Minoru Otani

List of Publications by Year
in descending order

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95	5,242	109137	85405
papers	citations	35 h-index	71 g-index

98	98	98	6132
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relationship between Electric Double-Layer Structure of MXene Electrode and Its Surface Functional Groups. Chemistry of Materials, 2022, 34, 2069-2075.	3.2	28
2	Electronic, adsorption, and hydration structures of water-contained Na-montmorillonite and Na-beidellite through the first-principles method combined with the classical solution theory. Physical Review Materials, 2022, 6, .	0.9	3
3	Study on the free corrosion potential at an interface between an Al electrode and an acidic aqueous NaCl solution through density functional theory combined with the reference interaction site model. Electrochimica Acta, 2021, 377, 138121.	2.6	19
4	Bias-dependent diffusion of a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> molecule on metal surfaces by the first-principles method under the grand-canonical ensemble. Physical Review Materials, 2021, 5, .	0.9	9
5	Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2021, 125, 154-164.	1.1	24
6	Computational Investigation of Electric Field Driven Lithium Intercalation Into Bilayer Graphene. ECS Meeting Abstracts, 2021, MA2021-02, 425-425.	0.0	0
7	Computational Investigation of Li-Ion Adsorption on Charged Graphene. ECS Meeting Abstracts, 2021, MA2021-02, 524-524.	0.0	0
8	Thermodynamic Analysis of Li-Intercalated Graphite by First-Principles Calculations with Vibrational and Configurational Contributions. Journal of Physical Chemistry C, 2021, 125, 27891-27900.	1.5	3
9	Two-Phase Reaction Mechanism for Fluorination and Defluorination in Fluoride-Shuttle Batteries: A First-Principles Study. ACS Applied Materials & Interfaces, 2020, 12, 428-435.	4.0	19
10	Pseudocapacitors: Capacitive versus Pseudocapacitive Storage in MXene (Adv. Funct. Mater. 47/2020). Advanced Functional Materials, 2020, 30, 2070312.	7.8	2
11	Capacitive versus Pseudocapacitive Storage in MXene. Advanced Functional Materials, 2020, 30, 2000820.	7.8	74
12	Structural Variation in Carbonate Electrolytes by the Addition of Li Salts Studied by Xâ€Ray Total Scattering. Physica Status Solidi (B): Basic Research, 2020, 257, 2000100.	0.7	2
13	Toward Engineering of Solution Microenvironments for the CO₂ Reduction Reaction: Unraveling pH and Voltage Effects from a Combined Density-Functionalâ€“Continuum Theory. Journal of Physical Chemistry Letters, 2020, 11, 4113-4118.	2.1	49
14	Specific ion effects at graphitic interfaces. Nature Communications, 2019, 10, 4858.	5.8	62
15	Dense Charge Accumulation in MXene with a Hydrate-Melt Electrolyte. Chemistry of Materials, 2019, 31, 5190-5196.	3.2	39
16	Negative dielectric constant of water confined in nanosheets. Nature Communications, 2019, 10, 850.	5.8	116
17	Li deposition and desolvation with electron transfer at a silicon/propylene-carbonate interface: transition-state and free-energy profiles by large-scale first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2018, 20, 11586-11591.	1.3	12
18	Analysis of Lithium Insertion/Desorption Reaction at Interfaces between Graphite Electrodes and Electrolyte Solution Using Density Functional + Implicit Solvation Theory. Journal of Physical Chemistry C, 2018, 122, 9804-9810.	1.5	41

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19	Origins and Implications of Interfacial Capacitance Enhancements in C₆₀-Modified Graphene Supercapacitors. ACS Applied Materials & Interfaces, 2018, 10, 36860-36865.	4.0	23
20	A Study of Electrochemical Interface and Reaction Simulations Using Density Functional Theory Calculations. Review of Polarography, 2018, 64, 79-89.	0.0	0
21	Electrode potential from density functional theory calculations combined with implicit solvation theory. Physical Review Materials, 2018, 2, .	0.9	60
22	First-principles molecular dynamics simulation for electrochemical hydrogen production by 4,4â€²-bipyridine molecular catalyst on silver electrode. Journal of Electroanalytical Chemistry, 2017, 800, 13-18.	1.9	10
23	Toward full simulation of the electrochemical oxygen reduction reaction on Pt using first-principles and kinetic calculations. Physical Chemistry Chemical Physics, 2017, 19, 4447-4453.	1.3	45
24	Hybrid solvation models for bulk, interface, and membrane: Reference interaction site methods coupled with density functional theory. Physical Review B, 2017, 96, .	1.1	131
25	Stable Liâ€“Organic Batteries with Nafionâ€Based Sandwichâ€Type Separators. Advanced Energy Materials, 2016, 6, 1501780.	10.2	61
26	Polyanthraquinone as a Reliable Organic Electrode for Stable and Fast Lithium Storage. Angewandte Chemie - International Edition, 2015, 54, 13947-13951.	7.2	333
27	Poly(benzoquinonyl sulfide) as a Highâ€Energy Organic Cathode for Rechargeable Li and Na Batteries. Advanced Science, 2015, 2, 1500124.	5.6	267
28	Potentialâ€Induced Electronic Structure Changes in Supercapacitor Electrodes Observed by In Operando Soft Xâ€Ray Spectroscopy. Advanced Materials, 2015, 27, 1512-1518.	11.1	25
29	Capacitive charge storage at an electrified interface investigated via direct first-principles simulations. Physical Review B, 2015, 91, .	1.1	25
30	Effect of thermal motion on catalytic activity of nanoparticles in polar solvent. Journal of Chemical Physics, 2014, 140, 044703.	1.2	2
31	A quinone-based oligomeric lithium salt for superior Liâ€“organic batteries. Energy and Environmental Science, 2014, 7, 4077-4086.	15.6	259
32	A method of orbital analysis for large-scale first-principles simulations. Journal of Chemical Physics, 2014, 140, 244105.	1.2	13
33	Vibrational Dynamics of Sulfate Anion Adsorption on Pt(111) Surface: Ab Initio Molecular Dynamics Simulations. ChemElectroChem, 2014, 1, 1632-1635.	1.7	2
34	Flexible metallic nanowires with self-adaptive contacts to semiconducting transition-metal dichalcogenide monolayers. Nature Nanotechnology, 2014, 9, 436-442.	15.6	228
35	First-Principles-Inspired Design Strategies for Graphene-Based Supercapacitor Electrodes. Journal of Physical Chemistry C, 2014, 118, 4-15.	1.5	136
36	Study of the lithium/nickel ions exchange in the layered LiNi0.42Mn0.42Co0.16O2 cathode material for lithium ion batteries: experimental and first-principles calculations. Energy and Environmental Science, 2014, 7, 1068.	15.6	195

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37	Gate-induced electron-state tuning of MoS₂: first-principles calculations. Journal of Physics Condensed Matter, 2014, 26, 135001.	0.7	30
38	Electrochemical reduction of an anion for ionic-liquid molecules on a lithium electrode studied by first-principles calculations. Chemical Physics Letters, 2014, 612, 240-244.	1.2	18
39	Self-Poisoning Dynamical Effects in the Oxygen Reduction Reaction on Pt(111) from a Top-Down Kinetic Analysis. Journal of Physical Chemistry C, 2014, 118, 13638-13643.	1.5	12
40	5ï¼Žé›»ä½å‹¾é…å¯¾ä¸‹ã§ã®é›»æ¥µç•Œé¢ã‚€ã‚Šã‚Ÿã‚¯ã‚·ãƒ§ãƒ³ã‚·ãƒŸãƒ¥ãƒ¬ãƒ¼ã‚·ãƒ§ãƒ³. Electrochemistry, 2014, 82, 1102-1107.	0.6	0
41	Absence of edge states near the 120<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mo>â˜</mml:mo></mml:msup></mml:math>corners of zigzag graphene nanoribbons. Physical Review B, 2013, 87, .	1.1	14
42	Improved modeling of electrified interfaces using the effective screening medium method. Physical Review B, 2013, 88, .	1.1	49
43	Inhibition of water dissociation on a pitted Pt(111) surface: First principles study. Catalysis Today, 2013, 202, 163-167.	2.2	9
44	Charge Manipulation in Molecules Encapsulated Inside Single-Wall Carbon Nanotubes. Physical Review Letters, 2013, 110, 086801.	2.9	18
45	Highly Ordered Cobaltâ€“Phthalocyanine Chains on Fractional Atomic Steps: One-Dimensionality and Electron Hybridization. ACS Nano, 2013, 7, 1317-1323.	7.3	19
46	High-Efficiency Photoelectric Conversion in Grapheneâ€“Diamond Hybrid Structures: Model and First-Principles Calculations. Applied Physics Express, 2013, 6, 045104.	1.1	8
47	Biased interface between solid ion conductor LiBH4 and lithium metal: A first principles molecular dynamics study. Applied Physics Letters, 2013, 103, .	1.5	15
48	Tunable Magnetic Properties of Rhombohedral Graphite Thin Films: Effects of Insulating Substrate on Magnetic Properties. Japanese Journal of Applied Physics, 2012, 51, 02BN04.	0.8	0
49	Large-scale first-principles molecular dynamics for electrochemical systems with O(N) methods. Journal of Chemical Physics, 2012, 136, 134101.	1.2	24
50	Electron-state engineering of bilayer graphene by ionic molecules. Applied Physics Letters, 2012, 101, 233106.	1.5	10
51	Magnetic-state tuning of the rhombohedral graphite film by interlayer spacing and thickness. Surface Science, 2012, 606, 253-257.	0.8	7
52	First-Principles Molecular Dynamics at a Constant Electrode Potential. Physical Review Letters, 2012, 109, 266101.	2.9	165
53	The charged interface between Pt and water: First principles molecular dynamics simulations. AIP Advances, 2012, 2, 032182.	0.6	19
54	Tunable Magnetic Properties of Rhombohedral Graphite Thin Films: Effects of Insulating Substrate on Magnetic Properties. Japanese Journal of Applied Physics, 2012, 51, 02BN04.	0.8	0

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55	Semiconducting Electronic Property of Graphene Adsorbed on (0001) Surfaces of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2011, 106, 106801.	2.9	171
56	Gate-controlled carrier injection into hexagonal boron nitride. Physical Review B, 2011, 83, .	1.1	19
57	First-principles Calculations under an External Electric Field: Electrochemical Reactions and Control of Electronic Structures. Journal of the Vacuum Society of Japan, 2011, 54, 512-517.	0.3	1
58	Reversible redox reaction and water configuration on a positively charged platinum surface: first principles molecular dynamics simulation. Physical Chemistry Chemical Physics, 2011, 13, 20223.	1.3	35
59	Electronâ€state control of hexagonal boron nitride: Carrier injection into interâ€layer band. Physica Status Solidi C: Current Topics in Solid State Physics, 2011, 8, 500-502.	0.8	0
60	Origin of the n-type transport behavior of azafullerene encapsulated single-walled carbon nanotubes. Applied Physics Letters, 2011, 99, 053105.	1.5	4
61	Field-Induced Free-Electron Carriers in Graphite. Journal of the Physical Society of Japan, 2010, 79, 073701.	0.7	38
62	Intrinsic magnetic moment on (0001) surfaces of rhombohedral graphite. Physical Review B, 2010, 81, .	1.1	64
63	Stability and electronic structure of potassium-intercalated hexagonal boron nitride from density functional calculations. Physical Review B, 2010, 81, .	1.1	14
64	Phase control of magnetic state of graphite thin films by electric field. Applied Physics Letters, 2010, 96, .	1.5	26
65	Electronic hyperpolarizability calculation without the periodic images error for a large nonlinear molecule. Physical Review B, 2010, 81, .	1.1	4
66	Comparative van der Waals density-functional study of graphene on metal surfaces. Physical Review B, 2010, 82, .	1.1	274
67	Influence of Disorder on Conductance in Bilayer Graphene under Perpendicular Electric Field. Nano Letters, 2010, 10, 3888-3892.	4.5	116
68	Greenâ€™s function method for elimination of the spurious multipole interaction in the surface/interface slab model. Physical Review B, 2009, 80, .	1.1	72
69	Intrinsic dipole moment on the capped carbon nanotubes. Physical Review B, 2009, 80, .	1.1	12
70	Title is missing!. Electrochemistry, 2009, 77, 241-247.	0.6	3
71	Structure of the water/platinum interfaceâ€“â€“a first principles simulation under bias potential. Physical Chemistry Chemical Physics, 2008, 10, 3609.	1.3	124
72	Optical Band Gap Modification of Single-Walled Carbon Nanotubes by Encapsulated Fullerenes. Journal of the American Chemical Society, 2008, 130, 4122-4128.	6.6	84

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73	Electrode Dynamics from First Principles. Journal of the Physical Society of Japan, 2008, 77, 024802.	0.7	133
74	Effect of encapsulated atoms on the electronic structure of the fullerene cage: A case study onLa2@C78andTi2C2@C78via ultraviolet photoelectron spectroscopy. Physical Review B, 2007, 75, .	1.1	21
75	The role of the phonon anomaly in the superconductivity of vanadium and selenium under high pressures. Journal of Physics Condensed Matter, 2007, 19, 125206.	0.7	14
76	First-principles molecular dynamics simulation of biased electrode/solution interface. Surface Science, 2007, 601, 5237-5240.	0.8	96
77	Formation of titanium-carbide in a nanospace of C78 fullerenes. Chemical Physics Letters, 2007, 438, 274-278.	1.2	9
78	First-principles calculations of charged surfaces and interfaces: A plane-wave nonrepeated slab approach. Physical Review B, 2006, 73, .	1.1	616
79	Enhanced Si and B diffusion in semiconductor-grade SiO2 and the effect of strain on diffusion. Thin Solid Films, 2006, 508, 270-275.	0.8	6
80	Electrochemical Tuning of Electronic Structure of C60 and C70 Fullerene Peapods:â€‰ In Situ Visible Near-Infrared and Raman Study. Journal of Physical Chemistry B, 2003, 107, 7666-7675.	1.2	75
81	Charge-state-dependent boron diffusion in SiO2. Physica B: Condensed Matter, 2003, 340-342, 949-952.	1.3	0
82	Theoretical study on stable structures and diffusion mechanisms of B in SiO2. Applied Surface Science, 2003, 216, 490-496.	3.1	6
83	Energetics and electronic structure of C70-peapods and one-dimensional chains of C70. New Journal of Physics, 2003, 5, 122-122.	1.2	22
84	Energetics and electronic structures of one-dimensional fullerene chains encapsulated in zigzag nanotubes. Physical Review B, 2003, 68, .	1.1	108
85	Mechanisms of Diffusion of Boron Impurities inSiO2. Physical Review Letters, 2003, 90, 075901.	2.9	23
86	First-principles calculations of boron-related defects inSiO2. Physical Review B, 2003, 68, .	1.1	22
87	Electron-state control of carbon nanotubes by space and encapsulated fullerenes. Physical Review B, 2003, 67, .	1.1	103
88	Pressure-Induced Composite Phase Transition of Solid Oxygen. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2003, 13, 212-217.	0.1	0
89	Theoretical study on the lattice dynamics and electronÂphonon interaction of vanadium under high pressures. Journal of Physics Condensed Matter, 2002, 14, 10869-10872.	0.7	38
90	Pressure-induced insulatorâ€“metal transition and collapse of magnetism in molecular solid oxygen. Polyhedron, 2001, 20, 1381-1385.	1.0	7

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91	Structural and superconducting transition in selenium at high pressure. Physical Review B, 2001, 63, .	1.1	19
92	Theoretical study of the magnetic properties of low-dimensional oxygen molecular assemblies. Physica B: Condensed Matter, 1999, 265, 60-63.	1.3	6
93	The pressure-induced insulator-metal transition of solid oxygen - band-structure calculations. Journal of Physics Condensed Matter, 1998, 10, 11603-11606.	0.7	8
94	First-Principles Calculations of Electronic Band Structures of High Pressure Phase of Solid Oxygen.. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 1998, 7, 178-180.	0.1	11
95	Theoretical Study on Organic One-Dimensional Ferrimagnets. Molecular Crystals and Liquid Crystals, 1997, 306, 339-344.	0.3	0