

Bi-Cai Pan

List of Publications by Year in descending order

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161
papers

12,754
citations

57758

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15725
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#	ARTICLE	IF	CITATIONS
1	Enhanced Photoresponsive Ultrathin Graphitic-Phase C ₃ N ₄ Nanosheets for Bioimaging. <i>Journal of the American Chemical Society</i> , 2013, 135, 18-21.	13.7	1,908
2	Oxygen Vacancies Confined in Ultrathin Indium Oxide Porous Sheets for Promoted Visible-Light Water Splitting. <i>Journal of the American Chemical Society</i> , 2014, 136, 6826-6829.	13.7	1,178
3	Ultrathin Spinel-Structured Nanosheets Rich in Oxygen Deficiencies for Enhanced Electrocatalytic Water Oxidation. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 7399-7404.	13.8	1,118
4	Structures of medium-sized silicon clusters. <i>Nature</i> , 1998, 392, 582-585.	27.8	622
5	Atomically-thin molybdenum nitride nanosheets with exposed active surface sites for efficient hydrogen evolution. <i>Chemical Science</i> , 2014, 5, 4615-4620.	7.4	455
6	Heterogeneous Spin States in Ultrathin Nanosheets Induce Subtle Lattice Distortion To Trigger Efficient Hydrogen Evolution. <i>Journal of the American Chemical Society</i> , 2016, 138, 5087-5092.	13.7	351
7	Design and Epitaxial Growth of MoSe ₂ -NiSe Vertical Heteronanostructures with Electronic Modulation for Enhanced Hydrogen Evolution Reaction. <i>Chemistry of Materials</i> , 2016, 28, 1838-1846.	6.7	310
8	Intralayered Ostwald Ripening to Ultrathin Nanomesh Catalyst with Robust Oxygen-Evolving Performance. <i>Advanced Materials</i> , 2017, 29, 1604765.	21.0	283
9	Giant Electron-Hole Interactions in Confined Layered Structures for Molecular Oxygen Activation. <i>Journal of the American Chemical Society</i> , 2017, 139, 4737-4742.	13.7	243
10	Oxygen vacancy associated single-electron transfer for photofixation of CO ₂ to long-chain chemicals. <i>Nature Communications</i> , 2019, 10, 788.	12.8	222
11	Pothole-rich Ultrathin WO ₃ Nanosheets that Trigger N≡N Bond Activation of Nitrogen for Direct Nitrate Photosynthesis. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 731-735.	13.8	202
12	Fast colloidal synthesis of scalable Mo-rich hierarchical ultrathin MoSe ₂ nanosheets for high-performance hydrogen evolution. <i>Nanoscale</i> , 2014, 6, 11046-11051.	5.6	200
13	Conductive Tungsten Oxide Nanosheets for Highly Efficient Hydrogen Evolution. <i>Nano Letters</i> , 2017, 17, 7968-7973.	9.1	195
14	Nature of Single Vacancy in Achiral Carbon Nanotubes. <i>Physical Review Letters</i> , 2004, 92, 105504.	7.8	184
15	Structural distortion in graphitic-C ₃ N ₄ realizing an efficient photoreactivity. <i>Nanoscale</i> , 2015, 7, 5152-5156.	5.6	178
16	Half-Metallicity in Single-Layered Manganese Dioxide Nanosheets by Defect Engineering. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1195-1199.	13.8	177
17	Electrochemical doping of anatase TiO ₂ in organic electrolytes for high-performance supercapacitors and photocatalysts. <i>Journal of Materials Chemistry A</i> , 2014, 2, 229-236.	10.3	172
18	Half-Metallic Ferromagnetism in Synthetic Co ₉ Se ₈ Nanosheets with Atomic Thickness. <i>Journal of the American Chemical Society</i> , 2012, 134, 11908-11911.	13.7	170

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19	Ionization of medium-sized silicon clusters and the geometries of the cations. Journal of Chemical Physics, 1998, 109, 9401-9409.	3.0	169
20	Atomic-layer-confined Doping for Atomic-level Insights into Visible-light Water Splitting. Angewandte Chemie - International Edition, 2015, 54, 9266-9270.	13.8	158
21	Local Electric Field Facilitates High-Performance Li-Ion Batteries. ACS Nano, 2017, 11, 8519-8526.	14.6	155
22	Promoting Photogenerated Holes Utilization in Pore-rich WO ₃ Ultrathin Nanosheets for Efficient Oxygen-evolving Photoanode. Advanced Energy Materials, 2016, 6, 1600437.	19.5	150
23	An environment-dependent tight-binding potential for Si. Journal of Physics Condensed Matter, 1999, 11, 2043-2049.	1.8	139
24	Highly Active Fe Sites in Ultrathin Pyrrhotite Fe ₇ S ₈ Nanosheets Realizing Efficient Electrocatalytic Oxygen Evolution. ACS Central Science, 2017, 3, 1221-1227.	11.3	136
25	Intercalated Iridium Diselenide Electrocatalysts for Efficient pH-universal Water Splitting. Angewandte Chemie - International Edition, 2019, 58, 14764-14769.	13.8	126
26	Highly efficient visible-light-driven photocatalytic activities in synthetic ordered monoclinic BiVO ₄ quantum tubes-graphene nanocomposites. Nanoscale, 2012, 4, 3761.	5.6	121
27	Electrochemical Doping of Halide Perovskites with Ion Intercalation. ACS Nano, 2017, 11, 1073-1079.	14.6	118
28	Ultrathin Nanosheets of MAX Phases with Enhanced Thermal and Mechanical Properties in Polymeric Compositions: Ti ₃ Si _{0.75} Al _{0.25} C ₂ . Angewandte Chemie - International Edition, 2013, 52, 4361-4365.	13.8	113
29	New-phase VO ₂ micro/nanostructures: investigation of phase transformation and magnetic property. New Journal of Chemistry, 2012, 36, 619-625.	2.8	108
30	Single atom accelerates ammonia photosynthesis. Science China Chemistry, 2018, 61, 1187-1196.	8.2	107
31	Synthesis of FeP ₂ /C nanohybrids and their performance for hydrogen evolution reaction. Journal of Materials Chemistry A, 2015, 3, 499-503.	10.3	91
32	Magnetic ions in wide band gap semiconductor nanocrystals for optimized thermoelectric properties. Materials Horizons, 2014, 1, 81-86.	12.2	87
33	Dissolving, trapping and detrapping mechanisms of hydrogen in bcc and fcc transition metals. AIP Advances, 2013, 3, .	1.3	82
34	Theoretical study on the tungsten-induced reduction of transition temperature and the degradation of optical properties for VO ₂ . Journal of Chemical Physics, 2013, 138, 114705.	3.0	76
35	Bionanofiber Assisted Decoration of Few-layered MoSe ₂ Nanosheets on 3D Conductive Networks for Efficient Hydrogen Evolution. Small, 2017, 13, 1602866.	10.0	67
36	Formation energies of topological defects in carbon nanotubes. Physical Review B, 2000, 62, 12652-12655.	3.2	64

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37	Oxygen vacancy engineering in spinel-structured nanosheet wrapped hollow polyhedra for electrochemical nitrogen fixation under ambient conditions. <i>Journal of Materials Chemistry A</i> , 2020, 8, 1652-1659.	10.3	59
38	Microscopic nature of Staebler-Wronski defect formation in amorphous silicon. <i>Applied Physics Letters</i> , 1998, 72, 371-373.	3.3	55
39	Wide Range Bandgap Modulation Based on ZnO-based Alloys and Fabrication of Solar Blind UV Detectors with High Rejection Ratio. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 14152-14158.	8.0	55
40	Structural Features and Electronic Properties of MgO Nanosheets and Nanobelts. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23130-23135.	3.1	53
41	Lithium-Boron (Li-B) Monolayers: First-Principles Cluster Expansion and Possible Two-Dimensional Superconductivity. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 2526-2532.	8.0	49
42	Enhanced stability of deuterium in silicon. <i>Applied Physics Letters</i> , 1998, 72, 3500-3502.	3.3	45
43	Theoretical study of size-dependent properties of BN nanotubes with intrinsic defects. <i>Physical Review B</i> , 2007, 76, .	3.2	42
44	The Nature of Radiative Transitions in O-Doped Boron Nitride Nanotubes. <i>Journal of the American Chemical Society</i> , 2009, 131, 4839-4845.	13.7	42
45	On the influence of short and medium range order on the material band gap in hydrogenated amorphous silicon. <i>Journal of Applied Physics</i> , 2004, 96, 3818-3826.	2.5	40
46	Electronic and vibrational properties of diamondlike hydrocarbons. <i>Physical Review B</i> , 2005, 72, .	3.2	40
47	Structures, Stability, Vibration Entropy and IR Spectra of Hydrated Calcium Ion Clusters [Ca(H ₂ O) _n] ²⁺ (n = 1~20, 27): A Systematic Investigation by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7595-7603.	2.5	39
48	Highly Dual-Heteroatom-Doped Ultrathin Carbon Nanosheets with Expanded Interlayer Distance for Efficient Energy Storage. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 3143-3153.	6.7	38
49	Noncovalent Functionalization of BN Nanotubes with Perylene Derivative Molecules: An <i>in situ</i> Study. <i>ACS Nano</i> , 2010, 4, 1313-1320.	14.6	37
50	Facilitating Lithium-Ion Diffusion in Layered Cathode Materials by Introducing Li ⁺ /Ni ²⁺ Antisite Defects for High-Rate Li-Ion Batteries. <i>Research</i> , 2019, 2019, 2198906.	5.7	36
51	Structure and optical properties of ternary alloy BeZnO and quaternary alloy BeMgZnO films growth by molecular beam epitaxy. <i>Applied Surface Science</i> , 2013, 274, 341-344.	6.1	35
52	Nature of the negative thermal expansion in antiperovskite compound Mn ₃ ZnN. <i>Journal of Applied Physics</i> , 2010, 108, .	2.5	33
53	Highly depressed temperature-induced metal-insulator transition in synthetic monodisperse 10-nm V ₂ O ₃ pseudocubes enclosed by {012} facets. <i>Nanoscale</i> , 2011, 3, 2609.	5.6	32
54	Ultrahigh Energy Density Realized by a Single-Layer $\text{Co}(\text{OH})_2$ All-Solid-State Asymmetric Supercapacitor. <i>Angewandte Chemie</i> , 2014, 126, 13003-13007.	2.0	32

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55	Geometric structures, electronic properties, and vibrational frequencies of small tellurium clusters. <i>Physical Review B</i> , 2002, 65, .	3.2	31
56	Solar-blind wurtzite MgZnO alloy films stabilized by Be doping. <i>Journal Physics D: Applied Physics</i> , 2013, 46, 245103.	2.8	31
57	Formation behavior of Be-doped ZnO alloys grown by plasma-assisted molecular beam epitaxy. <i>Applied Physics Letters</i> , 2013, 102, .	3.3	31
58	Intercalated Iridium Diselenide Electrocatalysts for Efficient pH-Universal Water Splitting. <i>Angewandte Chemie</i> , 2019, 131, 14906-14911.	2.0	30
59	Giant reduction of the phase transition temperature for beryllium doped VO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4687.	2.8	29
60	An energetic evaluation of dissolution corrosion capabilities of liquid metals on iron surface. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16837.	2.8	29
61	Interaction of hydrogen with vacancies in a (12,0) carbon nanotube. <i>Physical Review B</i> , 2005, 71, .	3.2	27
62	Hydrogen diffusion behavior in N doped ZnO: First-principles study. <i>Journal of Applied Physics</i> , 2008, 103, .	2.5	26
63	Quantum Tunneling of Magnetization in Ultrasmall Half-Metallic V ₃ O ₄ Quantum Dots: Displaying Quantum Superparamagnetic State. <i>Scientific Reports</i> , 2012, 2, 755.	3.3	25
64	Enhanced Exciton Binding Energy of ZnO by Long-Distance Perturbation of Doped Be Atoms. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1484-1489.	4.6	25
65	The composition-dependent mechanical properties of Ge/Si core-shell nanowires. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 3042-3048.	2.7	23
66	Elastic and Melting Properties of Crystalline SiC Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 8199-8205.	3.1	23
67	H-stabilized shallow acceptors in N-doped ZnO. <i>Physical Review B</i> , 2015, 92, .	3.2	23
68	Theoretical study of the new compound VO ₂ (D). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 3474-3477.	2.1	22
69	Mechanism of Proton Conduction in Doped Barium Cerates: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8024-8033.	3.1	22
70	Theoretical studies of neutral and cationic selenium clusters. <i>Physical Review B</i> , 2000, 62, 17026-17030.	3.2	21
71	Pothole-rich Ultrathin WO ₃ Nanosheets that Trigger N ₂ Bond Activation of Nitrogen for Direct Nitrate Photosynthesis. <i>Angewandte Chemie</i> , 2019, 131, 741-745.	2.0	21
72	Thermal Conductivity, Electrical Resistivity, and Microstructure of Cu/W Multilayered Nanofilms. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 8886-8896.	8.0	21

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73	Introducing a Pseudocapacitive Lithium Storage Mechanism into Graphite by Defect Engineering for Fast-Charging Lithium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 16279-16288.	8.0	21
74	Tuning electronic structure of graphene via tailoring structure: Theoretical study. <i>Journal of Applied Physics</i> , 2010, 107, .	2.5	20
75	The dynamical process of the phase transition from VO ₂ (M) to VO ₂ (R). <i>Journal of Applied Physics</i> , 2011, 110, .	2.5	20
76	Effect of irradiation defects on the corrosion behaviors of steels exposed to lead bismuth eutectic in ADS: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12292-12298.	2.8	20
77	Structures of W _x N _y Crystals and Their Intrinsic Properties: First-Principles Calculations. <i>Crystal Growth and Design</i> , 2018, 18, 2270-2278.	3.0	20
78	Structural features of silicon clusters (Si _n). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007, 368, 396-401.	2.1	19
79	Effects of nitrogen vacancies on transition-metal-doped GaN: An ab initio study. <i>Journal of Applied Physics</i> , 2009, 105, 103710.	2.5	19
80	A microstructure engineered perovskite super anode with Li-storage life of exceeding 10,000 cycles. <i>Nano Energy</i> , 2022, 94, 106972.	16.0	19
81	Low-lying isomers of Si _n ⁺ and Si _n ²⁺ (n=31-50) clusters. <i>Journal of Chemical Physics</i> , 2008, 128, 234302.	3.0	18
82	Strain-induced semiconducting-metallic transition for ZnO zigzag nanoribbons. <i>Journal of Applied Physics</i> , 2010, 107, .	2.5	18
83	Boron-tuning transition temperature of vanadium dioxide from rutile to monoclinic phase. <i>Journal of Chemical Physics</i> , 2014, 141, 194707.	3.0	18
84	Structural features and thermal properties of W/Cu compounds using tight-binding potential calculations. <i>Journal of Materials Science</i> , 2016, 51, 5948-5961.	3.7	18
85	Electronic structure regulation of Na ₂ FePO ₄ F cathode toward superior high-rate and high-temperature sodium-ion batteries. <i>Energy Storage Materials</i> , 2022, 45, 851-860.	18.0	18
86	Structure and simulation of hydrogenated nanocrystalline silicon. <i>Journal of Applied Physics</i> , 2004, 96, 6247-6252.	2.5	17
87	Interaction of Iron Atoms with Pristine and Defective (8, 0) Boron Nitride Nanotubes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13571-13578.	3.1	17
88	Development of a tight-binding model for Cu and its application to a Cu-heat-sink under irradiation. <i>Journal of Materials Science</i> , 2015, 50, 5684-5693.	3.7	17
89	Simulation of hydrogen evolution from nano-crystalline silicon. <i>Journal of Non-Crystalline Solids</i> , 2004, 333, 44-47.	3.1	16
90	Studies on structural defects in carbon nanotubes. <i>Frontiers of Physics in China</i> , 2009, 4, 297-306.	1.0	16

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91	High ICE Hard Carbon Anodes for Lithium-Ion Batteries Enabled by a High Work Function. ACS Applied Materials & Interfaces, 2021, 13, 46813-46820.	8.0	15
92	Tight-binding potential for hydrocarbons. Physical Review B, 2001, 64, .	3.2	14
93	Identifying structural distortion in doped VO ₂ with IR spectroscopy. Physical Chemistry Chemical Physics, 2012, 14, 7225.	2.8	14
94	Synthetic Potassium Vanadium Oxide K ₂ V ₆ O ₁₆ ·1.5H ₂ O Superlong Nanobelts: A 1D Room-Temperature Ferromagnetic Semiconductor. European Journal of Inorganic Chemistry, 2013, 2013, 3497-3505.	2.0	13
95	The influence of liquid Pb–Bi on the anti-corrosion behavior of Fe ₃ O ₄ : a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 7789-7796.	2.8	13
96	Observation of local electronic structures of adatom vacancies in Si(111)-(7×7) surface in real space. Physical Review B, 2007, 75, .	3.2	12
97	Effect of cation replacement on the phase stability of formamidinium lead iodide perovskite. Journal of Chemical Physics, 2019, 151, 134104.	3.0	11
98	Possible lowest-reactivity structure of the silicon cluster Si ₄₅ . Physical Review B, 2006, 73, .	3.2	10
99	Enhancing the topological structures of defected carbon nanotubes with adsorbed hydrocarbon radicals at low temperatures. Physical Review B, 2007, 75, .	3.2	10
100	Theoretical Study of the Site-Dependent Stabilities of Intrinsic Defects in a Polar BN Nanotube with Finite Length. Journal of Physical Chemistry C, 2008, 112, 19353-19359.	3.1	10
101	Electronic Structures and Vibrational Properties of a Carbon Nanotube with Adsorption of Small Hydrocarbon Radicals. Journal of Physical Chemistry C, 2008, 112, 18876-18881.	3.1	10
102	An atomistic insight into the corrosion of the oxide film in liquid lead–bismuth eutectic. Physical Chemistry Chemical Physics, 2014, 16, 7417.	2.8	10
103	Strain-dependent diffusion behavior of H within tungsten. Physica B: Condensed Matter, 2014, 443, 76-79.	2.7	10
104	Active-Site-Specific Structural Engineering Enabled Ultrahigh Rate Performance of the NaLi ₃ Fe ₃ (PO ₄) ₂ (P ₂ O ₇) ₂ Cathode for Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 11255-11263.	8.0	10
105	The Structural Features of the Hydrated Ferrous Ion Clusters: [Fe(H ₂ O) _n] ²⁺ (n=1–19). Journal of Cluster Science, 2012, 23, 311-324.	3.3	9
106	Stabilization of BeZnO alloy by S incorporation: A density functional theory investigation. Journal of Alloys and Compounds, 2016, 658, 636-641.	5.5	9
107	An empirical law for the elastic moduli of component-segregated W/Cu compounds. Journal of Alloys and Compounds, 2018, 766, 349-354.	5.5	9
108	Reactivity and Migration of Hydrogen in A-Si:H. Materials Research Society Symposia Proceedings, 1997, 467, 135.	0.1	8

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109	Transferable tight-binding potential for germanium. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 305802.	1.8	8
110	Interaction of H with stacking fault in W(111) film: A possible formation mechanism of H bubbles. <i>RSC Advances</i> , 2014, 4, 7030.	3.6	8
111	A machine learning based deep potential for seeking the low-lying candidates of Al clusters. <i>Journal of Chemical Physics</i> , 2020, 152, 114105.	3.0	8
112	Diffusion of small hydrocarbon radicals on the outer wall of a carbon nanotube. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 542-549.	2.7	7
113	Understanding the origin of phase segregation of nano-crystalline in a $\text{Be}_{1/3}\text{Zn}_{2/3}\text{O}$ random alloy: a novel phase of $\text{Be}_{1/3}\text{Zn}_{2/3}\text{O}$. <i>Nanoscale</i> , 2015, 7, 9852-9858.	5.6	7
114	Environment-Dependent Tight-Binding Potential Model. <i>Materials Research Society Symposia Proceedings</i> , 1997, 491, 211.	0.1	6
115	Structural phase transition and the related electronic and optical properties of MgZnO nanowires. <i>European Physical Journal B</i> , 2011, 80, 395-400.	1.5	6
116	An empirical law for the band gaps of MgZnO nanowires. <i>Journal of Applied Physics</i> , 2011, 110, 124315.	2.5	6
117	The wurtzite-“rocksalt” phase transition for a $\text{Be}_x\text{Mg}_{1-x}\text{Zn}_y\text{O}$ alloy: Be content vs Mg content. <i>Journal of Alloys and Compounds</i> , 2014, 608, 197-201.	5.5	6
118	The formation of H bubbles at small-angle tilt grain boundaries in W films. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 33103-33108.	2.8	6
119	Interaction between gallium atoms and the inner walls of single-walled carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 075706.	2.6	5
120	“Compressing liquid” An efficient global minima search strategy for clusters. <i>Journal of Chemical Physics</i> , 2009, 131, 034108.	3.0	5
121	Distribution and self-assisted diffusion of Be and Mg impurities in ZnO. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19631-19636.	2.8	5
122	An empirical law on the finite-size effects in electronic transport calculations of tungsten. <i>AIP Advances</i> , 2019, 9, .	1.3	5
123	The mechanism on retention of hydrogen in three representative tungsten nitride compounds in nuclear fusion reactors. <i>Journal of Nuclear Materials</i> , 2021, 544, 152687.	2.7	5
124	Non-thermal melting of tungsten under intense electronic excitations. <i>Acta Materialia</i> , 2021, 216, 117158.	7.9	5
125	H Evolution from Nano-Crystalline Silicon- Comparison of Simulation and Experiment. <i>Materials Research Society Symposia Proceedings</i> , 2004, 808, 101.	0.1	4
126	Improved endohedral fullerene-like structures of silicon clusters Si_31 – Si_39 by density functional calculations. <i>European Physical Journal D</i> , 2008, 47, 367-372.	1.3	4

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127	The elastic properties of $Mn_3(Cu_{1-x}Gex)N$ compounds. AIP Advances, 2011, 1, 042125.	1.3	4
128	Defects in SiC for Quantum Computing. MRS Advances, 2019, 4, 2217-2222.	0.9	4
129	Linear scaling algorithm for tight-binding molecular dynamics simulations. Journal of Chemical Physics, 2019, 150, 114107.	3.0	4
130	Performance of tungsten nitride compound surfaces to resist sputtering under intense irradiation in nuclear fusion reactors. Applied Surface Science, 2022, 600, 154072.	6.1	4
131	A Tight-Binding Model Beyond Two-Center Approximation. Materials Research Society Symposia Proceedings, 1995, 408, 37.	0.1	3
132	Electronic structures of an extra Si atom diffusing in the Si(111)($7\sqrt{3}\times 7$) surface. Surface Science, 2005, 599, 85-92.	1.9	3
133	Size- and surface-dependent electronic structures of crystalline SiC nanotubes. Journal of Applied Physics, 2011, 109, 084318.	2.5	3
134	The hydrogenation-dependent thermal expansion properties of hydrogenated graphene. European Physical Journal B, 2014, 87, 1.	1.5	3
135	The nucleation and growth of H blisters in dislocation loops in W{110}. Journal of Nuclear Materials, 2016, 478, 222-226.	2.7	3
136	Theoretical Simulations of Irradiation-Induced Sputtering at Tungsten Surface. Chinese Journal of Chemical Physics, 2017, 30, 77-82.	1.3	3
137	The thermal conductivity of defected copper at finite temperatures. Journal of Materials Science, 2020, 55, 4453-4463.	3.7	3
138	Flatband in a three-dimensional tungsten nitride compound. Journal of Chemical Physics, 2020, 152, 224503.	3.0	3
139	Atomistic Character of Nanocrystalline and Mixed Phase Silicon. Materials Research Society Symposia Proceedings, 2003, 762, 1141.	0.1	3
140	Microcrystalline and Nanocrystalline Silicon: Simulation of Material Properties. Materials Research Society Symposia Proceedings, 2005, 862, 2431.	0.1	2
141	Crystallized silicon nanostructures – experimental characterization and atomistic simulations. Canadian Journal of Physics, 2014, 92, 783-788.	1.1	2
142	Interplay of the doped Ge atoms and the N vacancies with the negative thermal expansion of $Mn_3(Cu_{1-x})N$. Journal of Applied Physics, 2023, 125, 045101.	2.3	2
143	A first-principles study on the negative thermal expansion material: $Mn_3(A_{0.5}B_{0.5})N$ (A=Cu, Zn, Ag, or Bi). Journal of Applied Physics, 2023, 125, 045101.	1.3	2
144	Atomic resolution on the (111)B surface of mercury cadmium telluride by scanning tunneling microscopy. Physical Review B, 2018, 97, .	3.2	2

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145	First-principles study of intrinsic point defects in MgSiAs ₂ . Physical Chemistry Chemical Physics, 2019, 21, 5295-5304.	2.8	2
146	Mechanical properties and phase transition of tungsten with edge dislocation under intensively-electronic excitation. Journal of Nuclear Materials, 2022, 561, 153540.	2.7	2
147	Simulation of Realistic Core-shell Silicon Nanowires. Materials Research Society Symposia Proceedings, 2006, 910, 4.	0.1	1
148	Identification of Silicon Clusters by Electron Diffraction Spectra. Journal of Physical Chemistry C, 2007, 111, 5850-5854.	3.1	1
149	Stability of Ga ₆ N ₆ clusters in a nitrogen environment. European Physical Journal D, 2007, 41, 121-125.	1.3	1
150	Diffusion of an Extra Ga Atom in GaAs(001)(2 × 4) Rich-As Surface. Chinese Journal of Chemical Physics, 2008, 21, 69-75.	1.3	1
151	Theoretical Study of H Diffusion Behavior and the Vibrational Properties of Li ⁺ H Complexes in ZnO. Journal of Physical Chemistry C, 2009, 113, 11381-11384.	3.1	1
152	New compounds Mg ₃ IV ₆ V ₈ (IV=Si, Ge, Sn; V=P, As, Sb) and their potential application to photovoltaic materials. Journal of Alloys and Compounds, 2019, 786, 434-439.	5.5	1
153	Dilute magnetism in Co-doped spinel Mg ₃ Si ₆ As ₈ . Journal of Applied Physics, 2020, 128, .	2.5	1
154	Theoretical study on the interaction of p-type impurities with hydrogen in ZnO. Scientia Sinica: Physica, Mechanica Et Astronomica, 2012, 42, 1124-1134.	0.4	1
155	Nonthermal effects in H-doped tungsten at high electronic temperatures. Journal of Nuclear Materials, 2022, 568, 153896.	2.7	1
156	INVESTIGATION OF A POSSIBLE GROWTH MECHANISM OF SYNTHETIC DIAMOND FILMS. Modern Physics Letters B, 1992, 06, 599-604.	1.9	0
157	STUDY OF ELECTRONIC STATES IN THE HYDROGEN-INDUCED STRUCTURAL PHASE TRANSITION FROM DIAMOND C(111)â€“(2 × 1) RECONSTRUCTION TO (1 × 1) STRUCTURE. Modern Physics Letters B, 1992, 06, 649-655. ^{1.9}	1.9	0
158	Nature of Charged Metastable Defects in Network Rebonding Model. Materials Research Society Symposia Proceedings, 2002, 715, 1131.	0.1	0
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