6	223
3	Ternary intermetallic LaCoSi as a catalyst for N2 activation. Nature Catalysis, 2018, 1, 178-185.	16.1	221
4	Water Durable Electride Y₅Si₃: Electronic Structure and Catalytic Activity for Ammonia Synthesis. Journal of the American Chemical Society, 2016, 138, 3970-3973.	6.6	217
5	Essential role of hydride ion in ruthenium-based ammonia synthesis catalysts. Chemical Science, 2016, 7, 4036-4043.	3.7	195
6	Highly Versatile Organostibine Mediators for Living Radical Polymerization. Journal of the American Chemical Society, 2004, 126, 13908-13909.	6.6	189
7	Discovery of hexagonal ternary phase Ti2InB2 and its evolution to layered boride TiB. Nature Communications, 2019, 10, 2284.	5.8	159
8	Selfâ€organized Ruthenium–Barium Coreâ€“Shell Nanoparticles on a Mesoporous Calcium Amide Matrix for Efficient Lowâ€Temperature Ammonia Synthesis. Angewandte Chemie - International Edition, 2018, 57, 2648-2652.	7.2	144
9	Rectifying Electron-Transport Properties through Stacks of Aromatic Molecules Inserted into a Self-Assembled Cage. Journal of the American Chemical Society, 2015, 137, 5939-5947.	6.6	126
10	Design principle for increasing charge mobility of Ï€-conjugated polymers using regularly localized molecular orbitals. Nature Communications, 2013, 4, 1691.	5.8	115
11	High-Throughput ab Initio Screening for Two-Dimensional Electride Materials. Inorganic Chemistry, 2014, 53, 10347-10358.	1.9	107
12	Low-Temperature Synthesis of Perovskite Oxynitride-Hydrides as Ammonia Synthesis Catalysts. Journal of the American Chemical Society, 2019, 141, 20344-20353.	6.6	106
13	Electron Transport through Single Molecules Comprising Aromatic Stacks Enclosed in Selfâ€Assembled Cages. Angewandte Chemie - International Edition, 2011, 50, 5708-5711.	7.2	92
14	Quantum Transport Effects in Nanosized Graphite Sheets. ChemPhysChem, 2002, 3, 1035-1037.	1.0	90
15	Copper-Based Intermetallic Electride Catalyst for Chemoselective Hydrogenation Reactions. Journal of the American Chemical Society, 2017, 139, 17089-17097.	6.6	90
16	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. Chemistry of Materials, 2020, 32, 6947-6957.	3.2	89
17	Exploration of Stable Strontium Phosphide-Based Electrides: Theoretical Structure Prediction and Experimental Validation. Journal of the American Chemical Society, 2017, 139, 15668-15680.	6.6	84
18	â€œDopingâ€•of Polyyne with an Organometallic Fragment Leads to Highly Conductive Metallapolyyne Molecular Wire. Journal of the American Chemical Society, 2018, 140, 10080-10084.	6.6	78

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19	Triphosphasumanene Trisulfide: High Out-of-Plane Anisotropy and Janus-Type Ï€-Surfaces. Journal of the American Chemical Society, 2017, 139, 5787-5792.	6.6	75
20	Characteristic fast Hâ¯ ion conduction in oxygen-substituted lanthanum hydride. Nature Communications, 2019, 10, 2578.	5.8	70
21	Highly Conductive [3Ã—n] Goldâ€Ion Clusters Enclosed within Selfâ€Assembled Cages. Angewandte Chemie - International Edition, 2013, 52, 6202-6205.	7.2	69
22	Single-Molecule Conductance of Ï€-Conjugated Rotaxane: New Method for Measuring Stipulated Electric Conductance of Ï€-Conjugated Molecular Wire Using STM Break Junction. Small, 2012, 8, 726-730.	5.2	67
23	Wire-Length Dependence of the Conductance of Oligo(p-phenylene) Dithiolate Wires:â€‰ A Consideration from Molecular Orbitals. Journal of Physical Chemistry A, 2004, 108, 9143-9149.	1.1	66
24	A theoretical measurement of the quantum transport through an optical molecular switch. Chemical Physics Letters, 2005, 412, 55-59.	1.2	66
25	Enhanced Catalytic Ammonia Synthesis with Transformed BaO. ACS Catalysis, 2018, 8, 10977-10984.	5.5	59
26	Greenâ€™s function formalism coupled with Gaussian broadening of discrete states for quantum transport: Application to atomic and molecular wires. Journal of Chemical Physics, 2004, 121, 8050.	1.2	55
27	Nonequilibrium Quantum Transport Properties of a Silver Atomic Switch. Nano Letters, 2007, 7, 2688-2692.	4.5	55
28	Resolving metal-molecule interfaces at single-molecule junctions. Scientific Reports, 2016, 6, 26606.	1.6	55
29	First-principles simulations on bulk Ta2O5 and Cu/Ta2O5/Pt heterojunction: Electronic structures and transport properties. Journal of Applied Physics, 2009, 106, .	1.1	51
30	Conductive Path Formation in the Ta₂O₅ Atomic Switch: First-Principles Analyses. ACS Nano, 2010, 4, 6477-6482.	7.3	50
31	Oscillation of Conductance in Molecular Junctions of Carbon Ladder Compounds. Journal of the American Chemical Society, 2004, 126, 14182-14189.	6.6	49
32	Triptycene Tripods for the Formation of Highly Uniform and Densely Packed Self-Assembled Monolayers with Controlled Molecular Orientation. Journal of the American Chemical Society, 2019, 141, 5995-6005.	6.6	48
33	Excess-silver-induced bridge formation in a silver sulfide atomic switch. Applied Physics Letters, 2008, 93, .	1.5	46
34	Organometallic molecular wires as versatile modules for energy-level alignment of the metalâ€“moleculeâ€“metal junction. Chemical Communications, 2016, 52, 5796-5799.	2.2	45
35	High Electron Density on Ru in Intermetallic YRu₂: The Application to Catalyst for Ammonia Synthesis. Journal of Physical Chemistry C, 2018, 122, 10468-10475.	1.5	43
36	Palladium-bearing intermetallic electride as anÂefficient and stable catalyst for Suzuki cross-coupling reactions. Nature Communications, 2019, 10, 5653.	5.8	43

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37	Semimetallic Two-Dimensional TiB₁₂: Improved Stability and Electronic Properties Tunable by Biaxial Strain. Chemistry of Materials, 2017, 29, 5922-5930.	3.2	41
38	Molecular design of electron transport with orbital rule: toward conductance-decay free molecular junctions. Physical Chemistry Chemical Physics, 2015, 17, 32099-32110.	1.3	40
39	A Stable, Soluble, and Crystalline Supramolecular System with a Triplet Ground State. Angewandte Chemie - International Edition, 2017, 56, 4261-4265.	7.2	40
40	Quantum Transport Effects in Nanosized Graphite Sheets. II. Enhanced Transport Effects by Heteroatoms. Journal of Physical Chemistry B, 2003, 107, 8789-8793.	1.2	35
41	Molecular Orbital Interactions in the Nanostar Dendrimer. Journal of Physical Chemistry B, 2003, 107, 14204-14210.	1.2	34
42	Large Oblate Hemispheroidal Ruthenium Particles Supported on Calcium Amide as Efficient Catalysts for Ammonia Decomposition. Chemistry - A European Journal, 2018, 24, 7976-7984.	1.7	34
43	Anchoring Bond between Ru and N Atoms of Ru/Ca₂NH Catalyst: Crucial for the High Ammonia Synthesis Activity. Journal of Physical Chemistry C, 2017, 121, 20900-20904.	1.5	33
44	Reverse Exponential Decay of Electrical Transmission in Nanosized Graphite Sheets. Journal of Physical Chemistry B, 2004, 108, 7565-7572.	1.2	31
45	Theoretical Measurements of Conductance in an (AT)12 DNA Molecule. ChemPhysChem, 2003, 4, 1256-1260.	1.0	30
46	Conduction paths in Cu/amorphous-Ta2O5/Pt atomic switch: First-principles studies. Journal of Applied Physics, 2014, 115, .	1.1	30
47	Realization of Mott-insulating electrides in dimorphic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">Y</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>5</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physi	1.1	30
48	Theoretical analysis of space charge layer formation at metal/ionic conductor interfaces. Solid State Ionics, 2011, 183, 20-25.	1.3	28
49	Room-Temperature Fast H^{â€“} Conduction in Oxygen-Substituted Lanthanum Hydride. Journal of the American Chemical Society, 2022, 144, 1523-1527.	6.6	27
50	Quantum Transport Effects in Copper(II) Phthalocyanine Sandwiched between Gold Nanoelectrodes. Journal of Physical Chemistry B, 2005, 109, 12443-12448.	1.2	26
51	Migration of Ag in low-temperature Ag2S from first principles. Journal of Chemical Physics, 2008, 128, 014704.	1.2	26
52	First-Principles and Microkinetic Study on the Mechanism for Ammonia Synthesis Using Ru-Loaded Hydride Catalyst. Journal of Physical Chemistry C, 2020, 124, 2070-2078.	1.5	25
53	Surface electron states on the quasi-two-dimensional excess-electron compounds<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ca</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Y</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:math>. Physical Review B, 2017, 95, .	1.1	21
54	Selfâ€organized Rutheniumâ€“Barium Coreâ€“Shell Nanoparticles on a Mesoporous Calcium Amide Matrix for Efficient Lowâ€Temperature Ammonia Synthesis. Angewandte Chemie, 2018, 130, 2678-2682.	1.6	21

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55	Single-molecule junctions of multinuclear organometallic wires: long-range carrier transport brought about by metalâ€“metal interaction. Chemical Science, 2021, 12, 4338-4344.	3.7	21
56	Controlling stacking order and charge transport in Ï€-stacks of aromatic molecules based on surface assembly. Chemical Communications, 2018, 54, 12443-12446.	2.2	20
57	Ring shape-dependent self-sorting of pillar[n]arenes assembled on a surface. Communications Chemistry, 2018, 1, .	2.0	19
58	How fluorine minimizes density fluctuations of silica glass: Molecular dynamics study with machine-learning assisted force-matching potential. Materials and Design, 2021, 197, 109210.	3.3	18
59	Anionic Stannaferrocene and Its Unique Electronic State. Chemistry Letters, 2019, 48, 163-165.	0.7	16
60	Difficulty of carrier generation in orthorhombic PbO. Journal of Applied Physics, 2016, 119, .	1.1	14
61	Molecular dynamics study on the coâ€doping effect of Al₂O₃ and fluorine to reduce Rayleigh scattering of silica glass. Journal of the American Ceramic Society, 2021, 104, 5001-5015.	1.9	13
62	Electrostatic and dynamical effects of an aqueous solution on the zero-bias conductance of a single molecule: A first-principles study. Physical Review B, 2009, 80, .	1.1	12
63	Molecular orbital concept on spin-flip transport in molecular junctions. Theoretical Chemistry Accounts, 2011, 130, 775-788.	0.5	12
64	Theoretical study on temperature effect of electronic structure and spin state in LaCoO3 by using density functional theory. Solid State Ionics, 2016, 285, 195-201.	1.3	12
65	First-Principles Study of the Adsorption Behavior of Triptycene Molecular Tripods on Au(111): Site Selectivity and Unambiguous Molecular Orientation. Journal of Physical Chemistry C, 2019, 123, 4401-4406.	1.5	12
66	Comparative Study of Charged and Neutral Oxygen Vacancies in Cubic Zirconia from First Principles. Applied Physics Express, 0, 2, 061402.	1.1	11
67	Single-Molecule Junction of a Cationic Rh(III) Polyyne Molecular Wire. Inorganic Chemistry, 2020, 59, 13254-13261.	1.9	11
68	Many-body calculations for periodic materials via restricted Boltzmann machine-based VQE. Quantum Science and Technology, 2021, 6, 025015.	2.6	11
69	Crystal and electronic structure engineering of tin monoxide by external pressure. Journal of Advanced Ceramics, 2021, 10, 565-577.	8.9	11
70	Suppression of Rayleigh Scattering in Silica Glass by Codoping Boron and Fluorine: Molecular Dynamics Simulations with Force-Matching and Neural Network Potentials. Journal of Physical Chemistry C, 2022, 126, 2264-2275.	1.5	11
71	Stabilization Factor of Anion-Excess Fluorite Phase for Fast Anion Conduction. Chemistry of Materials, 2021, 33, 1867-1874.	3.2	10
72	Computational Study on Stable Structures, Formation Energies, and Conductance of Single Benzene-dithiolate between Two Au Electrodes. Japanese Journal of Applied Physics, 2005, 44, 7729-7731.	0.8	9

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73	Parallel-sheets model analysis of space charge layer formation at metal/ionic conductor interfaces. Solid State Ionics, 2012, 226, 62-70.	1.3	9
74	The role of lattice vibration in the terahertz region for proton conduction in 2D metalâ€“organic frameworks. Chemical Science, 2020, 11, 1538-1541.	3.7	9
75	Control of dominant conduction orbitals by peripheral substituents in paddle-wheel diruthenium alkynyl molecular junctions. Chemical Science, 2021, 12, 10871-10877.	3.7	9
76	The contributions of chalcogen to the peierls instability in model crystals of charge-transfer complexes. Synthetic Metals, 1998, 95, 169-177.	2.1	8
77	One-hundred-nm-scale electronic structure and transport calculations of organic polymers on the K computer. AIP Conference Proceedings, 2016, , .	0.3	8
78	Interlayer states arising from anionic electrons in the honeycomb-lattice-based compounds AeAlSi () Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.1	8
79	Characteristic mechanism for fast <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msup><mml:mi mathvariant="normal">H</mml:mi><mml:mo>â’</mml:mo></mml:msup></mml:math> conduction in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si15.svg"><mml:mrow><mml:msub><mml:mtext>LaH</mml:mtext><mml:mrow><mml:mn>2.5</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>0.25</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>.	3.8	8
80	Molecular orbital approach to the Peierls instability in polyenes and its application to model crystals of charge-transfer complexes. International Journal of Quantum Chemistry, 1997, 64, 325-336.	1.0	7
81	Hybrid Molecular Junctions Using Auâ€“S and Auâ¯Ï€ Bindings. Journal of Physical Chemistry C, 2020, 124, 9261-9268.	1.5	7
82	First Principles Study of Oxygen Vacancies Near Nickel/Zirconia Interface. E-Journal of Surface Science and Nanotechnology, 2010, 8, 93-100.	0.1	6
83	Elastic Transient Energy Transport and Energy Balance in a Single-Level Quantum Dot System. Japanese Journal of Applied Physics, 2012, 51, 094303.	0.8	6
84	Anomalous metallic-like transport of Coâ€“Pd ferromagnetic nanoparticles cross-linked with Ï€-conjugated molecules having a rotational degree of freedom. Physical Chemistry Chemical Physics, 2014, 16, 288-296.	1.3	6
85	Predictive Microkinetic Model for Solid Oxide Fuel Cell Patterned Anode: Based on an Extensive Literature Survey and Exhaustive Simulations. Journal of Physical Chemistry C, 2017, 121, 19069-19079.	1.5	6
86	First Principles Evolutionary Search for New Electrides along the Dimensionality of Anionic Electrons. Journal of Computer Chemistry Japan, 2017, 16, 135-138.	0.0	6
87	Electronic Correlation Strength of Inorganic Electrides from First Principles. Journal of Physical Chemistry Letters, 2021, 12, 12020-12025.	2.1	6
88	An analytical molecular orbital approach for modeling of low-dimensional conductors in molecular crystals. International Journal of Quantum Chemistry, 2002, 86, 401-415.	1.0	5
89	An analytical molecular orbital approach in tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ). Molecular Physics, 2004, 102, 1891-1901.	0.8	5
90	Theoretical study of four-probe resistance in nanoscale measurements: Monatomic carbon chains and (5,5)-carbon nanotubes. Physical Review B, 2009, 79, .	1.1	5

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91	The Key Indicator for the Control of Metal Particle Sizes on Supports from First-Principles and Experimental Observation. Journal of Physical Chemistry C, 2016, 120, 21879-21887.	1.5	5
92	Dopant driven tuning of the hydrogen oxidation mechanism at the pore/nickel/zirconia triple phase boundary. Physical Chemistry Chemical Physics, 2018, 20, 12574-12588.	1.3	4
93	Organometallic Molecular Wires with Thioacetylene Backbones, transâ€{RSâ€(Câ‰¡C)_n}₂Ru(phosphine)₄: High Conductance through Nonâ€Aromatic Bridging Linkers. Chemistry - A European Journal, 2021, 27, 9666-9673.	3.7	4
94	Effects of energetic stability in transport measurements of single benzene-dithiolate by the STM break junction technique. Chemical Physics Letters, 2006, 428, 367-370.	1.2	3
95	Hyperfine switching triggered by resonant tunneling for the detection of a single nuclear spin qubit. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 6690-6693.	0.9	3
96	Inelastic transient electrical currents and phonon heating in a single-level quantum dot system. Journal of Applied Physics, 2013, 113, 123701.	1.1	3
97	First-Principles Study of Dopant Effect on Hydrogen Oxidation in Anode of Solid Oxide Fuel Cell. ECS Transactions, 2017, 78, 1469-1475.	0.3	3
98	Transition Metal-doped Ru Nanoparticles Loaded on Metal Hydrides for Efficient Ammonia Synthesis from First Principles. Journal of Physical Chemistry C, 2020, 124, 1529-1534.	1.5	3
99	Efficientab initiomolecular-orbital approach to quasi-one-dimensional molecular crystals based on neighboring-interaction-localized molecular orbitals. Physical Review B, 2002, 65, .	1.1	2
100	Poly(para-phenylene) with the end structure ofCH2â^'(C6H4)nâ^'Hprovides nearly zero band gaps in long chains withn>6. Physical Review B, 2002, 66, .	1.1	2
101	Submatrix inversion approach to the ab initio Green's function method for electrical transport. E-Journal of Surface Science and Nanotechnology, 2006, 4, 484-489.	0.1	2
102	Chemically Softened Boundary of Metal/Vacuum/Solid-Electrolyte from First Principles. Journal of Physical Chemistry C, 2009, 113, 17780-17786.	1.5	2
103	Parallelized Meso-Scale Kinetic Monte Carlo Simulations for SOFC Characterization. ECS Transactions, 2013, 57, 2437-2447.	0.3	2
104	Zirconium-peroxo embedded in non-stoichiometric yttria stabilized zirconia (110) from first-principles. Solid State Ionics, 2016, 285, 215-221.	1.3	2
105	Elastic Transient Energy Transport and Energy Balance in a Single-Level Quantum Dot System. Japanese Journal of Applied Physics, 2012, 51, 094303.	0.8	2
106	Tight-Binding Analysis of Surface Electronic Conduction Measured with Micro-Multipoint Scanning Tunneling Microscopy Probes. Japanese Journal of Applied Physics, 2006, 45, 2136-2139.	0.8	1
107	Effects of Molecular Dynamics on Electrical Conductance of Single Molecular Junction in Aqueous Solution: First Principles Calculations. E-Journal of Surface Science and Nanotechnology, 2010, 8, 38-43.	0.1	1
108	Inside Cover: Electron Transport through Single Molecules Comprising Aromatic Stacks Enclosed in Self-Assembled Cages (Angew. Chem. Int. Ed. 25/2011). Angewandte Chemie - International Edition, 2011, 50, 5588-5588.	7.2	1

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109	Multi-Scale, Multi-Physics Approach for Solid Oxide Fuel Cell Anode Reaction. ECS Transactions, 2017, 78, 2835-2844.	0.3	1
110	Wave-packet multi-scale simulations based on a non-linear tight-binding Hamiltonian for carrier transport in Ï€-conjugated polymers. Materials Chemistry Frontiers, 2018, 2, 1351-1359.	3.2	1
111	Non-equilibrium thermal transport simulation of conical carbon nanofibers. Transactions of the Materials Research Society of Japan, 2013, 38, 183-186.	0.2	1
112	Effects of resonant scattering by probe contacts on nanoscale four-probe resistance measurements. New Journal of Physics, 2010, 12, 083017.	1.2	0
113	Orbital Rule for Electron Transport of Molecular Junctions. , 2016, , 165-190.		0
114	Full Atomistic Kinetic Monte Carlo and First Principles Study on Electromotive Force of SOFC with Direct Counting Approach. ECS Transactions, 2017, 78, 2815-2822.	0.3	0
115	Accurate meso-scale dynamics by kinetic Monte Carlo simulation via free energy multicanonical sampling: oxygen vacancy diffusion in BaTiO3. Science and Technology of Advanced Materials Methods, 2021, 1, 109-122.	0.4	0
116	Simulation for Measurements of Electric Properties of Surface Nanostructures. , 2007, , 119-124.		0
117	Theoretical Study of Quantum Interference Effects on Nanoscale Four-probe Measurements. Hyomen Kagaku, 2010, 31, 374-379.	0.0	0