Naoto Umezawa

List of Publications by Year in descending order

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133	11,008	76326	29157
papers	citations	40 h-index	104 g-index

135	135	135	13953
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Crystal and electronic structure engineering of tin monoxide by external pressure. Journal of Advanced Ceramics, 2021, 10, 565-577.	17.4	11
2	B₅N₃ and B₇N₅ Monolayers with High Carrier Mobility and Excellent Optical Performance. Journal of Physical Chemistry Letters, 2021, 12, 4823-4832.	4.6	18
3	Photocatalysis and hydrogen production from water solution. , 2020, , 555-577.		0
4	Topological Dirac nodal loops in nonsymmorphic hydrogenated monolayer boron. Physical Review B, 2020, 101, .	3.2	19
5	Recent advances in computational studies of thin-film solar cell material BaSi₂. Japanese Journal of Applied Physics, 2020, 59, SF0803.	1.5	20
6	Combined first-principles and electromagnetic simulation study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type doped anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> for the applications in infrared surface plasmon photonics. Physical Review Materials, 2020, 4, .	2.4	2
7	Electronic states of Zintl-phase solar-cell material BaSi2. Scripta Materialia, 2019, 172, 43-46.	5.2	7
8	Constructing Sn(<scp>ii</scp>)-doped SrNb₂O₆ for visible light response driven H₂ and O₂ evolution from water. Catalysis Science and Technology, 2019, 9, 3619-3622.	4.1	4
9	Structure and optical properties of sputter deposited pseudobrookite Fe₂TiO₅ thin films. CrystEngComm, 2019, 21, 34-40.	2.6	30
10	Energetics of native defects in ZnRh2O4 spinel from hybrid density functional calculations. Journal of Applied Physics, 2019, 125, .	2.5	3
11	Optical properties of single crystalline copper iodide with native defects: Experimental and density functional theoretical investigation. Journal of Applied Physics, 2019, 125, .	2.5	26
12	Chapter 2. Theoretical Design of PEC Materials. RSC Energy and Environment Series, 2018, , 29-61.	0.5	1
13	Crystal structure and electronic properties of Sr-substituted barium disilicide Ba1-Sr Si2 for solar cells: Computational and experimental studies. Acta Materialia, 2018, 148, 492-498.	7.9	8
14	Growth of Large Single Crystals of Copper Iodide by a Temperature Difference Method Using Feed Crystal Under Ambient Pressure. Crystal Growth and Design, 2018, 18, 6748-6756.	3.0	12
15	Design of p-type transparent conducting oxides Sn₂GeO₄ by an ab initio evolutionary structure search. Journal of Materials Chemistry C, 2018, 6, 11202-11208.	5.5	11
16	Impact of Surface Energy on the Formation of Composite Metal Oxide Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 24350-24358.	3.1	9
17	Self-trapped holes in BaTiO3. Journal of Applied Physics, 2018, 124, .	2.5	12
18	Photocatalytic CO₂ Reduction Using a Pristine Cu₂ZnSnS₄ Film Electrode under Visible Light Irradiation. Journal of Physical Chemistry C, 2018, 122, 21695-21702.	3.1	35

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19	Evolutionary structure prediction of two-dimensional IrB₁₄: a promising gas sensor material. Journal of Materials Chemistry C, 2018, 6, 5803-5811.	5.5	13
20	Spontaneous Direct Band Gap, High Hole Mobility, and Huge Exciton Energy in Atomic-Thin TiO₂ Nanosheet. Chemistry of Materials, 2018, 30, 6449-6457.	6.7	50
21	A-Site Cation Bulk and Surface Diffusion in A-Site-Deficient BaZrO₃ and SrZrO₃ Perovskites. Journal of Physical Chemistry C, 2017, 121, 12220-12229.	3.1	11
22	Viable approach toward efficient p-type conductivity in Al-doped anatase TiO₂via strain engineering. RSC Advances, 2017, 7, 20542-20547.	3.6	4
23	Determination of Crystal Structure of Graphitic Carbon Nitride: Ab Initio Evolutionary Search and Experimental Validation. Chemistry of Materials, 2017, 29, 2694-2707.	6.7	83
24	Exploration of Stable Strontium Phosphide-Based Electrides: Theoretical Structure Prediction and Experimental Validation. Journal of the American Chemical Society, 2017, 139, 15668-15680.	13.7	84
25	Formation and Characterization of Hydrogen Boride Sheets Derived from MgB₂ by Cation Exchange. Journal of the American Chemical Society, 2017, 139, 13761-13769.	13.7	157
26	Extended screened exchange functional derived from transcorrelated density functional theory. Journal of Chemical Physics, 2017, 147, 104104.	3.0	3
27	Electronic Structures and Photoanodic Properties of Ilmenite-type MTiO₃ Epitaxial Films (M = Mn, Fe, Co, Ni). Journal of Physical Chemistry C, 2017, 121, 18717-18724.	3.1	26
28	Electronic and Optical Properties of TiO₂ Solid-Solution Nanosheets for Bandgap Engineering: A Hybrid Functional Study. Journal of Physical Chemistry C, 2017, 121, 18683-18691.	3.1	5
29	Barium disilicide as a promising thin-film photovoltaic absorber: structural, electronic, and defect properties. Journal of Materials Chemistry A, 2017, 5, 25293-25302.	10.3	68
30	Semimetallic Two-Dimensional TiB₁₂: Improved Stability and Electronic Properties Tunable by Biaxial Strain. Chemistry of Materials, 2017, 29, 5922-5930.	6.7	41
31	Energetics and optical properties of nitrogen impurities in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from hybrid density-functional calculations. Physical Review B, 2017, 95, .	3.2	12
32	Controlling the Electronic Structures of Perovskite Oxynitrides and their Solid Solutions for Photocatalysis. ChemSusChem, 2016, 9, 1027-1031.	6.8	14
33	Reduction of CO₂ with Water on Pt-Loaded Rutile TiO₂(110) Modeled with Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 9160-9164.	3.1	29
34	A metal sulfide photocatalyst composed of ubiquitous elements for solar hydrogen production. Chemical Communications, 2016, 52, 7470-7473.	4.1	81
35	Electronic properties of highly-active Ag₃AsO₄photocatalyst and its band gap modulation: an insight from hybrid-density functional calculations. Physical Chemistry Chemical Physics, 2016, 18, 23407-23411.	2.8	30
36	Growth of Ba_{1â^'x}Sr_xZrO₃ (0 â‰¤ x â‰¤ 1) nanoparticles in supercritical water. RSC Advances, 2016, 6, 67525-67533.	3.6	13

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37	Energetics of native defects in anatase TiO₂: a hybrid density functional study. Physical Chemistry Chemical Physics, 2016, 18, 30040-30046.	2.8	31
38	Examining the Performance of Refractory Conductive Ceramics as Plasmonic Materials: A Theoretical Approach. ACS Photonics, 2016, 3, 43-50.	6.6	126
39	Band engineering of ternary metal nitride system Ti_1-x Zr_xN for plasmonic applications. Optical Materials Express, 2016, 6, 29.	3.0	37
40	Mixed Valence Tin Oxides as Novel van der Waals Materials: Theoretical Predictions and Potential Applications. Advanced Energy Materials, 2016, 6, 1501190.	19.5	79
41	Bonding and Electron Energy-Level Alignment at Metal/TiO₂ Interfaces: A Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 5549-5556.	3.1	45
42	Insight into the band structure engineering of single-layer SnS₂ with in-plane biaxial strain. Physical Chemistry Chemical Physics, 2016, 18, 7860-7865.	2.8	13
43	In situ X-ray diffraction for millisecond-order dynamics of BaZrO 3 nanoparticle formation in supercritical water. Journal of Supercritical Fluids, 2016, 107, 746-752.	3.2	20
44	Mesoporous palladiumâ€“copper bimetallic electrodes for selective electrocatalytic reduction of aqueous CO₂to CO. Journal of Materials Chemistry A, 2016, 4, 4776-4782.	10.3	115
45	Anisotropic Nature of Anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> and Its Intrinsic (001) Surface Electronic States. Physical Review Applied, 2015, 4, .	3.8	24
46	Effects of cation concentration on photocatalytic performance over magnesium vanadates. APL Materials, 2015, 3, 104405.	5.1	11
47	Plasmon mediated cathodic photocurrent generation in sol-gel synthesized doped SrTiO3 nanofilms. APL Materials, 2015, 3, .	5.1	6
48	Oxygenâ€Assisted Synthesis of Mesoporous Palladium Nanoparticles as Highly Active Electrocatalysts. Chemistry - A European Journal, 2015, 21, 18671-18676.	3.3	6
49	Electronic structures of anatase (TiO₂)_{1â^'x}(TaON)_x solid solutions: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 17980-17988.	2.8	5
50	Structural, electronic and optical characteristics of SrGe2 and BaGe2: A combined experimental and computational study. Journal of Alloys and Compounds, 2015, 630, 126-132.	5.5	6
51	Promoted Câ€“C bond cleavage over intermetallic TaPt₃ catalyst toward low-temperature energy extraction from ethanol. Energy and Environmental Science, 2015, 8, 1685-1689.	30.8	43
52	Effective mineralization of organic dye under visible-light irradiation over electronic-structure-modulated Sn(Nb 1â^'x Ta x) 2 O 6 solid solutions. Applied Catalysis B: Environmental, 2015, 168-169, 243-249.	20.2	23
53	Sulfur and Silicon Doping in Ag₃PO₄. Journal of Physical Chemistry C, 2015, 119, 2284-2289.	3.1	18
54	Artificial layered perovskite oxides A(B0.5Bâ€²0.5)O3 as potential solar energy conversion materials. Journal of Applied Physics, 2015, 117, 055106.	2.5	4

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55	Band gap engineering of bulk and nanosheet SnO: an insight into the interlayer Snâ€“Sn lone pair interactions. Physical Chemistry Chemical Physics, 2015, 17, 17816-17820.	2.8	100
56	Novel visible-light sensitive vanadate photocatalysts for water oxidation: implications from density functional theory calculations. Journal of Materials Chemistry A, 2015, 3, 10720-10723.	10.3	27
57	Covalency-reinforced oxygen evolution reaction catalyst. Nature Communications, 2015, 6, 8249.	12.8	393
58	Photocatalytic reactivity of {121} and {211} facets of brookite TiO₂ crystals. Journal of Materials Chemistry A, 2015, 3, 2331-2337.	10.3	54
59	Correlation between the surface electronic structure and CO-oxidation activity of Pt alloys. Physical Chemistry Chemical Physics, 2015, 17, 4879-4887.	2.8	37
60	Sensitization of Perovskite Strontium Stannate SrSnO₃towards Visible-Light Absorption by Doping. International Journal of Photoenergy, 2014, 2014, 1-3.	2.5	15
61	Effect of cation arrangement on the electronic structures of the perovskite solid solutions <span class="aps-inline-formula"><math		

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73	Anatase TiO₂ Single Crystals Exposed with High-Reactive {111} Facets Toward Efficient H₂ Evolution. Chemistry of Materials, 2013, 25, 405-411.	6.7	248
74	Undoped visible-light-sensitive titania photocatalyst. Journal of Materials Science, 2013, 48, 108-114.	3.7	30
75	Theoretical design of highly active SrTiO3-based photocatalysts by a codoping scheme towards solar energy utilization for hydrogen production. Journal of Materials Chemistry A, 2013, 1, 4221.	10.3	106
76	Role of photoexcited electrons in hydrogen evolution from platinum co-catalysts loaded on anatase TiO2: a first-principles study. Journal of Materials Chemistry A, 2013, 1, 6664.	10.3	21
77	Native defects and hydrogen impurities in Ag<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>PO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	3.2	26
78	(Invited) Theoretical Perspectives in Defect and Impurity Physics toward Materials Design for Oxides. ECS Transactions, 2013, 50, 35-39.	0.5	2
79	Nano-Photocatalytic Materials for Solar Fuel Production. ECS Meeting Abstracts, 2013, , .	0.0	0
80	Theoretical model for artificial structure modulation of HfO2/SiOx/Si interface by deposition of a dopant material. Applied Physics Letters, 2012, 100, 092904.	3.3	3
81	Mechanism of photocatalytic activities in Cr-doped SrTiO3 under visible-light irradiation: an insight from hybrid density-functional calculations. Physical Chemistry Chemical Physics, 2012, 14, 1876.	2.8	73
82	Role of complex defects in photocatalytic activities of nitrogen-doped anatase TiO2. Physical Chemistry Chemical Physics, 2012, 14, 5924.	2.8	51
83	Surface-Alkalinization-Induced Enhancement of Photocatalytic H₂ Evolution over SrTiO₃-Based Photocatalysts. Journal of the American Chemical Society, 2012, 134, 1974-1977.	13.7	330
84	Nanoâ€photocatalytic Materials: Possibilities and Challenges. Advanced Materials, 2012, 24, 229-251.	21.0	3,375
85	Visible light photoactivity from a bonding assembly of titanium oxide nanocrystals. Chemical Communications, 2011, 47, 4219.	4.1	44
86	Theoretical study of high photocatalytic performance of Ag<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>PO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:mro	3.2	186
87	Facet Effect of Single-Crystalline Ag₃PO₄ Sub-microcrystals on Photocatalytic Properties. Journal of the American Chemical Society, 2011, 133, 6490-6492.	13.7	1,255
88	Electronic coupling assembly of semiconductor nanocrystals: self-narrowed band gap to promise solar energy utilization. Energy and Environmental Science, 2011, 4, 1684.	30.8	55
89	Self-doped SrTiO3â˜Ï´ photocatalyst with enhanced activity for artificial photosynthesis under visible light. Energy and Environmental Science, 2011, 4, 4211.	30.8	244
90	Energetics and electronic structure of graphene adsorbed on HfO2(111): Density functional theory calculations. Physical Review B, 2011, 83, .	3.2	63

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91	Computational study of the dielectric properties of [La,Sc]2O3 solid solutions. Journal of Applied Physics, 2010, 107, 074104.	2.5	0
92	Origin of high solubility of silicon in La2O3: A first-principles study. Applied Physics Letters, 2010, 97, .	3.3	12
93	Effects of capping HfO2 with multivalent oxides toward reducing the number of charged defects. Applied Physics Letters, 2010, 96, 162906.	3.3	9
94	Hybrid functional studies of the oxygen vacancy in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 81, .	3.2	554
95	Effects of barium incorporation into HfO2 gate dielectrics on reduction in charged defects: First-principles study. Applied Physics Letters, 2009, 94, 022903.	3.3	12
96	Effect of Annealing on Electronic Characteristics of HfSiON Films fabricated by Damascene Gate Process. ECS Transactions, 2009, 16, 521-526.	0.5	0
97	Stability of Si impurity in high-Î¤ oxides. Microelectronic Engineering, 2009, 86, 1780-1781.	2.4	0
98	Observation of Leakage Sites in High-k Gate Dielectrics in MOSFET Devices by Electron-Beam-Induced Current Technique. Solid State Phenomena, 2008, 131-133, 449-454.	0.3	1
99	Physical model of the PBTI and TDDB of la incorporated HfSiON gate dielectrics with pre-existing and stress-induced defects. , 2008, , .		18
100	Reduction in charged defects associated with oxygen vacancies in hafnia by magnesium incorporation: First-principles study. Applied Physics Letters, 2008, 93, .	3.3	25
101	Local-density approximation for orbital densities applied to the self-interaction correction. Journal of Chemical Physics, 2008, 128, 044105.	3.0	1
102	Electronic Structure Study of Local Dielectric Properties of Lanthanoid Oxide Clusters. Japanese Journal of Applied Physics, 2008, 47, 205-211.	1.5	17
103	Landscape of Combinatorial Materials Exploration and High Throughput Characterizations for the Post-CMOS Devices. International Power Modulator Symposium and High-Voltage Workshop, 2008, , .	0.0	1
104	Chemical controllability of charge states of nitrogen-related defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>HfO</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub First-principles calculations. Physical Review B, 2008, 77, .	3.2	13
105	Optimizing optical absorption of TiO2 by alloying with TiS2. Applied Physics Letters, 2008, 92, .	3.3	24
106	1,3,5-trinitro-1,3,5-triazine decomposition and chemisorption on Al(111) surface: First-principles molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234702.	3.0	34
107	Characterization of Metal/High-kStructures Using Monoenergetic Positron Beams. Japanese Journal of Applied Physics, 2007, 46, 3214-3218.	1.5	9
108	Hafnium 4f Core-level Shifts Caused by Nitrogen Incorporation in Hf-based High-kGate Dielectrics. Japanese Journal of Applied Physics, 2007, 46, 3507-3509.	1.5	13

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109	Guiding Principle of Energy Level Controllability of Silicon Dangling Bonds in HfSiON. Japanese Journal of Applied Physics, 2007, 46, 1891-1894.	1.5	0
110	Quantum Monte Carlo study of first-row atoms using transcorrelated variational Monte Carlo trial functions. Journal of Chemical Physics, 2007, 126, 164109.	3.0	13
111	Suppression of oxygen vacancy formation in Hf-based high-k dielectrics by lanthanum incorporation. Applied Physics Letters, 2007, 91, .	3.3	64
112	Role of the Ionicity in Defect Formation in Hf-Based Dielectrics. ECS Transactions, 2007, 11, 199-211.	0.5	1
113	Role of Nitrogen Atoms in Reduction of Electron Charge Traps in Hf-Based High- $kappa$ Dielectrics. IEEE Electron Device Letters, 2007, 28, 363-365.	3.9	19
114	Study of highâ€k gate dielectrics by means of positron annihilation. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 3599-3604.	0.8	0
115	Recent Developments in Quantum Monte Carlo: Methods and Applications. AIP Conference Proceedings, 2007, , .	0.4	0
116	Effects of nitrogen atom doping on dielectric constants of Hf-based gate oxides. Applied Physics Letters, 2006, 88, 112903.	3.3	24
117	Explicit density-functional exchange potential with correct asymptotic behavior. Physical Review A, 2006, 74, .	2.5	24
118	Modified Oxygen Vacancy Induced Fermi Level Pinning Model Extendable to P-Metal Pinning. Japanese Journal of Applied Physics, 2006, 45, L1289-L1292.	1.5	101
119	Introduction of defects into HfO2 gate dielectrics by metal-gate deposition studied using x-ray photoelectron spectroscopy and positron annihilation. Journal of Applied Physics, 2006, 100, 064501.	2.5	12
120	Role of the one-body Jastrow factor in the transcorrelated self-consistent field equation. International Journal of Quantum Chemistry, 2006, 106, 1477-1486.	2.0	6
121	Unique behavior of F-centers in high-k Hf-based oxides. Physica B: Condensed Matter, 2006, 376-377, 392-394.	2.7	13
122	Determination of simple correlated wave functions for few-electron systems using a Jastrow factor. Physical Review A, 2006, 73, .	2.5	5
123	Characterization of HfSiON gate dielectrics using monoenergetic positron beams. Journal of Applied Physics, 2006, 99, 054507.	2.5	22
124	Orbital-dependent nonlocal correlation energy functional constructed from a Jastrow function: Application to atoms and ions. Physical Review A, 2006, 73, .	2.5	3
125	Physics of Metal/High-k Interfaces. ECS Transactions, 2006, 3, 129-140.	0.5	14
126	Characteristics of Dry-Band Arcing on Fiber Ropes for Wiring Works Near Transmission Lines. IEEJ Transactions on Power and Energy, 2006, 126, 1149-1156.	0.2	0

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127	Role of Nitrogen Incorporation into Hf-Based High-kGate Dielectrics for Termination of Local Current Leakage Paths. Japanese Journal of Applied Physics, 2005, 44, L1333-L1336.	1.5	15
128	A practical treatment for the three-body interactions in the transcorrelated variational Monte Carlo method: Application to atoms from lithium to neon. Journal of Chemical Physics, 2005, 122, 224101.	3.0	24
129	First-principles studies of the intrinsic effect of nitrogen atoms on reduction in gate leakage current through Hf-based high-k dielectrics. Applied Physics Letters, 2005, 86, 143507.	3.3	147
130	Ground-state correlation energy for the homogeneous electron gas calculated by the transcorrelated method. Physical Review B, 2004, 69, .	3.2	29
131	Excited electronic state calculations by the transcorrelated variational Monte Carlo method: Application to a helium atom. Journal of Chemical Physics, 2004, 121, 7070-7075.	3.0	17
132	Transcorrelated self-consistent calculation for electronic systems with variational Monte Carlo method. International Journal of Quantum Chemistry, 2003, 91, 184-190.	2.0	9
133	Transcorrelated method for electronic systems coupled with variational Monte Carlo calculation. Journal of Chemical Physics, 2003, 119, 10015-10031.	3.0	58