

Tomofumi Tada

List of Publications by Year in descending order

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117
papers

4,658
citations

94381

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106281

65
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125
all docs

125
docs citations

125
times ranked

4603
citing authors

#	ARTICLE	IF	CITATIONS
1	Suppression of Rayleigh Scattering in Silica Glass by Codoping Boron and Fluorine: Molecular Dynamics Simulations with Force-Matching and Neural Network Potentials. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2264-2275.	1.5	11
2	Room-Temperature Fast H ⁺ Conduction in Oxygen-Substituted Lanthanum Hydride. <i>Journal of the American Chemical Society</i> , 2022, 144, 1523-1527. Characteristic mechanism for fast H^+ conduction in	6.6	27
3	$\text{LaH}_{2.5}\text{O}_{0.25}$	3.8	8
4	How fluorine minimizes density fluctuations of silica glass: Molecular dynamics study with machine-learning assisted force-matching potential. <i>Materials and Design</i> , 2021, 197, 109210.	3.3	18
5	Accurate meso-scale dynamics by kinetic Monte Carlo simulation via free energy multicanonical sampling: oxygen vacancy diffusion in BaTiO ₃ . <i>Science and Technology of Advanced Materials Methods</i> , 2021, 1, 109-122.	0.4	0
6	Stabilization Factor of Anion-Excess Fluorite Phase for Fast Anion Conduction. <i>Chemistry of Materials</i> , 2021, 33, 1867-1874.	3.2	10
7	Many-body calculations for periodic materials via restricted Boltzmann machine-based VQE. <i>Quantum Science and Technology</i> , 2021, 6, 025015.	2.6	11
8	Molecular dynamics study on the codoping effect of Al ₂ O ₃ and fluorine to reduce Rayleigh scattering of silica glass. <i>Journal of the American Ceramic Society</i> , 2021, 104, 5001-5015.	1.9	13
9	Crystal and electronic structure engineering of tin monoxide by external pressure. <i>Journal of Advanced Ceramics</i> , 2021, 10, 565-577.	8.9	11
10	Organometallic Molecular Wires with Thioacetylene Backbones, $\text{[Ru}(\text{phosphine})_4\text{]}_2$: High Conductance through Non-Aromatic Bridging Linkers. <i>Chemistry - A European Journal</i> , 2021, 27, 9666-9673.	2.7	4
11	Control of dominant conduction orbitals by peripheral substituents in paddle-wheel diruthenium alkynyl molecular junctions. <i>Chemical Science</i> , 2021, 12, 10871-10877.	3.7	9
12	Single-molecule junctions of multinuclear organometallic wires: long-range carrier transport brought about by metal-metal interaction. <i>Chemical Science</i> , 2021, 12, 4338-4344.	3.7	21
13	Electronic Correlation Strength of Inorganic Electrides from First Principles. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12020-12025.	2.1	6
14	The role of lattice vibration in the terahertz region for proton conduction in 2D metal-organic frameworks. <i>Chemical Science</i> , 2020, 11, 1538-1541.	3.7	9
15	First-Principles and Microkinetic Study on the Mechanism for Ammonia Synthesis Using Ru-Loaded Hydride Catalyst. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2070-2078.	1.5	25
16	Transition Metal-doped Ru Nanoparticles Loaded on Metal Hydrides for Efficient Ammonia Synthesis from First Principles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1529-1534.	1.5	3
17	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. <i>Chemistry of Materials</i> , 2020, 32, 6947-6957.	3.2	89
18	Vacancy-enabled N ₂ activation for ammonia synthesis on an Ni-loaded catalyst. <i>Nature</i> , 2020, 583, 391-395.	13.7	309

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19	Single-Molecule Junction of a Cationic Rh(III) Polyynes Molecular Wire. <i>Inorganic Chemistry</i> , 2020, 59, 13254-13261.	1.9	11
20	Hybrid Molecular Junctions Using Au-S and Au-Te Bindings. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9261-9268.	1.5	7
21	Characteristic fast H ⁺ ion conduction in oxygen-substituted lanthanum hydride. <i>Nature Communications</i> , 2019, 10, 2578.	5.8	70
22	Discovery of hexagonal ternary phase Ti ₂ InB ₂ and its evolution to layered boride TiB. <i>Nature Communications</i> , 2019, 10, 2284.	5.8	159
23	Triptycene Tripods for the Formation of Highly Uniform and Densely Packed Self-Assembled Monolayers with Controlled Molecular Orientation. <i>Journal of the American Chemical Society</i> , 2019, 141, 5995-6005.	6.6	48
24	First-Principles Study of the Adsorption Behavior of Triptycene Molecular Tripods on Au(111): Site Selectivity and Unambiguous Molecular Orientation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4401-4406.	1.5	12
25	Low-Temperature Synthesis of Perovskite Oxynitride-Hydrides as Ammonia Synthesis Catalysts. <i>Journal of the American Chemical Society</i> , 2019, 141, 20344-20353.	6.6	106
26	Palladium-bearing intermetallic electride as an efficient and stable catalyst for Suzuki cross-coupling reactions. <i>Nature Communications</i> , 2019, 10, 5653.	5.8	43
27	Anionic Stannaferrocene and Its Unique Electronic State. <i>Chemistry Letters</i> , 2019, 48, 163-165.	0.7	16
28	High Electron Density on Ru in Intermetallic YRu ₂ : The Application to Catalyst for Ammonia Synthesis. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10468-10475.	1.5	43
29	Dopant driven tuning of the hydrogen oxidation mechanism at the pore/nickel/zirconia triple phase boundary. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12574-12588.	1.3	4
30	Large Oblate Hemispheroidal Ruthenium Particles Supported on Calcium Amide as Efficient Catalysts for Ammonia Decomposition. <i>Chemistry - A European Journal</i> , 2018, 24, 7976-7984.	1.7	34
31	Self-Organized Ruthenium-Barium Core-Shell Nanoparticles on a Mesoporous Calcium Amide Matrix for Efficient Low-Temperature Ammonia Synthesis. <i>Angewandte Chemie</i> , 2018, 130, 2678-2682.	1.6	21
32	Self-Organized Ruthenium-Barium Core-Shell Nanoparticles on a Mesoporous Calcium Amide Matrix for Efficient Low-Temperature Ammonia Synthesis. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 2648-2652.	7.2	144
33	Ternary intermetallic LaCoSi as a catalyst for N ₂ activation. <i>Nature Catalysis</i> , 2018, 1, 178-185.	16.1	221
34	Ring shape-dependent self-sorting of pillar[n]arenes assembled on a surface. <i>Communications Chemistry</i> , 2018, 1, .	2.0	19
35	Realization of novel insulating electrides in dimorphic $\text{Yb}_3\text{Mg}_2\text{Si}_2$ and $\text{Yb}_3\text{Mg}_2\text{Si}_2$. <i>Chemical Communications</i> , 2018, 1, .	1.1	30
36	Controlling stacking order and charge transport in π -stacks of aromatic molecules based on surface assembly. <i>Chemical Communications</i> , 2018, 54, 12443-12446.	2.2	20

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37	Enhanced Catalytic Ammonia Synthesis with Transformed BaO. ACS Catalysis, 2018, 8, 10977-10984.	5.5	59
38	“Doping” of Polyyne with an Organometallic Fragment Leads to Highly Conductive Metallapolyne Molecular Wire. Journal of the American Chemical Society, 2018, 140, 10080-10084.	6.6	78
39	Wave-packet multi-scale simulations based on a non-linear tight-binding Hamiltonian for carrier transport in π -conjugated polymers. Materials Chemistry Frontiers, 2018, 2, 1351-1359.	3.2	1
40	Triphosphasumanene Trisulfide: High Out-of-Plane Anisotropy and Janus-Type π -Surfaces. Journal of the American Chemical Society, 2017, 139, 5787-5792.	6.6	75
41	A Stable, Soluble, and Crystalline Supramolecular System with a Triplet Ground State. Angewandte Chemie - International Edition, 2017, 56, 4261-4265.	7.2	40
42	Interlayer states arising from anionic electrons in the honeycomb-lattice-based compounds $AeAlSi_2$. <i>Journal of Physical Chemistry C</i> , 2017, 121, 10787-10792.	1.1	8
43	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
44	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
45	Multi-Scale, Multi-Physics Approach for Solid Oxide Fuel Cell Anode Reaction. ECS Transactions, 2017, 78, 2835-2844.	0.3	1
46	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
47	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
48	Copper-Based Intermetallic Electride Catalyst for Chemoselective Hydrogenation Reactions. Journal of the American Chemical Society, 2017, 139, 17089-17097.	6.6	90
49	Semimetallic Two-Dimensional TiB_{12} : Improved Stability and Electronic Properties Tunable by Biaxial Strain. Chemistry of Materials, 2017, 29, 5922-5930.	3.2	41
50	Surface electron states on the quasi-two-dimensional excess-electron compounds $Ca_{2}N$ and Ca_2Y . <i>Physical Review B</i> , 2017, 95, .	1.1	21
51	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
52	Anchoring Bond between Ru and N Atoms of Ru/Ca_2NH Catalyst: Crucial for the High Ammonia Synthesis Activity. Journal of Physical Chemistry C, 2017, 121, 20900-20904.	1.5	33
53	Essential role of hydride ion in ruthenium-based ammonia synthesis catalysts. Chemical Science, 2016, 7, 4036-4043.	3.7	195
54	One-hundred-nm-scale electronic structure and transport calculations of organic polymers on the K computer. AIP Conference Proceedings, 2016, , .	0.3	8

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55	Resolving metal-molecule interfaces at single-molecule junctions. <i>Scientific Reports</i> , 2016, 6, 26606.	1.6	55
56	Orbital Rule for Electron Transport of Molecular Junctions. , 2016, , 165-190.		0
57	Zirconium-peroxo embedded in non-stoichiometric yttria stabilized zirconia (110) from first-principles. <i>Solid State Ionics</i> , 2016, 285, 215-221.	1.3	2
58	The Key Indicator for the Control of Metal Particle Sizes on Supports from First-Principles and Experimental Observation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21879-21887.	1.5	5
59	Difficulty of carrier generation in orthorhombic PbO. <i>Journal of Applied Physics</i> , 2016, 119, .	1.1	14
60	Organometallic molecular wires as versatile modules for energy-level alignment of the metalâ€“moleculeâ€“metal junction. <i>Chemical Communications</i> , 2016, 52, 5796-5799.	2.2	45
61	Water Durable Electride $Y_{5-x}Si_x$: Electronic Structure and Catalytic Activity for Ammonia Synthesis. <i>Journal of the American Chemical Society</i> , 2016, 138, 3970-3973.	6.6	217
62	Theoretical study on temperature effect of electronic structure and spin state in LaCoO ₃ by using density functional theory. <i>Solid State Ionics</i> , 2016, 285, 195-201.	1.3	12
63	Molecular design of electron transport with orbital rule: toward conductance-decay free molecular junctions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 32099-32110.	1.3	40
64	Rectifying Electron-Transport Properties through Stacks of Aromatic Molecules Inserted into a Self-Assembled Cage. <i>Journal of the American Chemical Society</i> , 2015, 137, 5939-5947.	6.6	126
65	Conduction paths in Cu/amorphous-Ta ₂ O ₅ /Pt atomic switch: First-principles studies. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	30
66	Anomalous metallic-like transport of Coâ€“Pd ferromagnetic nanoparticles cross-linked with Î€-conjugated molecules having a rotational degree of freedom. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 288-296.	1.3	6
67	High-Throughput ab Initio Screening for Two-Dimensional Electride Materials. <i>Inorganic Chemistry</i> , 2014, 53, 10347-10358.	1.9	107
68	Design principle for increasing charge mobility of Î€-conjugated polymers using regularly localized molecular orbitals. <i>Nature Communications</i> , 2013, 4, 1691.	5.8	115
69	Parallelized Meso-Scale Kinetic Monte Carlo Simulations for SOFC Characterization. <i>ECS Transactions</i> , 2013, 57, 2437-2447.	0.3	2
70	Highly Conductive [3Åâ€“ <i>n</i>] Goldâ€“ion Clusters Enclosed within Selfâ€“Assembled Cages. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6202-6205.	7.2	69
71	Inelastic transient electrical currents and phonon heating in a single-level quantum dot system. <i>Journal of Applied Physics</i> , 2013, 113, 123701.	1.1	3
72	Non-equilibrium thermal transport simulation of conical carbon nanofibers. <i>Transactions of the Materials Research Society of Japan</i> , 2013, 38, 183-186.	0.2	1

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73	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
74	Parallel-sheets model analysis of space charge layer formation at metal/ionic conductor interfaces. Solid State Ionics, 2012, 226, 62-70.	1.3	9
75	Single-Molecule Conductance of π -Conjugated Rotaxane: New Method for Measuring Stipulated Electric Conductance of π -Conjugated Molecular Wire Using STM Break Junction. Small, 2012, 8, 726-730.	5.2	67
76	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
77	Molecular orbital concept on spin-flip transport in molecular junctions. Theoretical Chemistry Accounts, 2011, 130, 775-788.	0.5	12
78	Electron Transport through Single Molecules Comprising Aromatic Stacks Enclosed in Self-Assembled Cages. Angewandte Chemie - International Edition, 2011, 50, 5708-5711.	7.2	92
79	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
80	Theoretical analysis of space charge layer formation at metal/ionic conductor interfaces. Solid State Ionics, 2011, 183, 20-25.	1.3	28
81	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
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	Conductive Path Formation in the Ta ₂ O ₅ Atomic Switch: First-Principles Analyses. ACS Nano, 2010, 4, 6477-6482.	7.3	50
84	Effects of resonant scattering by probe contacts on nanoscale four-probe resistance measurements. New Journal of Physics, 2010, 12, 083017.	1.2	0
85	Theoretical Study of Quantum Interference Effects on Nanoscale Four-probe Measurements. Hyomen Kagaku, 2010, 31, 374-379.	0.0	0
86	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
87	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
88	First-principles simulations on bulk Ta ₂ O ₅ and Cu/Ta ₂ O ₅ /Pt heterojunction: Electronic structures and transport properties. Journal of Applied Physics, 2009, 106, .	1.1	51
89	Chemically Softened Boundary of Metal/Vacuum/Solid-Electrolyte from First Principles. Journal of Physical Chemistry C, 2009, 113, 17780-17786.	1.5	2
90	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

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91	Orbital Views of the Electron Transport in Molecular Devices. <i>Journal of the American Chemical Society</i> , 2008, 130, 9406-9413.	6.6	223
92	Migration of Ag in low-temperature Ag ₂ S from first principles. <i>Journal of Chemical Physics</i> , 2008, 128, 014704.	1.2	26
93	Excess-silver-induced bridge formation in a silver sulfide atomic switch. <i>Applied Physics Letters</i> , 2008, 93, .	1.5	46
94	Nonequilibrium Quantum Transport Properties of a Silver Atomic Switch. <i>Nano Letters</i> , 2007, 7, 2688-2692.	4.5	55
95	Simulation for Measurements of Electric Properties of Surface Nanostructures. , 2007, , 119-124.		0
96	Submatrix inversion approach to the ab initio Green's function method for electrical transport. <i>E-Journal of Surface Science and Nanotechnology</i> , 2006, 4, 484-489.	0.1	2
97	Effects of energetic stability in transport measurements of single benzene-dithiolate by the STM break junction technique. <i>Chemical Physics Letters</i> , 2006, 428, 367-370.	1.2	3
98	Tight-Binding Analysis of Surface Electronic Conduction Measured with Micro-Multipoint Scanning Tunneling Microscopy Probes. <i>Japanese Journal of Applied Physics</i> , 2006, 45, 2136-2139.	0.8	1
99	A theoretical measurement of the quantum transport through an optical molecular switch. <i>Chemical Physics Letters</i> , 2005, 412, 55-59.	1.2	66
100	Computational Study on Stable Structures, Formation Energies, and Conductance of Single Benzene-dithiolate between Two Au Electrodes. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 7729-7731.	0.8	9
101	Quantum Transport Effects in Copper(II) Phthalocyanine Sandwiched between Gold Nanoelectrodes. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12443-12448.	1.2	26
102	Green's function formalism coupled with Gaussian broadening of discrete states for quantum transport: Application to atomic and molecular wires. <i>Journal of Chemical Physics</i> , 2004, 121, 8050.	1.2	55
103	Oscillation of Conductance in Molecular Junctions of Carbon Ladder Compounds. <i>Journal of the American Chemical Society</i> , 2004, 126, 14182-14189.	6.6	49
104	An analytical molecular orbital approach in tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ). <i>Molecular Physics</i> , 2004, 102, 1891-1901.	0.8	5
105	Reverse Exponential Decay of Electrical Transmission in Nanosized Graphite Sheets. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7565-7572.	1.2	31
106	Wire-Length Dependence of the Conductance of Oligo(p-phenylene) Dithiolate Wires: A Consideration from Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9143-9149.	1.1	66
107	Highly Versatile Organostibine Mediators for Living Radical Polymerization. <i>Journal of the American Chemical Society</i> , 2004, 126, 13908-13909.	6.6	189
108	Theoretical Measurements of Conductance in an (AT) ₁₂ DNA Molecule. <i>ChemPhysChem</i> , 2003, 4, 1256-1260.	1.0	30

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109	Molecular Orbital Interactions in the Nanostar Dendrimer. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14204-14210.	1.2	34
110	Quantum Transport Effects in Nanosized Graphite Sheets. II. Enhanced Transport Effects by Heteroatoms. <i>Journal of Physical Chemistry B</i> , 2003, 107, 8789-8793.	1.2	35
111	Efficient ab initio molecular-orbital approach to quasi-one-dimensional molecular crystals based on neighboring-interaction-localized molecular orbitals. <i>Physical Review B</i> , 2002, 65, .	1.1	2
112	Poly(para-phenylene) with the end structure of $\text{CH}_2^{\sim}(\text{C}_6\text{H}_4)_n^{\sim}\text{H}$ provides nearly zero band gaps in long chains with $n > 6$. <i>Physical Review B</i> , 2002, 66, .	1.1	2
113	Quantum Transport Effects in Nanosized Graphite Sheets. <i>ChemPhysChem</i> , 2002, 3, 1035-1037.	1.0	90
114	An analytical molecular orbital approach for modeling of low-dimensional conductors in molecular crystals. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 401-415.	1.0	5
115	The contributions of chalcogen to the Peierls instability in model crystals of charge-transfer complexes. <i>Synthetic Metals</i> , 1998, 95, 169-177.	2.1	8
116	Molecular orbital approach to the Peierls instability in polyenes and its application to model crystals of charge-transfer complexes. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 325-336.	1.0	7
117	Comparative Study of Charged and Neutral Oxygen Vacancies in Cubic Zirconia from First Principles. <i>Applied Physics Express</i> , 0, 2, 061402.	1.1	11