Tatsuhiko Ohto

List of Publications by Year in descending order

65 papers	2,504 citations	159585 30 h-index	197818 49 g-index
69 all docs	69 docs citations	69 times ranked	3187 citing authors

#	Article	IF	Citations
1	Boosting electrochemical water splitting via ternary NiMoCo hybrid nanowire arrays. Journal of Materials Chemistry A, 2019, 7, 2156-2164.	10.3	163
2	Highly Luminescent 2Dâ€Type Slab Crystals Based on a Molecular Chargeâ€Transfer Complex as Promising Organic Lightâ€Emitting Transistor Materials. Advanced Materials, 2017, 29, 1701346.	21.0	111
3	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
4	Toward ab initio molecular dynamics modeling for sum-frequency generation spectra; an efficient algorithm based on surface-specific velocity-velocity correlation function. Journal of Chemical Physics, 2015, 143, 124702.	3.0	100
5	Cooperation between holey graphene and NiMo alloy for hydrogen evolution in an acidic electrolyte. ACS Catalysis, 2018, 8, 3579-3586.	11.2	98
6	Molecular Structure and Modeling of Waterâ€“Air and Iceâ€“Air Interfaces Monitored by Sum-Frequency Generation. Chemical Reviews, 2020, 120, 3633-3667.	47.7	97
7	Acceleration of Electrochemical CO₂ Reduction to Formate at the Sn/Reduced Graphene Oxide Interface. ACS Catalysis, 2021, 11, 3310-3318.	11.2	92
8	Chemical Dopants on Edge of Holey Graphene Accelerate Electrochemical Hydrogen Evolution Reaction. Advanced Science, 2019, 6, 1900119.	11.2	90
9	Chemisorbed and Physisorbed Water at the TiO₂/Water Interface. Journal of Physical Chemistry Letters, 2017, 8, 2195-2199.	4.6	89
10	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
11	Catalytic activity of graphene-covered non-noble metals governed by proton penetration in electrochemical hydrogen evolution reaction. Nature Communications, 2021, 12, 203.	12.8	77
12	Electrochemical TERS Elucidates Potentialâ€Induced Molecular Reorientation of Adenine/Au(111). Angewandte Chemie - International Edition, 2017, 56, 9796-9801.	13.8	76
13	Lipid Carbonyl Groups Terminate the Hydrogen Bond Network of Membrane-Bound Water. Journal of Physical Chemistry Letters, 2015, 6, 4499-4503.	4.6	74
14	Multifunctional Octamethyltetrasila[2.2]cyclophanes: Conformational Variations, Circularly Polarized Luminescence, and Organic Electroluminescence. Journal of the American Chemical Society, 2017, 139, 11214-11221.	13.7	73
15	The surface roughness, but not the water molecular orientation varies with temperature at the waterâ€“air interface. Physical Chemistry Chemical Physics, 2015, 17, 23559-23564.	2.8	60
16	Effect of Graphene Encapsulation of NiMo Alloys on Oxygen Evolution Reaction. ACS Catalysis, 2020, 10, 792-799.	11.2	60
17	Thermopower of Benzenedithiol and C₆₀ Molecular Junctions with Ni and Au Electrodes. Nano Letters, 2014, 14, 5276-5280.	9.1	57
18	Graphene Layer Encapsulation of Non-Noble Metal Nanoparticles as Acid-Stable Hydrogen Evolution Catalysts. ACS Energy Letters, 2018, 3, 1539-1544.	17.4	57

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19	Structure and dynamics of water at waterâ€“graphene and waterâ€“hexagonal boron-nitride sheet interfaces revealed by ab initio sum-frequency generation spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 12979-12985.	2.8	53
20	Vibrational couplings and energy transfer pathways of waterâ€™s bending mode. Nature Communications, 2020, 11, 5977.	12.8	50
21	Orientational Distribution of Free O-H Groups of Interfacial Water is Exponential. Physical Review Letters, 2018, 121, 246101.	7.8	49
22	Definition of Free Oâ€“H Groups of Water at the Airâ€“Water Interface. Journal of Chemical Theory and Computation, 2018, 14, 357-364.	5.3	46
23	Aggregation-Induced Emission Enhancement from Disilane-Bridged Donorâ€“Acceptorâ€“Donor Luminogens Based on the Triarylamine Functionality. ACS Applied Materials & Interfaces, 2018, 10, 12164-12172.	8.0	45
24	Ab Initio Liquid Water Dynamics in Aqueous TMAO Solution. Journal of Physical Chemistry B, 2015, 119, 10597-10606.	2.6	44
25	Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Waterâ€“Air Interface. Journal of Physical Chemistry Letters, 2019, 10, 4914-4919.	4.6	43
26	Ï€⁺â€“Ï€⁺ stacking of imidazolium cations enhances molecular layering of room temperature ionic liquids at their interfaces. Physical Chemistry Chemical Physics, 2017, 19, 2850-2856.	2.8	42
27	Surface tension of ab initio liquid water at the water-air interface. Journal of Chemical Physics, 2016, 144, 204705.	3.0	39
28	Molecular Modeling of Water Interfaces: From Molecular Spectroscopy to Thermodynamics. Journal of Physical Chemistry B, 2016, 120, 3785-3796.	2.6	39
29	Trimethylamine-N-oxide: its hydration structure, surface activity, and biological function, viewed by vibrational spectroscopy and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 6909-6920.	2.8	39
30	Unveiling the Amphiphilic Nature of TMAO by Vibrational Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 17435-17443.	3.1	33
31	Influence of surface polarity on water dynamics at the water/rutile TiO₂(110) interface. Journal of Physics Condensed Matter, 2014, 26, 244102.	1.8	30
32	Polarizable Site Charge Model at Liquid/Solid Interfaces for Describing Surface Polarity: Application to Structure and Molecular Dynamics of Water/Rutile TiO₂(110) Interface. Journal of Chemical Theory and Computation, 2013, 9, 1193-1201.	5.3	29
33	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
34	Large Hydrogen-Bond Mismatch between TMAO and Urea Promotes Their Hydrophobic Association. CheM, 2018, 4, 2615-2627.	11.7	27
35	Ab initiotheory for current-induced molecular switching: Melamine on Cu(001). Physical Review B, 2013, 87, .	3.2	25
36	Impact of intermolecular vibrational coupling effects on the sum-frequency generation spectra of the water/air interface. Molecular Physics, 2020, 118, 1620358.	1.7	22

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37	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. Journal of Physical Chemistry Letters, 2020, 11, 2422-2429.	4.6	22
38	Polyethylene Glycol Covered Sn Catalysts Accelerate the Formation Rate of Formate by Carbon Dioxide Reduction. ACS Catalysis, 2021, 11, 9962-9969.	11.2	22
39	Mechanical switching of currentâ€“voltage characteristics in spiropyran single-molecule junctions. Nanoscale, 2020, 12, 7527-7531.	5.6	19
40	Structure and Dynamics of Water at the Waterâ€“Air Interface Using First-Principles Molecular Dynamics Simulations within Generalized Gradient Approximation. Journal of Chemical Theory and Computation, 2019, 15, 595-602.	5.3	18
41	Single-molecule rectifiers based on voltage-dependent deformation of molecular orbitals in carbazole oligomers. Nanoscale, 2018, 10, 19818-19824.	5.6	17
42	Highly Planar and Completely Insulated Oligothiophenes: Effects of Ï€-Conjugation on Hopping Charge Transport. Journal of Physical Chemistry Letters, 2019, 10, 3197-3204.	4.6	17
43	Improving Intramolecular Hopping Charge Transport via Periodical Segmentation of Ï€-Conjugation in a Molecule. Journal of the American Chemical Society, 2021, 143, 599-603.	13.7	14
44	Phase-Dependent Electrochemical CO₂ Reduction Ability of NiSn Alloys for Formate Generation. ACS Applied Energy Materials, 2021, 4, 7122-7128.	5.1	13
45	Electrochemical TERS Elucidates Potentialâ€Induced Molecular Reorientation of Adenine/Au(111). Angewandte Chemie, 2017, 129, 9928-9933.	2.0	12
46	Structure and Dynamics of Water at the Waterâ€“Air Interface Using First-Principles Molecular Dynamics Simulations. II. NonLocal vs Empirical van der Waals Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3836-3843.	5.3	12
47	Effects of cisâ€“trans Conformation between Thiophene Rings on Conductance of Oligothiophenes. Journal of Physical Chemistry Letters, 2019, 10, 5292-5296.	4.6	11
48	Decoding the molecular water structure at complex interfaces through surface-specific spectroscopy of the water bending mode. Physical Chemistry Chemical Physics, 2020, 22, 10934-10940.	2.8	11
49	Correlation between the Dipole Moment of Nonfullerene Acceptors and the Active Layer Morphology of Green-Solvent-Processed P3HT-Based Organic Solar Cells. ACS Sustainable Chemistry and Engineering, 2020, 8, 19013-19022.	6.7	10
50	Vibrational mode frequency correction of liquid water in density functional theory molecular dynamics simulations with van der Waals correction. Physical Chemistry Chemical Physics, 2020, 22, 12785-12793.	2.8	9
51	Control of dominant conduction orbitals by peripheral substituents in paddle-wheel diruthenium alkynyl molecular junctions. Chemical Science, 2021, 12, 10871-10877.	7.4	9
52	Enhancement of Carrier Mobility through Deformation Potential in Metal-Containing Insulated Molecular Wires. Journal of Physical Chemistry C, 2016, 120, 26637-26644.	3.1	8
53	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
54	Geometric model of 3D curved graphene with chemical dopants. Carbon, 2021, 182, 223-232.	10.3	7

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55	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
56	Three site molecular orbital controlled single-molecule rectifiers based on perpendicularly linked porphyrinâ€“imide dyads. Nanoscale, 2019, 11, 22724-22729.	5.6	5
57	Singleâ€Molecule Conductance of a Ï€â€Hybridized Tripodal Anchor while Maintaining Electronic Communication. Small, 2021, 17, 2006709.	10.0	3
58	Optical and redox properties of phenyl-capped cyclohexa[c]-oligothiophenes. Synthetic Metals, 2013, 181, 1-9.	3.9	2
59	Determination of the mechanism behind the organic magnetoresistance (OMAR) effect by using impedance spectroscopy. International Journal of Nanotechnology, 2015, 12, 238.	0.2	2
60	Analysis of Single Molecule Conductance of Heterogeneous Porphyrin Arrays by Partial Transmission Probabilities. ChemistrySelect, 2017, 2, 7484-7488.	1.5	2
61	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
62	Sun etÂal. Reply:. Physical Review Letters, 2019, 123, 099602.	7.8	1
63	Magnetic field effect on pentacene-doped sexithiophene diodes. Applied Physics Letters, 2017, 111, 203303.	3.3	0
64	Singleâ€Molecule Electronics: Singleâ€Molecule Conductance of a Ï€â€Hybridized Tripodal Anchor while Maintaining Electronic Communication (Small 3/2021). Small, 2021, 17, 2170012.	10.0	0
65	Charge Transport Mechanisms in Oligothiophene Molecular Junctions Studied by Electrical Conductance and Thermopower Measurements. Advances in Atom and Single Molecule Machines, 2017, , 341-353.	0.0	0