Bi-Cai Pan

List of Publications by Year
in descending order

		57758	23533
161	12,754	44	111
papers	citations	h-index	g-index

168	168	168	15725
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic structure regulation of Na2FePO4F cathode toward superior high-rate and high-temperature sodium-ion batteries. Energy Storage Materials, 2022, 45, 851-860.	18.0	18
2	A microstructure engineered perovskite super anode with Li-storage life of exceeding 10,000 cycles. Nano Energy, 2022, 94, 106972.	16.0	19
3	Mechanical properties and phase transition of tungsten with edge dislocation under intensively-electronic excitation. Journal of Nuclear Materials, 2022, 561, 153540.	2.7	2
4	Active-Site-Specific Structural Engineering Enabled Ultrahigh Rate Performance of the NaLi₃Fe₃(PO₄)₂(P₂O₇) Cathode for Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 11255-11263.	8.0	10
5	Introducing a Pseudocapacitive Lithium Storage Mechanism into Graphite by Defect Engineering for Fast-Charging Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 16279-16288.	8.0	21
6	Nonthermal effects in H-doped tungsten at high electronic temperatures. Journal of Nuclear Materials, 2022, 568, 153896.	2.7	1
7	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
8	The mechanism on retention of hydrogen in three representative tungsten nitride compounds in nuclear fusion reactors. Journal of Nuclear Materials, 2021, 544, 152687.	2.7	5
9	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
10	Non-thermal melting of tungsten under intense electronic excitations. Acta Materialia, 2021, 216, 117158.	7.9	5
11	Oxygen vacancy engineering in spinel-structured nanosheet wrapped hollow polyhedra for electrochemical nitrogen fixation under ambient conditions. Journal of Materials Chemistry A, 2020, 8, 1652-1659.	10.3	59
12	The thermal conductivity of defected copper at finite temperatures. Journal of Materials Science, 2020, 55, 4453-4463.	3.7	3
13	Dilute magnetism in Co-doped spinel Mg3Si6As8. Journal of Applied Physics, 2020, 128, .	2.5	1
14	Flatband in a three-dimensional tungsten nitride compound. Journal of Chemical Physics, 2020, 152, 224503.	3.0	3
15	A machine learning based deep potential for seeking the low-lying candidates of Al clusters. Journal of Chemical Physics, 2020, 152, 114105.	3.0	8
16	Thermal Conductivity, Electrical Resistivity, and Microstructure of Cu/W Multilayered Nanofilms. ACS Applied Materials & Interfaces, 2020, 12, 8886-8896.	8.0	21
17	Mechanism of Proton Conduction in Doped Barium Cerates: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 8024-8033.	3.1	22
18	Potholeâ€rich Ultrathin WO₃ Nanosheets that Trigger Nâ‰¡N Bond Activation of Nitrogen for Direct Nitrate Photosynthesis. Angewandte Chemie, 2019, 131, 741-745.	2.0	21

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19	Defects in SiC for Quantum Computing. MRS Advances, 2019, 4, 2217-2222.	0.9	4
20	An empirical law on the finite-size effects in electronic transport calculations of tungsten. AIP Advances, 2019, 9, .	1.3	5
21	Intercalated Iridium Diselenide Electrocatalysts for Efficient pHâ€Universal Water Splitting. Angewandte Chemie - International Edition, 2019, 58, 14764-14769.	13.8	126
22	Intercalated Iridium Diselenide Electrocatalysts for Efficient pHâ€Universal Water Splitting. Angewandte Chemie, 2019, 131, 14906-14911.	2.0	30
23	Effect of cation replacement on the phase stability of formamidinium lead iodide perovskite. Journal of Chemical Physics, 2019, 151, 134104.	3.0	11
24	Linear scaling algorithm for tight-binding molecular dynamics simulations. Journal of Chemical Physics, 2019, 150, 114107.	3.0	4
25	First-principles study of intrinsic point defects in MgSiAs2. Physical Chemistry Chemical Physics, 2019, 21, 5295-5304.	2.8	2
26	New compounds Mg3IV6V8 (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
27	Oxygen vacancy associated single-electron transfer for photofixation of CO2 to long-chain chemicals. Nature Communications, 2019, 10, 788.	12.8	222
28	Potholeâ€rich Ultrathin WO₃ Nanosheets that Trigger Nâ‰¡N Bond Activation of Nitrogen for Direct Nitrate Photosynthesis. Angewandte Chemie - International Edition, 2019, 58, 731-735.	13.8	202
29	Facilitating Lithium-Ion Diffusion in Layered Cathode Materials by Introducing Li ⁺ /Ni ²⁺ Antisite Defects for High-Rate Li-Ion Batteries. Research, 2019, 2019, 2198906.	5.7	36
30	Structures of WxNy Crystals and Their Intrinsic Properties: First-Principles Calculations. Crystal Growth and Design, 2018, 18, 2270-2278.	3.0	20
31	Highly Dual-Heteroatom-Doped Ultrathin Carbon Nanosheets with Expanded Interlayer Distance for Efficient Energy Storage. ACS Sustainable Chemistry and Engineering, 2018, 6, 3143-3153.	6.7	38
32	Atomic resolution on the (111)B surface of mercury cadmium telluride by scanning tunneling microscopy. Physical Review B, 2018, 97, .	3.2	2
33	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
34	Single atom accelerates ammonia photosynthesis. Science China Chemistry, 2018, 61, 1187-1196.	8.2	107
35	Intralayered Ostwald Ripening to Ultrathin Nanomesh Catalyst with Robust Oxygenâ€Evolving Performance. Advanced Materials, 2017, 29, 1604765.	21.0	283
36	Electrochemical Doping of Halide Perovskites with Ion Intercalation. ACS Nano, 2017, 11, 1073-1079.	14.6	118

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37	Giant Electronâ€“Hole Interactions in Confined Layered Structures for Molecular Oxygen Activation. Journal of the American Chemical Society, 2017, 139, 4737-4742.	13.7	243
38	Carbon Nanofibers: Bionanofiber Assisted Decoration of Fewâ€Layered MoSe₂ Nanosheets on 3D Conductive Networks for Efficient Hydrogen Evolution (Small 7/2017). Small, 2017, 13, .	10.0	0
39	Bionanofiber Assisted Decoration of Fewâ€Layered MoSe₂ Nanosheets on 3D Conductive Networks for Efficient Hydrogen Evolution. Small, 2017, 13, 1602866.	10.0	67
40	Highly Active Fe Sites in Ultrathin Pyrrhotite Fe₇S₈Nanosheets Realizing Efficient Electrocatalytic Oxygen Evolution. ACS Central Science, 2017, 3, 1221-1227.	11.3	136
41	Local Electric Field Facilitates High-Performance Li-Ion Batteries. ACS Nano, 2017, 11, 8519-8526.	14.6	155
42	Conductive Tungsten Oxide Nanosheets for Highly Efficient Hydrogen Evolution. Nano Letters, 2017, 17, 7968-7973.	9.1	195
43	Theoretical Simulations of Irradiation-Induced Sputtering at Tungsten Surface. Chinese Journal of Chemical Physics, 2017, 30, 77-82.	1.3	3
44	The formation of H bubbles at small-angle tilt grain boundaries in W films. Physical Chemistry Chemical Physics, 2016, 18, 33103-33108.	2.8	6
45	Enhanced Exciton Binding Energy of ZnO by Long-Distance Perturbation of Doped Be Atoms. Journal of Physical Chemistry Letters, 2016, 7, 1484-1489.	4.6	25
46	Distribution and self-assisted diffusion of Be and Mg impurities in ZnO. Physical Chemistry Chemical Physics, 2016, 18, 19631-19636.	2.8	5
47	Promoting Photogenerated Holes Utilization in Poreâ€Rich WO₃ Ultrathin Nanosheets for Efficient Oxygenâ€Evolving Photoanode. Advanced Energy Materials, 2016, 6, 1600437.	19.5	150
48	A first-principles study on the negative thermal expansion material: Mn3(A0.5B0.5)N (A=Cu, Zn, Ag, or) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.3	2
49	The nucleation and growth of H blisters in dislocation loops in W{110}. Journal of Nuclear Materials, 2016, 478, 222-226.	2.7	3
50	Lithiumâ€“Boron (Liâ€“B) Monolayers: First-Principles Cluster Expansion and Possible Two-Dimensional Superconductivity. ACS Applied Materials & Interfaces, 2016, 8, 2526-2532.	8.0	49
51	Heterogeneous Spin States in Ultrathin Nanosheets Induce Subtle Lattice Distortion To Trigger Efficient Hydrogen Evolution. Journal of the American Chemical Society, 2016, 138, 5087-5092.	13.7	351
52	Structural features and thermal properties of W/Cu compounds using tight-binding potential calculations. Journal of Materials Science, 2016, 51, 5948-5961.	3.7	18
53	The influence of liquid Pbâ€“Bi on the anti-corrosion behavior of Fe₃O₄: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 7789-7796.	2.8	13
54	Design and Epitaxial Growth of MoSe₂â€“NiSe Vertical Heteronanostructures with Electronic Modulation for Enhanced Hydrogen Evolution Reaction. Chemistry of Materials, 2016, 28, 1838-1846.	6.7	310

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55	Stabilization of BeZnO alloy by S incorporation: A density functional theory investigation. Journal of Alloys and Compounds, 2016, 658, 636-641.	5.5	9
56	H-stabilized shallow acceptors in N-doped ZnO. Physical Review B, 2015, 92, .	3.2	23
57	Atomicâ€Layerâ€Confined Doping for Atomicâ€Level Insights into Visibleâ€Light Water Splitting. Angewandte Chemie - International Edition, 2015, 54, 9266-9270.	13.8	158
58	Structural distortion in graphitic-C₃N₄realizing an efficient photoreactivity. Nanoscale, 2015, 7, 5152-5156.	5.6	178
59	Understanding the origin of phase segregation of nano-crystalline in a BexZn1â^'xO random alloy: a novel phase of Be1/3Zn2/3O. Nanoscale, 2015, 7, 9852-9858.	5.6	7
60	Development of a tight-binding model for Cu and its application to a Cu-heat-sink under irradiation. Journal of Materials Science, 2015, 50, 5684-5693.	3.7	17
61	Ultrathin Spinelâ€Structured Nanosheets Rich in Oxygen Deficiencies for Enhanced Electrocatalytic Water Oxidation. Angewandte Chemie - International Edition, 2015, 54, 7399-7404.	13.8	1,118
62	Effect of irradiation defects on the corrosion behaviors of steels exposed to lead bismuth eutectic in ADS: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 12292-12298.	2.8	20
63	Synthesis of FeP₂/C nanohybrids and their performance for hydrogen evolution reaction. Journal of Materials Chemistry A, 2015, 3, 499-503.	10.3	91
64	Halfâ€Metallicity in Singleâ€Layered Manganese Dioxide Nanosheets by Defect Engineering. Angewandte Chemie - International Edition, 2015, 54, 1195-1199.	13.8	177
65	Boron-tuning transition temperature of vanadium dioxide from rutile to monoclinic phase. Journal of Chemical Physics, 2014, 141, 194707.	3.0	18
66	Ultrahigh Energy Density Realized by a Singleâ€Layer Î²â€Co(OH)₂ Allâ€Solidâ€State Asymmetric Supercapacitor. Angewandte Chemie, 2014, 126, 13003-13007.	2.0	32
67	Crystallized silicon nanostructures â€" experimental characterization and atomistic simulations. Canadian Journal of Physics, 2014, 92, 783-788.	1.1	2
68	Interplay of the doped Ge atoms and the N vacancies with the negative thermal expansion of M3(Cu1â^'x) Tj ETQq0 0 0 rgBT /Overlock 1	2.3	2
69	The hydrogenation-dependent thermal expansion properties of hydrogenated graphene. European Physical Journal B, 2014, 87, 1.	1.5	3
70	The wurtziteâ€"rocksalt phase transition for a BexMgyZn1â^'xâ^'yO alloy: Be content vs Mg content. Journal of Alloys and Compounds, 2014, 608, 197-201.	5.5	6
71	Magnetic ions in wide band gap semiconductor nanocrystals for optimized thermoelectric properties. Materials Horizons, 2014, 1, 81-86.	12.2	87
72	Electrochemical doping of anatase TiO₂in organic electrolytes for high-performance supercapacitors and photocatalysts. Journal of Materials Chemistry A, 2014, 2, 229-236.	10.3	172

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73	An atomistic insight into the corrosion of the oxide film in liquid leadâ€“bismuth eutectic. Physical Chemistry Chemical Physics, 2014, 16, 7417.	2.8	10
74	Wide Range Bandgap Modulation Based on ZnO-based Alloys and Fabrication of Solar Blind UV Detectors with High Rejection Ratio. ACS Applied Materials & Interfaces, 2014, 6, 14152-14158.	8.0	55
75	Fast colloidal synthesis of scalable Mo-rich hierarchical ultrathin MoSe_{2â^'x}nanosheets for high-performance hydrogen evolution. Nanoscale, 2014, 6, 11046-11051.	5.6	200
76	Atomically-thin molybdenum nitride nanosheets with exposed active surface sites for efficient hydrogen evolution. Chemical Science, 2014, 5, 4615-4620.	7.4	455
77	Interaction of H with stacking fault in W(111) film: A possible formation mechanism of H bubbles. RSC Advances, 2014, 4, 7030.	3.6	8
78	An energetic evaluation of dissolution corrosion capabilities of liquid metals on iron surface. Physical Chemistry Chemical Physics, 2014, 16, 16837.	2.8	29
79	Strain-dependent diffusion behavior of H within tungsten. Physica B: Condensed Matter, 2014, 443, 76-79.	2.7	10
80	Oxygen Vacancies Confined in Ultrathin Indium Oxide Porous Sheets for Promoted Visible-Light Water Splitting. Journal of the American Chemical Society, 2014, 136, 6826-6829.	13.7	1,178
81	Giant reduction of the phase transition temperature for beryllium doped VO2. Physical Chemistry Chemical Physics, 2013, 15, 4687.	2.8	29
82	Enhanced Photoresponsive Ultrathin Graphitic-Phase C₃N₄ Nanosheets for Bioimaging. Journal of the American Chemical Society, 2013, 135, 18-21.	13.7	1,908
83	Structure and optical properties of ternary alloy BeZnO and quaternary alloy BeMgZnO films growth by molecular beam epitaxy. Applied Surface Science, 2013, 274, 341-344.	6.1	35
84	Synthetic Potassium Vanadium Oxide K2V6O16Â·1.5H2O Superlong Nanobelts: A 1D Room-Temperature Ferromagnetic Semiconductor. European Journal of Inorganic Chemistry, 2013, 2013, 3497-3505.	2.0	13
85	Solar-blind wurtzite MgZnO alloy films stabilized by Be doping. Journal Physics D: Applied Physics, 2013, 46, 245103.	2.8	31
86	Dissolving, trapping and detrapping mechanisms of hydrogen in bcc and fcc transition metals. AIP Advances, 2013, 3, .	1.3	82
87	Formation behavior of BexZn1â^'xO alloys grown by plasma-assisted molecular beam epitaxy. Applied Physics Letters, 2013, 102, .	3.3	31
88	Theoretical study on the tungsten-induced reduction of transition temperature and the degradation of optical properties for VO2. Journal of Chemical Physics, 2013, 138, 114705.	3.0	76
89	Ultrathin Nanosheets of MAX Phases with Enhanced Thermal and Mechanical Properties in Polymeric Compositions: Ti₃Si_{0.75}Al_{0.25}C₂. Angewandte Chemie - International Edition, 2013, 52, 4361-4365.	13.8	113
90	Transferable tight-binding potential for germanium. Journal of Physics Condensed Matter, 2012, 24, 305802.	1.8	8

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91	Identifying structural distortion in doped VO2 with IR spectroscopy. Physical Chemistry Chemical Physics, 2012, 14, 7225.	2.8	14
92	Half-Metallic Ferromagnetism in Synthetic Co₉Se₈ Nanosheets with Atomic Thickness. Journal of the American Chemical Society, 2012, 134, 11908-11911.	13.7	170
93	Structural Features and Electronic Properties of MgO Nanosheets and Nanobelts. Journal of Physical Chemistry C, 2012, 116, 23130-23135.	3.1	53
94	New-phase VO2 micro/nanostructures: investigation of phase transformation and magnetic property. New Journal of Chemistry, 2012, 36, 619-625.	2.8	108
95	Quantum Tunneling of Magnetization in Ultrasmall Half-Metallic V3O4 Quantum Dots: Displaying Quantum Superparamagnetic State. Scientific Reports, 2012, 2, 755.	3.3	25
96	Highly efficient visible-light-driven photocatalytic activities in synthetic ordered monoclinic BiVO4 quantum tubesâ€“graphene nanocomposites. Nanoscale, 2012, 4, 3761.	5.6	121
97	The Structural Features of the Hydrated Ferrous Ion Clusters: [Fe(H2O) n]2+ (nÂ=Â1â€“19). Journal of Cluster Science, 2012, 23, 311-324.	3.3	9
98	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
99	Highly depressed temperature-induced metal-insulator transition in synthetic monodisperse 10-nm V2O3 pseudocubes enclosed by {012} facets. Nanoscale, 2011, 3, 2609.	5.6	32
100	The elastic properties of Mn3(Cu1â^'xGex)N compounds. AIP Advances, 2011, 1, 042125.	1.3	4
101	Theoretical study of the new compound VO2 (D). Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 3474-3477.	2.1	22
102	Structural phase transition and the related electronic and optical properties of MgZnO nanowires. European Physical Journal B, 2011, 80, 395-400.	1.5	6
103	The dynamical process of the phase transition from VO2(M) to VO2(R). Journal of Applied Physics, 2011, 110, .	2.5	20
104	An empirical law for the band gaps of MgZnO nanowires. Journal of Applied Physics, 2011, 110, 124315.	2.5	6
105	Size- and surface-dependent electronic structures of crystalline SiC nanotubes. Journal of Applied Physics, 2011, 109, 084318.	2.5	3
106	The effect of hydrogen and oxygen atoms on the adsorbed gallium inside defective carbon nanotubes. European Physical Journal B, 2010, 73, 413-416.	1.5	0
107	Tuning electronic structure of graphene via tailoring structure: Theoretical study. Journal of Applied Physics, 2010, 107, .	2.5	20
108	Nature of the negative thermal expansion in antiperovskite compound Mn3ZnN. Journal of Applied Physics, 2010, 108, .	2.5	33

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109	Elastic and Melting Properties of Crystalline SiC Nanotubes. Journal of Physical Chemistry C, 2010, 114, 8199-8205.	3.1	23
110	Strain-induced semiconducting-metallic transition for ZnO zigzag nanoribbons. Journal of Applied Physics, 2010, 107, .	2.5	18
111	Structures, Stability, Vibration Entropy and IR Spectra of Hydrated Calcium Ion Clusters [Ca(H₂O)_n]²⁺ (n = 1â^'20, 27): A Systematic Investigation by Density Functional Theory. Journal of Physical Chemistry A, 2010, 114, 7595-7603.	2.5	39
112	Noncovalent Functionalization of BN Nanotubes with Perylene Derivative Molecules: An ab Initio Study. ACS Nano, 2010, 4, 1313-1320.	14.6	37
113	Lattice strain effects in graphane and partially-hydrogenated graphene sheets. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	0
114	Effects of nitrogen vacancies on transition-metal-doped GaN: An ab initio study. Journal of Applied Physics, 2009, 105, 103710.	2.5	19
115	Studies on structural defects in carbon nanotubes. Frontiers of Physics in China, 2009, 4, 297-306.	1.0	16
116	The Nature of Radiative Transitions in O-Doped Boron Nitride Nanotubes. Journal of the American Chemical Society, 2009, 131, 4839-4845.	13.7	42
117	â€œCompressing liquidâ€: An efficient global minima search strategy for clusters. Journal of Chemical Physics, 2009, 131, 034108.	3.0	5
118	Theoretical Study of H Diffusion Behavior and the Vibrational Properties of Liâ^'H Complexes in ZnO. Journal of Physical Chemistry C, 2009, 113, 11381-11384.	3.1	1
119	Diffusion of small hydrocarbon radicals on the outer wall of a carbon nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 542-549.	2.7	7
120	The composition-dependent mechanical properties of Ge/Si coreâ€“shell nanowires. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 3042-3048.	2.7	23
121	Improved endohedral fullerenelike structures of silicon clusters Si31â€“Si39 by density functional calculations. European Physical Journal D, 2008, 47, 367-372.	1.3	4
122	Interaction of Iron Atoms with Pristine and Defective (8, 0) Boron Nitride Nanotubes. Journal of Physical Chemistry C, 2008, 112, 13571-13578.	3.1	17
123	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
124	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
125	Low-lying isomers of Sin+ and Sinâ^' (n=31â€“50) clusters. Journal of Chemical Physics, 2008, 128, 234302.	3.0	18
126	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

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127	Interaction between gallium atoms and the inner walls of single-walled carbon nanotubes. Nanotechnology, 2008, 19, 075706.	2.6	5
128	Hydrogen diffusion behavior in N doped ZnO: First-principles study. Journal of Applied Physics, 2008, 103, .	2.5	26
129	Observation of local electronic structures of adatom vacancies inSi(111)â^'(7Ã—7)surface in real space. Physical Review B, 2007, 75, .	3.2	12
130	Theoretical study of size-dependent properties of BN nanotubes with intrinsic defects. Physical Review B, 2007, 76, .	3.2	42
131	Enhancing the topological structures of defected carbon nanotubes with adsorbed hydrocarbon radicals at low temperatures. Physical Review B, 2007, 75, .	3.2	10
132	Identification of Silicon Clusters by Electron Diffraction Spectra. Journal of Physical Chemistry C, 2007, 111, 5850-5854.	3.1	1
133	Stability of Ga6N6 clusters in a nitrogen environment. European Physical Journal D, 2007, 41, 121-125.	1.3	1
134	Structural features of silicon clusters (). Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 368, 396-401.	2.1	19
135	Simulation of Realistic Core-shell Silicon Nanowires. Materials Research Society Symposia Proceedings, 2006, 910, 4.	0.1	1
136	Possible lowest-reactivity structure of the silicon clusterSi45. Physical Review B, 2006, 73, .	3.2	10
137	Electronic structures of an extra Si atom diffusing in the Si(111)(7Ã—7) surface. Surface Science, 2005, 599, 85-92.	1.9	3
138	Electronic and vibrational properties of diamondlike hydrocarbons. Physical Review B, 2005, 72, .	3.2	40
139	Interaction of hydrogen with vacancies in a (12,0) carbon nanotube. Physical Review B, 2005, 71, .	3.2	27
140	Microcrystalline and Nanocrystalline Silicon: Simulation of Material Properties. Materials Research Society Symposia Proceedings, 2005, 862, 2431.	0.1	2
141	Nature of Single Vacancy in Achiral Carbon Nanotubes. Physical Review Letters, 2004, 92, 105504.	7.8	184
142	On the influence of short and medium range order on the material band gap in hydrogenated amorphous silicon. Journal of Applied Physics, 2004, 96, 3818-3826.	2.5	40
143	H Evolution from Nano-Crystalline Silicon- Comparison of Simulation and Experiment. Materials Research Society Symposia Proceedings, 2004, 808, 101.	0.1	4
144	Structure and simulation of hydrogenated nanocrystalline silicon. Journal of Applied Physics, 2004, 96, 6247-6252.	2.5	17

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145	Simulation of hydrogen evolution from nano-crystalline silicon. Journal of Non-Crystalline Solids, 2004, 333, 44-47.	3.1	16
146	Atomistic Character of Nanocrystalline and Mixed Phase Silicon. Materials Research Society Symposia Proceedings, 2003, 762, 1141.	0.1	3
147	Geometric structures, electronic properties, and vibrational frequencies of small tellurium clusters. Physical Review B, 2002, 65, .	3.2	31
148	Nature of Charged Metastable Defects in Network Rebonding Model. Materials Research Society Symposia Proceedings, 2002, 715, 1131.	0.1	0
149	Tight-binding potential for hydrocarbons. Physical Review B, 2001, 64, .	3.2	14
150	Formation energies of topological defects in carbon nanotubes. Physical Review B, 2000, 62, 12652-12655.	3.2	64
151	Theoretical studies of neutral and cationic selenium clusters. Physical Review B, 2000, 62, 17026-17030.	3.2	21
152	An environment-dependent tight-binding potential for Si. Journal of Physics Condensed Matter, 1999, 11, 2043-2049.	1.8	139
153	Structures of medium-sized silicon clusters. Nature, 1998, 392, 582-585.	27.8	622
154	Microscopic nature of Staebler-Wronski defect formation in amorphous silicon. Applied Physics Letters, 1998, 72, 371-373.	3.3	55
155	Ionization of medium-sized silicon clusters and the geometries of the cations. Journal of Chemical Physics, 1998, 109, 9401-9409.	3.0	169
156	Enhanced stability of deuterium in silicon. Applied Physics Letters, 1998, 72, 3500-3502.	3.3	45
157	Reactivity and Migration of Hydrogen in A-SI:H. Materials Research Society Symposia Proceedings, 1997, 467, 135.	0.1	8
158	Environment-Dependent Tight-Binding Potential Model. Materials Research Society Symposia Proceedings, 1997, 491, 211.	0.1	6
159	A Tight-Binding Model Beyond Two-Center Approximation. Materials Research Society Symposia Proceedings, 1995, 408, 37.	0.1	3
160	INVESTIGATION OF A POSSIBLE GROWTH MECHANISM OF SYNTHETIC DIAMOND FILMS. Modern Physics Letters B, 1992, 06, 599-604.	1.9	0
161	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	0