

Yuan Ping Feng

List of Publications by Year in descending order

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519
papers

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all docs

525
docs citations

525
times ranked

27763
citing authors

#	ARTICLE	IF	CITATIONS
1	Uniaxial Strain on Graphene: Raman Spectroscopy Study and Band-Gap Opening. ACS Nano, 2008, 2, 2301-2305.	14.6	1,409
2	Graphene Thickness Determination Using Reflection and Contrast Spectroscopy. Nano Letters, 2007, 7, 2758-2763.	9.1	1,034
3	Room-Temperature Ferromagnetism in Carbon-Doped ZnO. Physical Review Letters, 2007, 99, 127201.	7.8	775
4	Carbon Nanotubes for Supercapacitor. Nanoscale Research Letters, 2010, 5, 654-668.	5.7	650
5	Hollow Mo-doped CoP nanoarrays for efficient overall water splitting. Nano Energy, 2018, 48, 73-80.	16.0	608
6	Structural and electronic properties of h-BN. Physical Review B, 2003, 68, .	3.2	455
7	Ferromagnetism in Dilute Magnetic Semiconductors through Defect Engineering: Li-Doped ZnO. Physical Review Letters, 2010, 104, 137201.	7.8	428
8	Electronic phase separation at the LaAlO ₃ /SrTiO ₃ interface. Nature Communications, 2011, 2, 188.	12.8	366
9	Dual-Functional N Dopants in Edges and Basal Plane of MoS ₂ Nanosheets Toward Efficient and Durable Hydrogen Evolution. Advanced Energy Materials, 2017, 7, 1602086.	19.5	286
10	Copper Single Atoms Anchored in Porous Nitrogen-Doped Carbon as Efficient pH-Universal Catalysts for the Nitrogen Reduction Reaction. ACS Catalysis, 2019, 9, 10166-10173.	11.2	284
11	Carbon nanowalls and related materials. Journal of Materials Chemistry, 2004, 14, 469.	6.7	275
12	Mechanism of ferromagnetism in nitrogen-doped ZnO: First-principle calculations. Physical Review B, 2008, 78, .	3.2	269
13	Chemically Exfoliated VSe ₂ Monolayers with Room-Temperature Ferromagnetism. Advanced Materials, 2019, 31, e1903779.	21.0	251
14	Spatially Resolved Electronic Structures of Atomically Precise Armchair Graphene Nanoribbons. Scientific Reports, 2012, 2, 983.	3.3	246
15	Growth of Single-Crystalline Ni and Co Nanowires via Electrochemical Deposition and Their Magnetic Properties. Journal of Physical Chemistry B, 2005, 109, 3094-3098.	2.6	240
16	Tuning the Electronic Structure of Graphene by an Organic Molecule. Journal of Physical Chemistry B, 2009, 113, 2-5.	2.6	219
17	NIR Schottky Photodetectors Based on Individual Single-Crystalline GeSe Nanosheet. ACS Applied Materials & Interfaces, 2013, 5, 9594-9604.	8.0	214
18	Room-Temperature Ferromagnetism of Cu-Doped ZnO Films Probed by Soft X-Ray Magnetic Circular Dichroism. Physical Review Letters, 2010, 105, 207201.	7.8	205

#	ARTICLE	IF	CITATIONS
19	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. Scientific Data, 2019, 6, 86.	5.3	201
20	Review of borophene and its potential applications. Frontiers of Physics, 2019, 14, 1.	5.0	201
21	Giant Phononic Anisotropy and Unusual Anharmonicity of Phosphorene: Interlayer Coupling and Strain Engineering. Advanced Functional Materials, 2015, 25, 2230-2236.	14.9	198
22	Efficient Hydrogen Evolution of Oxidized Ni ₃ Defective Sites for Alkaline Freshwater and Seawater Electrolysis. Advanced Materials, 2021, 33, e2003846.	21.0	198
23	Topological Properties Determined by Atomic Buckling in Self-Assembled Ultrathin Bi(110). Nano Letters, 2015, 15, 80-87.	9.1	191
24	Synergizing Mo Single Atoms and Mo ₂ C Nanoparticles on CNTs Synchronizes Selectivity and Activity of Electrocatalytic N ₂ Reduction to Ammonia. Advanced Materials, 2020, 32, e2002177. and optical properties of the monolayer group-IV monochalcogenides	21.0	190
25			

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37	Graphene-based bipolar spin diode and spin transistor: Rectification and amplification of spin-polarized current. <i>Physical Review B</i> , 2011, 83, .	3.2	145
38	Electronic and transport properties of phosphorene nanoribbons. <i>Physical Review B</i> , 2015, 92, .	3.2	145
39	Elemental Ferroelectricity and Antiferroelectricity in Group V Monolayer. <i>Advanced Functional Materials</i> , 2018, 28, 1707383.	14.9	145
40	Controlling the magnetic anisotropy in Cr ₂ Ge ₂ Te ₆ by electrostatic gating. <i>Nature Electronics</i> , 2020, 3, 460-465.	26.0	145
41	Greatly enhanced adsorption and catalytic activity of Au and Pt clusters on defective graphene. <i>Journal of Chemical Physics</i> , 2010, 132, 194704.	3.0	138
42	High-throughput screening of transition metal single atom catalysts anchored on molybdenum disulfide for nitrogen fixation. <i>Nano Energy</i> , 2020, 68, 104304.	16.0	136
43	Ferromagnetism in ZnO Nanowires Derived from Electrodeposition on AAO Template and Subsequent Oxidation. <i>Advanced Materials</i> , 2008, 20, 1170-1174.	21.0	135
44	Density-functional characterization of antiferromagnetism in oxygen-deficient anatase and rutile TiO_2 . <i>Physical Review B</i> , 2010, 81, .	3.2	135
45	Large valley splitting in monolayer WS ₂ by proximity coupling to an insulating antiferromagnetic substrate. <i>Physical Review B</i> , 2018, 97, .	3.2	134
46	Silicon Carbide Nanotubes As Potential Gas Sensors for CO and HCN Detection. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15985-15988.	3.1	133
47	Dynamics of Bound Exciton Complexes in CdS Nanobelts. <i>ACS Nano</i> , 2011, 5, 3660-3669.	14.6	132
48	Growth Intermediates for CVD Graphene on Cu(111): Carbon Clusters and Defective Graphene. <i>Journal of the American Chemical Society</i> , 2013, 135, 8409-8414.	13.7	132
49	Raman spectroscopic investigation of carbon nanowalls. <i>Journal of Chemical Physics</i> , 2006, 124, 204703.	3.0	131
50	High oscillator strength interlayer excitons in two-dimensional heterostructures for mid-infrared photodetection. <i>Nature Nanotechnology</i> , 2020, 15, 675-682.	31.5	129
51	Semiconductor Nanowires and Nanotubes: Effects of Size and Surface-to-Volume Ratio. <i>ACS Nano</i> , 2008, 2, 2410-2414.	14.6	125
52	Cu-doped GaN: A dilute magnetic semiconductor from first-principles study. <i>Applied Physics Letters</i> , 2006, 89, 062505.	3.3	121
53	Origin of \tilde{d} magnetic anisotropy in II-VI and III-V semiconductors by substitutional doping at anion site. <i>Physical Review B</i> , 2010, 81, .	3.2	121
54	Charge-Transfer-Based Mechanism for Half-Metallicity and Ferromagnetism in One-Dimensional Organometallic Sandwich Molecular Wires. <i>Journal of the American Chemical Society</i> , 2008, 130, 13956-13960.	13.7	118

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55	Supercapacitor Electrodes from Tubes-in-Tube Carbon Nanostructures. <i>Chemistry of Materials</i> , 2007, 19, 6120-6125.	6.7	116
56	Tailoring sample-wide pseudo-magnetic fields on a graphene/black phosphorus heterostructure. <i>Nature Nanotechnology</i> , 2018, 13, 828-834.	31.5	113
57	Effects of edge passivation by hydrogen on electronic structure of armchair graphene nanoribbon and band gap engineering. <i>Applied Physics Letters</i> , 2009, 94, .	3.3	112
58	Strain-Enhanced Stabilization and Catalytic Activity of Metal Nanoclusters on Graphene. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16541-16546.	3.1	108
59	Optical limiting properties of metal nanowires. <i>Applied Physics Letters</i> , 2006, 88, 223106.	3.3	106
60	Ferromagnetism in Mg-doped AlN from ab initio study. <i>Applied Physics Letters</i> , 2006, 89, 142501.	3.3	104
61	High anisotropy of fully hydrogenated borophene. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31424-31430.	2.8	104
62	Symmetrical Negative Differential Resistance Behavior of a Resistive Switching Device. <i>ACS Nano</i> , 2012, 6, 2517-2523.	14.6	103
63	Atomically Thin 2D Transition Metal Oxides: Structural Reconstruction, Interaction with Substrates, and Potential Applications. <i>Advanced Materials Interfaces</i> , 2019, 6, 1801160.	3.7	100
64	Size-dependent magnetism and spin-glass behavior of amorphous NiO bulk, clusters, and nanocrystals: Experiments and first-principles calculations. <i>Physical Review B</i> , 2007, 76, .	3.2	96
65	Mutual Ferromagnetic/Ferroelectric Coupling in Multiferroic Copper-Doped ZnO. <i>Advanced Materials</i> , 2011, 23, 1635-1640.	21.0	96
66	Magnetic Transition in Monolayer VSe ₂ via Interface Hybridization. <i>ACS Nano</i> , 2019, 13, 8997-9004.	14.6	94
67	Density functional theory study of BN-doped graphene superlattice: Role of geometrical shape and size. <i>Journal of Applied Physics</i> , 2010, 108, .	2.5	93
68	Strain effects on hydrogen storage capability of metal-decorated graphene: A first-principles study. <i>Applied Physics Letters</i> , 2010, 97, .	3.3	92
69	Single-crystal growth of metallic nanowires with preferred orientation. <i>Nanotechnology</i> , 2005, 16, 1559-1564.	2.6	91
70	Heterostructures of phosphorene and transition metal dichalcogenides for excitonic solar cells: A first-principles study. <i>Applied Physics Letters</i> , 2016, 108, .	3.3	90
71	Linear tuning of charge carriers in graphene by organic molecules and charge-transfer complexes. <i>Physical Review B</i> , 2010, 81, .	3.2	88
72	Origin of Long-Range Ferromagnetic Ordering in Metal-Organic Frameworks with Antiferromagnetic Dimeric-Cu(II) Building Units. <i>Journal of the American Chemical Society</i> , 2012, 134, 17286-17290.	13.7	86

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73	Ab initio study of electronic and optical properties of multiwall carbon nanotube structures made up of a single rolled-up graphite sheet. <i>Physical Review B</i> , 2005, 72, .	3.2	84
74	Room Temperature Ferromagnetism of Monolayer Chromium Telluride with Perpendicular Magnetic Anisotropy. <i>Advanced Materials</i> , 2021, 33, e2103360.	21.0	84
75	First-principles calculation of the thermodynamics of $\text{In}_x\text{Ga}_{1-x}$ alloys: Effect of lattice vibrations. <i>Physical Review B</i> , 2006, 73, .	3.2	83
76	Orientation-Dependent Raman Spectroscopy of Single Wurtzite CdS Nanowires. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1865-1870.	3.1	83
77	Statistical composition-structure-property correlation and glass-forming ability based on the full icosahedra in Cu-Zr metallic glasses. <i>Applied Physics Letters</i> , 2010, 96, .	3.3	83
78	Giant enhancement in vertical conductivity of stacked CVD graphene sheets by self-assembled molecular layers. <i>Nature Communications</i> , 2014, 5, 5461.	12.8	83
79	Monte Carlo simulation of a cluster system with strong interaction and random anisotropy. <i>Physical Review B</i> , 2001, 64, .	3.2	76
80	Hexagonal close-packed Ni nanostructures grown on the (001) surface of MgO. <i>Applied Physics Letters</i> , 2005, 86, 131915.	3.3	76
81	Review on charge transfer and chemical activity of TiO ₂ : Mechanism and applications. <i>Progress in Surface Science</i> , 2016, 91, 183-202.	8.3	76
82	High-Throughput Computational Screening of Vertical 2D van der Waals Heterostructures for High-efficiency Excitonic Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 32142-32150.	8.0	75
83	Recent progress and challenges in magnetic tunnel junctions with 2D materials for spintronic applications. <i>Applied Physics Reviews</i> , 2021, 8, .	11.3	74
84	Stimulated Electrocatalytic Hydrogen Evolution Activity of MOF-Derived MoS ₂ Basal Domains via Charge Injection through Surface Functionalization and Heteroatom Doping. <i>Advanced Science</i> , 2019, 6, 1900140.	11.2	73
85	Hydrogen storage of ZnO and Mg doped ZnO nanowires. <i>Nanotechnology</i> , 2006, 17, 2963-2967.	2.6	72
86	Band-Gap Engineering with Hybrid Graphene-Graphene Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20841-20844.	3.1	66
87	Impact of oxide defects on band offset at GeO ₂ /Ge interface. <i>Applied Physics Letters</i> , 2009, 94, 142903.	3.3	66
88	From nucleation to coexistence. <i>Applied Physics Letters</i> , 2005, 87, 162513.	3.3	65
89	Nanostructured trimetallic Pt/FeRuC, Pt/NiRuC, and Pt/CoRuC catalysts for methanol electrooxidation. <i>Journal of Materials Chemistry</i> , 2012, 22, 13643.	6.7	65
90	Effect of nitrogen doping on optical properties and electronic structures of SrTiO ₃ films. <i>Applied Physics Letters</i> , 2006, 89, 231922.	3.3	63

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91	Charge and spin transport in graphene-based heterostructure. <i>Applied Physics Letters</i> , 2011, 98, 053101.	3.3	62
92	Energy-Gap Opening in a Bi(110) Nanoribbon Induced by Edge Reconstruction. <i>Physical Review Letters</i> , 2012, 109, 246804.	7.8	62
93	Energy-band alignments at ZrO ₂ /Si, SiGe, and Ge interfaces. <i>Applied Physics Letters</i> , 2004, 85, 4418.	3.3	61
94	Switching and rectification of a single light-sensitive diarylethene molecule sandwiched between graphene nanoribbons. <i>Journal of Chemical Physics</i> , 2011, 135, 184703.	3.0	60
95	Nanoscale Magnetization Reversal Caused by Electric Field-Induced Ion Migration and Redistribution in Cobalt Ferrite Thin Films. <i>ACS Nano</i> , 2015, 9, 4210-4218.	14.6	60
96	Relativistic band structure of ternary II-VI semiconductor alloys containing Cd, Zn, Se and Te. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 2783-2799.	1.8	59
97	Effect of nitrogen incorporation on the electronic structure and thermal stability of HfO ₂ gate dielectric. <i>Applied Physics Letters</i> , 2006, 88, 192103.	3.3	59
98	Graphene-based spin logic gates. <i>Applied Physics Letters</i> , 2011, 98, .	3.3	59
99	Phase stability of magnesium-rare earth binary systems from first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2011, 509, 6899-6907.	5.5	59
100	The stability of aluminium oxide monolayer and its interface with two-dimensional materials. <i>Scientific Reports</i> , 2016, 6, 29221.	3.3	59
101	First-principles study of ZrO ₂ /Si interfaces: Energetics and band offsets. <i>Physical Review B</i> , 2005, 72, .	3.2	58
102	Wide V_{fb} and V_{th} Tunability for Metal-Gated MOS Devices With HfLaO Gate Dielectrics. <i>IEEE Electron Device Letters</i> , 2007, 28, 258-260.	3.9	57
103	First principles study of the electric field effect on magnetization and magnetic anisotropy of FeCo/MgO(001) thin film. <i>Applied Physics Letters</i> , 2011, 99, .	3.3	57
104	Multiple unpinned Dirac points in group-Va single-layers with phosphorene structure. <i>Npj Computational Materials</i> , 2016, 2, .	8.7	57
105	Quadratic contact point semimetal: Theory and material realization. <i>Physical Review B</i> , 2018, 98, .	3.2	57
106	Room temperature ferromagnetism in Teflon due to carbon dangling bonds. <i>Nature Communications</i> , 2012, 3, 727.	12.8	56
107	Pt-W C nano-composites as an efficient electrochemical catalyst for oxygen reduction reaction. <i>Nano Energy</i> , 2013, 2, 28-39.	16.0	56
108	Electrically Tunable In-Plane Anisotropic Magnetoresistance in Topological Insulator BiSbTeSe ₂ Nanodevices. <i>Nano Letters</i> , 2015, 15, 2061-2066.	9.1	56

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109	Graphene with line defect as a membrane for gas separation: Design via a first-principles modeling. <i>Surface Science</i> , 2013, 607, 153-158.	1.9	55
110	Elastic constants of B2-MgRE (RE= Sc, Y, La-Lu) calculated with first-principles. <i>Solid State Communications</i> , 2008, 148, 314-318.	1.9	54
111	Tungsten Carbide Supports for Single-Atom Platinum-Based Fuel-Cell Catalysts: First-Principles Study on the Metal-Support Interactions and O ₂ Dissociation on W ₂ C Low-Index Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13525-13538.	3.1	54
112	High-Throughput Identification of Exfoliable Two-Dimensional Materials with Active Basal Planes for Hydrogen Evolution. <i>ACS Energy Letters</i> , 2020, 5, 2313-2321.	17.4	54
113	Efficient charge-spin conversion and magnetization switching through the Rashba effect at topological-insulator/Ag interfaces. <i>Physical Review B</i> , 2018, 97, .	3.2	53
114	Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. <i>Journal of Materials Chemistry C</i> , 2019, 7, 8868-8873.	5.5	52
115	Diverse Transport Behaviors in Cyclo[18]carbon-Based Molecular Devices. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2611-2617.	4.6	52
116	Ab initio study of OH-functionalized single-wall carbon nanotubes. <i>Physical Review B</i> , 2004, 70, .	3.2	51
117	Novel CdS Nanostructures: Synthesis and Field Emission. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11227-11230.	3.1	49
118	Magnetic and transport properties of Mn ₃ Ga/MgO/Mn ₃ Ga magnetic tunnel junctions: A first-principles study. <i>Applied Physics Letters</i> , 2012, 100, .	3.3	49
119	Negative-U property of oxygen vacancy in cubic HfO ₂ . <i>Applied Physics Letters</i> , 2005, 87, 062105.	3.3	48
120	Two-dimensional graphene superlattice made with partial hydrogenation. <i>Applied Physics Letters</i> , 2010, 96, 193115.	3.3	48
121	Observation of room-temperature high-energy resonant excitonic effects in graphene. <i>Physical Review B</i> , 2011, 84, .	3.2	48
122	Electron transmission modes in electrically biased graphene nanoribbons and their effects on device performance. <i>Physical Review B</i> , 2012, 86, .	3.2	48
123	Constructing metallic nanoroads on a MoS ₂ monolayer via hydrogenation. <i>Nanoscale</i> , 2014, 6, 1691-1697.	5.6	48
124	Metallic 1T Phase, 3d ¹ Electronic Configuration and Charge Density Wave Order in Molecular Beam Epitaxy Grown Monolayer Vanadium Diteelluride. <i>ACS Nano</i> , 2019, 13, 12894-12900.	14.6	48
125	A Facile and Effective Method for Patching Sulfur Vacancies of WS ₂ via Nitrogen Plasma Treatment. <i>Small</i> , 2019, 15, e1901791.	10.0	48
126	Cooling-rate dependence of the density of Pd ₄₀ Ni ₁₀ Cu ₃₀ P ₂₀ bulk metallic glass. <i>Physical Review B</i> , 2001, 64, .	3.2	47

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127	Investigation of the non-volatile resistance change in noncentrosymmetric compounds. Scientific Reports, 2012, 2, 587.	3.3	47
128	Transition metal atoms pathways on rutile TiO ₂ (110) surface: Distribution of Ti ³⁺ states and evidence of enhanced peripheral charge accumulation. Journal of Chemical Physics, 2013, 138, 154711.	3.0	47
129	Separation of glass transition and crystallization in metallic glasses by temperature-modulated differential scanning calorimetry. Philosophical Magazine Letters, 1998, 78, 213-220.	1.2	46
130	Magnetism in phosphorene: Interplay between vacancy and strain. Applied Physics Letters, 2015, 107, .	3.3	46
131	Reactive Co magic cluster formation on Si(111) (7Å ⁻¹). Physical Review B, 2005, 72, .	3.2	45
132	Stability and electronic structure of two dimensional C _x (BN) _y compound. Applied Physics Letters, 2011, 98, .	3.3	45
133	Ultra-low magnetic damping of perovskite La _{0.7} Sr _{0.3} MnO ₃ thin films. Applied Physics Letters, 2017, 110, .	3.3	45
134	Impact of interface structure on Schottky-barrier height for Ni ²⁺ /ZrO ₂ (001) interfaces. Applied Physics Letters, 2005, 86, 132103.	3.3	43
135	Calculation of the thermodynamic properties of B2 AIRE (RE=Sc, Y, La, Ce~Lu). Physica B: Condensed Matter, 2007, 399, 27-32.	2.7	43
136	Ab initio calculation of the total energy and elastic properties of Laves phase C15 Al ₂ RE (RE=Sc, Y, La, Tj ETQq0 0 0 rgBT /Overlock 10 T	3.6	43
137	Li ⁺ ionic conductivities and diffusion mechanisms in Li-based imides and lithium amide. Physical Chemistry Chemical Physics, 2012, 14, 1596-1606.	2.8	43
138	Magnetocrystalline anisotropy and its electric-field-assisted switching of Heusler-compound-based perpendicular magnetic tunnel junctions. New Journal of Physics, 2014, 16, 103033.	2.9	43
139	Synthesis and Characterization of a New Ternary Imide Li ₂ Ca(NH) ₂ . Inorganic Chemistry, 2007, 46, 517-521.	4.0	42
140	Enhancement of room temperature ferromagnetism in C-doped ZnO films by nitrogen codoping. Journal of Applied Physics, 2009, 105, 07C513.	2.5	42
141	Glass forming abilities of binary Cu _{100-x} Zr _x (34, 35.5, and 38.2 at.%) metallic glasses: A LAMMPS study. Journal of Applied Physics, 2009, 105, .	2.5	42
142	Band gap engineering in graphene and hexagonal BN antidot lattices: A first principles study. Applied Physics Letters, 2011, 98, 023105.	3.3	42
143	Surface ferromagnetism in hydrogenated-ZnO film. Applied Physics Letters, 2011, 98, .	3.3	42
144	Tunable and low-loss correlated plasmons in Mott-like insulating oxides. Nature Communications, 2017, 8, 15271.	12.8	42

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145	Anisotropy of electron-phonon coupling in single wurtzite CdS nanowires. Applied Physics Letters, 2007, 91, .	3.3	41
146	Disorder and surface effects on work function of Ni-Pt metal gates. Physical Review B, 2008, 78, .	3.2	41
147	New crystal structure prediction of fully hydrogenated borophene by first principles calculations. Scientific Reports, 2017, 7, 609.	3.3	41
148	One-dimensional thermoelectrics induced by Rashba spin-orbit coupling in two-dimensional BiSb monolayer. Nano Energy, 2018, 52, 163-170.	16.0	41
149	Chemical tuning of band alignments for metal gate/high- κ oxide interfaces. Physical Review B, 2006, 73, .	3.2	40
150	Enthalpies of formation for the Al-Cu-Ni-Zr quaternary alloys calculated via a combined approach of geometric model and Miedema theory. Journal of Alloys and Compounds, 2006, 420, 175-181.	5.5	39
151	Efficient Spin Injection into Graphene through a Tunnel Barrier: Overcoming the Spin-Conductance Mismatch. Physical Review Applied, 2014, 2, .	3.8	39
152	Electron Transport at the TiO ₂ Surfaces of Rutile, Anatase, and Strontium Titanate: The Influence of Orbital Corrugation. ACS Applied Materials & Interfaces, 2015, 7, 24616-24621.	8.0	39
153	Discovery of Hidden Classes of Layered Electrides by Extensive High-Throughput Material Screening. Chemistry of Materials, 2019, 31, 1860-1868.	6.7	39
154	Configuration-Dependent Interface Charge Transfer at a Molecule-Metal Junction. Journal of the American Chemical Society, 2006, 128, 8003-8007.	13.7	38
155	Ab initio study of single-wall BC ₂ N nanotubes. Physical Review B, 2006, 74, .	3.2	38
156	High pressure photoluminescence and Raman investigations of CdSe/ZnS core/shell quantum dots. Applied Physics Letters, 2007, 90, 021921.	3.3	38
157	Ab initio calculations of mechanical and thermodynamic properties for the B ₂ -based AlRE. Computational Materials Science, 2007, 40, 226-233.	3.0	38
158	The basic polyhedral clusters, the optimum glass formers, and the composition-structure-property (glass-forming ability) correlation in Cu-Zr metallic glasses. Journal of Applied Physics, 2010, 107, .	2.5	38
159	Evolution of Topological Surface States in Antimony Ultra-Thin Films. Scientific Reports, 2013, 3, 2010.	3.3	38
160	Dipole Orientation Dependent Symmetry Reduction of Chloroaluminum Phthalocyanine on Cu(111). Journal of Physical Chemistry C, 2013, 117, 1013-1019.	3.1	38
161	Biaxial strain-induced transport property changes in atomically tailored SrTiO ₃ systems. Physical Review B, 2014, 90, .	3.2	38
162	Interplay of electronic reconstructions, surface oxygen vacancies, and lattice distortions in insulator-metal transition of LaAlO ₃ . Physical Review B, 2015, 92, .	3.2	38

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163	Tailoring Self-Polarization of BaTiO ₃ Thin Films by Interface Engineering and Flexoelectric Effect. <i>Advanced Materials Interfaces</i> , 2016, 3, 1600737.	3.7	37
164	Experimental evidences of topological surface states of $\hat{\Gamma}^2$ -Ag ₂ Te. <i>AIP Advances</i> , 2013, 3, 032123.	1.3	36
165	First-principles GGA+ <i>U</i> study of the different conducting properties in pentavalent-ion-doped anatase and rutile TiO ₂ . <i>Journal Physics D: Applied Physics</i> , 2014, 47, 275101.	2.8	36
166	High catalytic activity of oxygen-induced (200) surface of Ta ₂ O ₅ nanolayer towards durable oxygen evolution reaction. <i>Nano Energy</i> , 2016, 25, 60-67.	16.0	36
167	Empirical pseudopotential band-structure calculation for Zn _{1-x} Cd _x SySe _{1-y} quaternary alloy. <i>Journal of Applied Physics</i> , 1993, 74, 3948-3955.	2.5	35
168	Band structure of Mg _{1-x} Zn _x SySe _{1-y} . <i>Semiconductor Science and Technology</i> , 1994, 9, 349-355.	2.0	35
169	First-principles calculations of the thermodynamic and elastic properties of the L ₁ ₂ -based Al ₃ RE (RE = Sc, Y, La-Lu). <i>International Journal of Materials Research</i> , 2008, 99, 582-588.	0.3	35
170	C-doped ZnO nanowires: Electronic structures, magnetic properties, and a possible spintronic device. <i>Journal of Chemical Physics</i> , 2011, 134, 104706.	3.0	35
171	Hydrogen adsorption by tungsten carbide nanotube. <i>Applied Physics Letters</i> , 2007, 90, 223104.	3.3	34
172	Strain effects on work functions of pristine and potassium-decorated carbon nanotubes. <i>Journal of Chemical Physics</i> , 2009, 131, 224701.	3.0	34
173	Mn-doped thiolated Au ₂₅ nanoclusters: Atomic configuration, magnetic properties, and a possible high-performance spin filter. <i>Applied Physics Letters</i> , 2011, 98, .	3.3	34
174	Atomic-orbital-free intrinsic ferromagnetism in electrenes. <i>Physical Review B</i> , 2020, 102, .	3.2	34
175	Electronic structure of germanium nitride considered for gate dielectrics. <i>Journal of Applied Physics</i> , 2007, 102, 013507.	2.5	33
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177	Boron diffusion induced symmetry reduction and scattering in CoFeB/MgO/CoFeB magnetic tunnel junctions. <i>Physical Review B</i> , 2013, 87, .	3.2	33
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