

Tatsuhiko Ohto

List of Publications by Year in descending order

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65
papers

2,504
citations

159585

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all docs

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docs citations

69
times ranked

3187
citing authors

#	ARTICLE	IF	CITATIONS
1	Single-Molecule Conductance of a π -Hybridized Tripodal Anchor while Maintaining Electronic Communication. <i>Small</i> , 2021, 17, 2006709.	10.0	3
2	Improving Intramolecular Hopping Charge Transport via Periodical Segmentation of π -Conjugation in a Molecule. <i>Journal of the American Chemical Society</i> , 2021, 143, 599-603.	13.7	14
3	Single-Molecule Electronics: Single-Molecule Conductance of a π -Hybridized Tripodal Anchor while Maintaining Electronic Communication (<i>Small</i> 3/2021). <i>Small</i> , 2021, 17, 2170012.	10.0	0
4	Acceleration of Electrochemical CO ₂ Reduction to Formate at the Sn/Reduced Graphene Oxide Interface. <i>ACS Catalysis</i> , 2021, 11, 3310-3318.	11.2	92
5	Phase-Dependent Electrochemical CO ₂ Reduction Ability of NiSn Alloys for Formate Generation. <i>ACS Applied Energy Materials</i> , 2021, 4, 7122-7128.	5.1	13
6	Polyethylene Glycol Covered Sn Catalysts Accelerate the Formation Rate of Formate by Carbon Dioxide Reduction. <i>ACS Catalysis</i> , 2021, 11, 9962-9969.	11.2	22
7	Geometric model of 3D curved graphene with chemical dopants. <i>Carbon</i> , 2021, 182, 223-232.	10.3	7
8	Control of dominant conduction orbitals by peripheral substituents in paddle-wheel diruthenium alkynyl molecular junctions. <i>Chemical Science</i> , 2021, 12, 10871-10877.	7.4	9
9	Catalytic activity of graphene-covered non-noble metals governed by proton penetration in electrochemical hydrogen evolution reaction. <i>Nature Communications</i> , 2021, 12, 203.	12.8	77
10	Impact of intermolecular vibrational coupling effects on the sum-frequency generation spectra of the water/air interface. <i>Molecular Physics</i> , 2020, 118, 1620358.	1.7	22
11	Effect of Graphene Encapsulation of NiMo Alloys on Oxygen Evolution Reaction. <i>ACS Catalysis</i> , 2020, 10, 792-799.	11.2	60
12	Correlation between the Dipole Moment of Nonfullerene Acceptors and the Active Layer Morphology of Green-Solvent-Processed P3HT-Based Organic Solar Cells. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 19013-19022.	6.7	10
13	Vibrational couplings and energy transfer pathways of water's bending mode. <i>Nature Communications</i> , 2020, 11, 5977.	12.8	50
14	Vibrational mode frequency correction of liquid water in density functional theory molecular dynamics simulations with van der Waals correction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12785-12793.	2.8	9
15	Hydrogen Bonds and Molecular Orientations of Supramolecular Structure between Barbituric Acid and Melamine Derivative at the Air/Water Interface Revealed by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2422-2429.	4.6	22
16	Molecular Structure and Modeling of Water-Air and Ice-Air Interfaces Monitored by Sum-Frequency Generation. <i>Chemical Reviews</i> , 2020, 120, 3633-3667.	47.7	97
17	Mechanical switching of current-voltage characteristics in spiropyran single-molecule junctions. <i>Nanoscale</i> , 2020, 12, 7527-7531.	5.6	19
18	Decoding the molecular water structure at complex interfaces through surface-specific spectroscopy of the water bending mode. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10934-10940.	2.8	11

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19	Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water–Air Interface. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4914-4919.	4.6	43
20	Effects of <i>cis</i> – <i>trans</i> Conformation between Thiophene Rings on Conductance of Oligothiophenes. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5292-5296.	4.6	11
21	Sun <i>et al.</i> Reply. <i>Physical Review Letters</i> , 2019, 123, 099602.	7.8	1
22	Boosting electrochemical water splitting <i>via</i> ternary NiMoCo hybrid nanowire arrays. <i>Journal of Materials Chemistry A</i> , 2019, 7, 2156-2164.	10.3	163
23	Highly Planar and Completely Insulated Oligothiophenes: Effects of π -Conjugation on Hopping Charge Transport. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3197-3204.	4.6	17
24	Structure and Dynamics of Water at the Water–Air Interface Using First-Principles Molecular Dynamics Simulations. II. NonLocal vs Empirical van der Waals Corrections. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3836-3843.	5.3	12
25	Chemical Dopants on Edge of Holey Graphene Accelerate Electrochemical Hydrogen Evolution Reaction. <i>Advanced Science</i> , 2019, 6, 1900119.	11.2	90
26	Three site molecular orbital controlled single-molecule rectifiers based on perpendicularly linked porphyrin–imide dyads. <i>Nanoscale</i> , 2019, 11, 22724-22729.	5.6	5
27	Structure and Dynamics of Water at the Water–Air Interface Using First-Principles Molecular Dynamics Simulations within Generalized Gradient Approximation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 595-602.	5.3	18
28	Aggregation-Induced Emission Enhancement from Disilane-Bridged Donor–Acceptor–Donor Luminogens Based on the Triarylamine Functionality. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 12164-12172.	8.0	45
29	Structure and dynamics of water at water–graphene and water–hexagonal boron-nitride sheet interfaces revealed by <i>ab initio</i> sum-frequency generation spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12979-12985.	2.8	53
30	Cooperation between holey graphene and NiMo alloy for hydrogen evolution in an acidic electrolyte. <i>ACS Catalysis</i> , 2018, 8, 3579-3586.	11.2	98
31	Definition of Free O–H Groups of Water at the Air–Water Interface. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 357-364.	5.3	46
32	Single-molecule rectifiers based on voltage-dependent deformation of molecular orbitals in carbazole oligomers. <i>Nanoscale</i> , 2018, 10, 19818-19824.	5.6	17
33	Oriental Distribution of Free O-H Groups of Interfacial Water is Exponential. <i>Physical Review Letters</i> , 2018, 121, 246101.	7.8	49
34	Large Hydrogen-Bond Mismatch between TMAO and Urea Promotes Their Hydrophobic Association. <i>Chem</i> , 2018, 4, 2615-2627.	11.7	27
35	Graphene Layer Encapsulation of Non-Noble Metal Nanoparticles as Acid-Stable Hydrogen Evolution Catalysts. <i>ACS Energy Letters</i> , 2018, 3, 1539-1544.	17.4	57
36	Trimethylamine-N-oxide: its hydration structure, surface activity, and biological function, viewed by vibrational spectroscopy and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6909-6920.	2.8	39

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37	Chemisorbed and Physisorbed Water at the TiO ₂ /Water Interface. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2195-2199.	4.6	89
38	Electrochemical TERS Elucidates Potential-Induced Molecular Reorientation of Adenine/Au(111). <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9796-9801.	13.8	76
39	π-π stacking of imidazolium cations enhances molecular layering of room temperature ionic liquids at their interfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2850-2856.	2.8	42
40	Multifunctional Octamethyltetrasila[2.2]cyclophanes: Conformational Variations, Circularly Polarized Luminescence, and Organic Electroluminescence. <i>Journal of the American Chemical Society</i> , 2017, 139, 11214-11221.	13.7	73
41	Electrochemical TERS Elucidates Potential-Induced Molecular Reorientation of Adenine/Au(111). <i>Angewandte Chemie</i> , 2017, 129, 9928-9933.	2.0	12
42	Magnetic field effect on pentacene-doped sexithiophene diodes. <i>Applied Physics Letters</i> , 2017, 111, 203303.	3.3	0
43	Analysis of Single Molecule Conductance of Heterogeneous Porphyrin Arrays by Partial Transmission Probabilities. <i>ChemistrySelect</i> , 2017, 2, 7484-7488.	1.5	2
44	Highly Luminescent 2D-Type Slab Crystals Based on a Molecular Charge-Transfer Complex as Promising Organic Light-Emitting Transistor Materials. <i>Advanced Materials</i> , 2017, 29, 1701346.	21.0	111
45	Charge Transport Mechanisms in Oligothiophene Molecular Junctions Studied by Electrical Conductance and Thermopower Measurements. <i>Advances in Atom and Single Molecule Machines</i> , 2017, , 341-353.	0.0	0
46	Surface tension of ab initio liquid water at the water-air interface. <i>Journal of Chemical Physics</i> , 2016, 144, 204705.	3.0	39
47	Unveiling the Amphiphilic Nature of TMAO by Vibrational Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17435-17443.	3.1	33
48	Enhancement of Carrier Mobility through Deformation Potential in Metal-Containing Insulated Molecular Wires. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26637-26644.	3.1	8
49	Molecular Modeling of Water Interfaces: From Molecular Spectroscopy to Thermodynamics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3785-3796.	2.6	39
50	Toward <i>ab initio</i> molecular dynamics modeling for sum-frequency generation spectra; an efficient algorithm based on surface-specific velocity-velocity correlation function. <i>Journal of Chemical Physics</i> , 2015, 143, 124702.	3.0	100
51	Determination of the mechanism behind the organic magnetoresistance (OMAR) effect by using impedance spectroscopy. <i>International Journal of Nanotechnology</i> , 2015, 12, 238.	0.2	2
52	<i>Ab Initio</i> Liquid Water Dynamics in Aqueous TMAO Solution. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10597-10606.	2.6	44
53	Lipid Carbonyl Groups Terminate the Hydrogen Bond Network of Membrane-Bound Water. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4499-4503.	4.6	74
54	The surface roughness, but not the water molecular orientation varies with temperature at the water-air interface. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23559-23564.	2.8	60

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55	Influence of surface polarity on water dynamics at the water/rutile TiO ₂ (110) interface. Journal of Physics Condensed Matter, 2014, 26, 244102.	1.8	30
56	Single Molecular Resistive Switch Obtained via Sliding Multiple Anchoring Points and Varying Effective Wire Length. Journal of the American Chemical Society, 2014, 136, 7327-7332.	13.7	101
57	Thermopower of Benzenedithiol and C ₆₀ Molecular Junctions with Ni and Au Electrodes. Nano Letters, 2014, 14, 5276-5280.	9.1	57
58	Optical and redox properties of phenyl-capped cyclohexa[c]-oligothiophenes. Synthetic Metals, 2013, 181, 1-9.	3.9	2
59	Polarizable Site Charge Model at Liquid/Solid Interfaces for Describing Surface Polarity: Application to Structure and Molecular Dynamics of Water/Rutile TiO ₂ (110) Interface. Journal of Chemical Theory and Computation, 2013, 9, 1193-1201.	5.3	29
60	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
61	Chirality dependence of quantum thermal transport in carbon nanotubes at low temperatures: A first-principles study. Journal of Chemical Physics, 2013, 139, 044711.	3.0	6
62	<i>Ab initio</i> theory for current-induced molecular switching: Melamine on Cu(001). Physical Review B, 2013, 87, .	3.2	25
63	First-principles study of electronic structure and charge transport at PTCDA molecular layers on Ag(111) and Al(111) electrodes. Physical Review B, 2011, 84, .	3.2	7
64	Effect of Anchoring Group Position on Formation and Conductance of a Single Disubstituted Benzene Molecule Bridging Au Electrodes: Change of Conductive Molecular Orbital and Electron Pathway. Journal of Physical Chemistry C, 2010, 114, 22254-22261.	3.1	86
65	First-principles study of charge-density waves on Cu surfaces covered by In, Pb, and Bi atoms: Analysis of electronic structure and surface phonons. Physical Review B, 2010, 82, .	3.2	1