Jerry Bernholc

List of Publications by Year
in descending order

258 papers	19,170 citations	13099 68 h-index	11939 134 g-index
265 all docs	265 docs citations	265 times ranked	12526 citing authors

#	Article	IF	Citations
1	Nanomechanics of Carbon Tubes: Instabilities beyond Linear Response. Physical Review Letters, 1996, 76, 2511-2514.	7.8	2,450
2	Structural flexibility of carbon nanotubes. Journal of Chemical Physics, 1996, 104, 2089-2092.	3.0	1,115
3	Mn Interstitial Diffusion in(Ga,Mn)As. Physical Review Letters, 2004, 92, 037201.	7.8	476
4	High strain rate fracture and C-chain unraveling in carbon nanotubes. Computational Materials Science, 1997, 8, 341-348.	3.0	475
5	Brittle and Ductile Behavior in Carbon Nanotubes. Physical Review Letters, 1998, 81, 4656-4659.	7.8	475
6	Native defects in gallium nitride. Physical Review B, 1995, 51, 17255-17258.	3.2	444
7	Mechanism of strain release in carbon nanotubes. Physical Review B, 1998, 57, R4277-R4280.	3.2	441
8	Negative-electron-affinity effects on the diamond (100) surface. Physical Review B, 1994, 50, 5803-5806.	3.2	369
9	Mechanical and Electrical Properties of Nanotubes. Annual Review of Materials Research, 2002, 32, 347-375.	9.3	343
10	Nitrogen and potentialn-type dopants in diamond. Physical Review Letters, 1991, 66, 2010-2013.	7.8	342
11	Real-space multigrid-based approach to large-scale electronic structure calculations. Physical Review B, 1996, 54, 14362-14375.	3.2	341
12	Self-Consistent Method for Point Defects in Semiconductors: Application to the Vacancy in Silicon. Physical Review Letters, 1978, 41, 895-899.	7.8	317
13	Towards the Identification of the Dominant Donor in GaN. Physical Review Letters, 1995, 75, 296-299.	7.8	295
14	Ab InitioInvestigations of Lithium Diffusion in Carbon Nanotube Systems. Physical Review Letters, 2002, 88, 075506.	7.8	254
15	Ab initiophonon dispersions of wurtzite AlN, GaN, and InN. Physical Review B, 2000, 61, 6720-6725.	3.2	253
16	Ultimate strength of carbon nanotubes: A theoretical study. Physical Review B, 2002, 65, .	3.2	239
17	Doping properties of C, Si, and Ge impurities in GaN and AlN. Physical Review B, 1997, 56, 9496-9505.	3.2	233
18	Scattering-theoretic method for defects in semiconductors. I. Tight-binding description of vacancies in Si, Ge, and GaAs. Physical Review B, 1978, 18, 1780-1789.	3.2	229

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19	Scattering-theoretic method for defects in semiconductors. II. Self-consistent formulation and application to the vacancy in silicon. Physical Review B, 1980, 21, 3545-3562.	3.2	228
20	Towards grid-basedO(N)density-functional theory methods: Optimized nonorthogonal orbitals and multigrid acceleration. Physical Review B, 2000, 62, 1713-1722.	3.2	220
21	Enhancement of the dielectric response in polymer nanocomposites with low dielectric constant fillers. Nanoscale, 2017, 9, 10992-10997.	5.6	216
22	Spontaneous polarization and piezoelectricity in boron nitride nanotubes. Physical Review B, 2003, 67, .	3.2	211
23	Carbon Nanotubeâˆ'Metal Cluster Composites:Â A New Road to Chemical Sensors?. Nano Letters, 2005, 5, 847-851.	9.1	209
24	Large-scale electronic-structure calculations with multigrid acceleration. Physical Review B, 1995, 52, R5471-R5474.	3.2	208
25	Structure and dynamics of solidC60. Physical Review Letters, 1991, 66, 2633-2636.	7.8	203
26	Ferroelectric polymers exhibiting behaviour reminiscent of a morphotropic phase boundary. Nature, 2018, 562, 96-100.	27.8	200
27	Atomic structure and doping of microtubules. Physical Review B, 1993, 47, 1708-1711.	3.2	168
28	Mechanism of self-diffusion in diamond. Physical Review Letters, 1988, 61, 2689-2692.	7.8	162
29	Mechanical properties, defects and electronic behavior of carbon nanotubes. Carbon, 2000, 38, 1703-1711.	10.3	162
30	Consistent methodology for calculating surface and interface energies. Physical Review B, 1998, 57, 7281-7291.	3.2	161
31	Formation energies, abundances, and the electronic structure of native defects in cubic SiC. Physical Review B, 1988, 38, 12752-12755.	3.2	145
32	Kinetics of metal-catalyzed growth of single-walled carbon nanotubes. Physical Review B, 1997, 55, R6097-R6100.	3.2	142
33	Mechanical deformations and coherent transport in carbon nanotubes. Physical Review B, 1999, 60, R16338-R16341.	3.2	137
34	Polarization field effects on the electron-hole recombination dynamics in In0.2Ga0.8N/In1âˆ'xGaxN multiple quantum wells. Applied Physics Letters, 1997, 71, 3135-3137.	3.3	125
35	Theory of growth and mechanical properties of nanotubes. Applied Physics A: Materials Science and Processing, 1998, 67, 39-46.	2.3	124
36	Optical Absorption of Water: Coulomb Effects versus Hydrogen Bonding. Physical Review Letters, 2005, 94, 037404.	7.8	123

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37	High-entropy polymer produces a giant electrocaloric effect at low fields. Nature, 2021, 600, 664-669.	27.8	121
38	Pressure effects on self-diffusion in silicon. Physical Review B, 1989, 40, 10643-10646.	3.2	120
39	Electronic and field emission properties of boron nitride/carbon nanotube superlattices. Applied Physics Letters, 2002, 81, 46-48.	3.3	118
40	Ab InitioStudies of Polarization and Piezoelectricity in Vinylidene Fluoride and BN-Based Polymers. Physical Review Letters, 2004, 92, 115504.	7.8	116
41	Kinetics of cluster formation in the laser vaporization source: Carbon clusters. Journal of Chemical Physics, 1986, 85, 3258-3267.	3.0	115
42	O(N)real-space method forab initioquantum transport calculations: Application to carbon nanotubeâ€"metal contacts. Physical Review B, 2001, 64, .	3.2	115
43	Isomerization of C60 fullerenes. Journal of Chemical Physics, 1992, 96, 8634-8636.	3.0	110
44	Ab InitioStudies of the Diffusion Barriers at Single-Height Si(100) Steps. Physical Review Letters, 1995, 75, 101-104.	7.8	107
45	Theory of carbon nanotube growth. Physical Review B, 1995, 52, 14850-14858.	3.2	106
46	Amphoteric properties of substitutional carbon impurity in GaN and AlN. Applied Physics Letters, 1996, 69, 233-235.	3.3	106
47	Structure and energetics of single and multilayer fullerene cages. Physical Review Letters, 1993, 70, 3023-3026.	7.8	105
48	Ad-dimers on Strained Carbon Nanotubes: A New Route for Quantum Dot Formation?. Physical Review Letters, 1999, 83, 4132-4135.	7.8	104
49	Growth Energetics of Carbon Nanotubes. Physical Review Letters, 1994, 73, 2468-2471.	7.8	103
50	Strain effects on the interface properties of nitride semiconductors. Physical Review B, 1997, 55, R7323-R7326.	3.2	101
51	Theory of surface morphology of wurtzite GaN (0001) surfaces. Physical Review B, 1997, 56, R12725-R12728.	3.2	100
52	High-temperature polymers with record-high breakdown strength enabled by rationally designed chain-packing behavior in blends. Matter, 2021, 4, 2448-2459.	10.0	100
53	Structural distortions in metal clusters. Physical Review Letters, 1991, 67, 1594-1597.	7.8	96
54	Theoretical STM signatures and transport properties of native defects in carbon nanotubes. Physical Review B, 2000, 61, 14194-14203.	3.2	96

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55	Chirality-induced relaxor properties in ferroelectric polymers. Nature Materials, 2020, 19, 1169-1174.	27.5	93
56	Lip-Lip Interactions and the Growth of Multiwalled Carbon Nanotubes. Physical Review Letters, 1998, 80, 313-316.	7.8	91
57	Surface structures and electron affinities of bare and hydrogenated diamond C(100) surfaces. Physical Review B, 1995, 51, 5291-5296.	3.2	89
58	Generating high dielectric constant blends from lower dielectric constant dipolar polymers using nanostructure engineering. Nano Energy, 2017, 32, 73-79.	16.0	89
59	Theory of binding energies of acceptors in semiconductors. Physical Review B, 1977, 15, 4935-4947.	3.2	87
60	Understanding reflectance anisotropy: Surface-state signatures and bulk-related features in the optical spectrum ofInP(001)(2Ã—4). Physical Review B, 2000, 61, R16335-R16338.	3.2	87
61	Collective polarization effects inÎ²-polyvinylidene fluoride and its copolymers with tri- and tetrafluoroethylene. Physical Review B, 2005, 72, .	3.2	87
62	Structural Insight in the Interfacial Effect in Ferroelectric Polymer Nanocomposites. Advanced Materials, 2020, 32, e2005431.	21.0	84
63	Phase Equilibria in High Energy Density PVDF-Based Polymers. Physical Review Letters, 2007, 99, 047801.	7.8	77
64	Precursors toC60fullerene formation. Physical Review B, 1992, 46, 7326-7328.	3.2	75
65	Intrinsic electron transport properties of carbon nanotube Y-junctions. Applied Physics Letters, 2002, 81, 5234-5236.	3.3	74
66	Relaxor ferroelectric polymer exhibits ultrahigh electromechanical coupling at low electric field. Science, 2022, 375, 1418-1422.	12.6	74
67	Kinetics of aggregation of carbon clusters. Physical Review B, 1986, 33, 7395-7398.	3.2	73
68	Broensted acid sites in transition metal oxide catalysts: modeling of structure, acid strengths, and support effects. The Journal of Physical Chemistry, 1987, 91, 1526-1530.	2.9	73
69	Mechanism of copper(II)-induced misfolding of Parkinson's disease protein. Scientific Reports, 2011, 1, 11.	3.3	71
70	Electronic structure of deepsp-bonded substitutional impurities in silicon. Physical Review B, 1982, 26, 5706-5715.	3.2	67
71	Structural transitions in aluminum clusters. Chemical Physics Letters, 1990, 174, 461-466.	2.6	66
72	Nonequilibrium Quantum Transport Properties of Organic Molecules on Silicon. Physical Review Letters, 2005, 95, 206805.	7.8	65

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73	Electronic Structure of the Jahn-Teller Distorted Vacancy in Silicon. Physical Review Letters, 1979, 43, 1354-1357.	7.8	64
74	Seamless Staircase Electrical Contact to Semiconducting Graphene Nanoribbons. Nano Letters, 2017, 17, 6241-6247.	9.1	64
75	Recent developments and applications of the real-space multigrid method. Journal of Physics Condensed Matter, 2008, 20, 294205.	1.8	63
76	Quantum-Interference-Controlled Three-Terminal Molecular Transistors Based on a Single Ring-Shaped Molecule Connected to Graphene Nanoribbon Electrodes. Physical Review Letters, 2010, 105, 236803.	7.8	63
77	Supramolecular Self-Assembly of Ï€-Conjugated Hydrocarbons via 2D Cooperative CH/Ï€ Interaction. ACS Nano, 2012, 6, 566-572.	14.6	63
78	Nanotubes. Current Opinion in Solid State and Materials Science, 1997, 2, 706-715.	11.5	61
79	Terrace and step contributions to the optical anisotropy of Si(001) surfaces. Physical Review B, 2001, 63, .	3.2	61
80	Local Spin-Density Description of Multiple Metal-Metal Bonding:Mo2andCr2. Physical Review Letters, 1983, 50, 1451-1454.	7.8	60
81	Structural defects and the shape of large fullerenes. Chemical Physics Letters, 1994, 219, 473-478.	2.6	59
82	(2Ã—4)GaP(001) surface: Atomic structure and optical anisotropy. Physical Review B, 1999, 60, 2488-2494.	3.2	58
83	Enzymatic Mechanism of Copper-Containing Nitrite Reductase. Biochemistry, 2015, 54, 1233-1242.	2.5	58
84	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. Nature Communications, 2017, 8, 14815.	12.8	58
85	Structure of monatomic steps on the Si(001) surface. Physical Review Letters, 1994, 72, 3694-3697.	7.8	56
86	Surface sensitivity of impurity incorporation: Mg at GaN (0001) surfaces. Physical Review B, 1999, 59, 9771-9774.	3.2	56
87	Mechanisms of NH3 and NO2 detection in carbon-nanotube-based sensors: An ab initio investigation. Carbon, 2016, 101, 177-183.	10.3	56
88	Growth of carbon nanotubes: a molecular dynamics study. Chemical Physics Letters, 1995, 236, 150-155.	2.6	54
89	Structural mechanics of carbon nanotubes: From continuum elasticity to atomistic fracture. Journal of Computer-Aided Materials Design, 1996, 3, 173-182.	0.7	53
90	GaAs(001): Surface Structure and Optical Properties. Physica Status Solidi A, 2001, 188, 1401-1409.	1.7	53

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91	Theory of Zn-enhanced disordering in GaAs/AlAs superlattices. Physical Review Letters, 1992, 69, 3789-3792.	7.8	52
92	Negative Differential Resistance in C₆₀-Based Electronic Devices. ACS Nano, 2010, 4, 7205-7210.	14.6	52
93	Identification and Properties of Defects in GaP. Physical Review Letters, 1981, 47, 413-416.	7.8	51
94	GaP(001) and InP(001): Reflectance anisotropy and surface geometry. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1999, 17, 1691.	1.6	50
95	Theory of native defects, doping and diffusion in diamond and silicon carbide. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1992, 11, 265-272.	3.5	48
96	Electronic structure and identification of deep defects in GaP. Physical Review B, 1984, 29, 3269-3282.	3.2	46
97	Impurity incorporation and doping of diamond. Physica B: Condensed Matter, 1993, 185, 144-149.	2.7	45
98	Computational Materials Science: The Era of Applied Quantum Mechanics. Physics Today, 1999, 52, 30-35.	0.3	45
99	Structural and electronic properties of carbon nanotube tapers. Physical Review B, 2001, 64, .	3.2	45
100	Optimizing nanostructure to achieve high dielectric response with low loss in strongly dipolar polymers. Nano Energy, 2015, 16, 227-234.	16.0	44
101	Structural fingerprints in the reflectance anisotropy spectra ofInP(001)(2Ã—4)surfaces. Physical Review B, 1999, 59, 2234-2239.	3.2	43
102	Electric Field Induced Phase Transitions in Polymers: A Novel Mechanism for High Speed Energy Storage. Physical Review Letters, 2012, 108, 087802.	7.8	43
103	Intrinsic localized defect states in a-Se associated with dihedral angle distortions. Journal of Non-Crystalline Solids, 1987, 97-98, 1171-1174.	3.1	42
104	Hybridab initioKohn-Sham density functional theory/frozen-density orbital-free density functional theory simulation method suitable for biological systems. Journal of Chemical Physics, 2008, 128, 014101.	3.0	42
105	Edge States and Optical Transition Energies in Carbon Nanoribbons. Physical Review Letters, 2008, 101, 246803.	7.8	40
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109	Functional implications of multistage copper binding to the prion protein. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11576-11581.	7.1	35
110	Equivalence of dipole correction and Coulomb cutoff techniques in supercell calculations. Physical Review B, 2008, 77, .	3.2	34
111	Computer simulation studies of the growth of strained layers by molecular-beam epitaxy. Physical Review B, 1990, 42, 2914-2922.	3.2	33
112	Selective sensing of ethylene and glucose using carbon-nanotube-based sensors: an ab initio investigation. Nanoscale, 2017, 9, 1687-1698.	5.6	33
113	Resonant coupling and negative differential resistance in metal/ferrocenyl alkanethiolate/STM structures. Physical Review B, 2006, 74, .	3.2	32
114	(Negative) Electron Affinity of AlN and AlGaN Alloys. Materials Research Society Symposia Proceedings, 1995, 395, 777.	0.1	31
115	Interplay of surface reconstruction and surface electric fields in the optical anisotropy of GaAs(001). Physical Review B, 2002, 66, .	3.2	31
116	Structural transitions in metal clusters. Faraday Discussions, 1991, 92, 217.	3.2	30
117	Surface Segregation of Ge at SiGe(001) by Concerted Exchange Pathways. Physical Review Letters, 2002, 88, 166101.	7.8	30
118	Nanowire-induced optical anisotropy of the Si(111)-In surface. Physical Review B, 2003, 68, .	3.2	30
119	Localized states and the electronic properties of a hydrogenated defect in amorphous silicon. Physical Review B, 1983, 28, 3246-3257.	3.2	29
120	Understanding reflectance anisotropy: Surface-state signatures and bulk-related features. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2000, 18, 2215.	1.6	29
121	Fermi-level effects on the electronic structure and magnetic couplings in (Ga,Mn)N. Physical Review B, 2005, 72, .	3.2	28
122	The shapes of firstâ€stage sinters. Journal of Applied Physics, 1989, 65, 3219-3225.	2.5	27
123	Gallium-rich reconstructions on GaAs(001). Physica Status Solidi (B): Basic Research, 2003, 240, 91-98.	1.5	27
124	Binding of Copper and Cisplatin to Atox1 Is Mediated by Glutathione through the Formation of Metalâ€"Sulfur Clusters. Biochemistry, 2017, 56, 3129-3141.	2.5	27
125	Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence. ACS Nano, 2020, 14, 5090-5098.	14.6	27
126	Morphology-induced dielectric enhancement in polymer nanocomposites. Nanoscale, 2021, 13, 10933-10942.	5.6	27

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127	Reactivity, stability, and formation of fullerenes. Physical Review B, 1993, 48, 5724-5727.	3.2	26
128	Surface segregation and interface stability of AlN/GaN, GaN/InN, and AlN/InN {0001} epitaxial systems. Physical Review B, 2000, 61, 10820-10826.	3.2	26
129	Cycloaddition reaction versus dimer cleavage at theSi(001):C5H8interface. Physical Review B, 2003, 68, .	3.2	26
130	Theory of nitrogen doping of carbon nanoribbons: Edge effects. Journal of Chemical Physics, 2012, 136, 014702.	3.0	26
131	SELF-ENERGY EFFECTS IN THE OPTICAL ANISOTROPY OF GaP(001). Surface Review and Letters, 1999, 06, 1159-1165.	1.1	25
132	GaAs(001) surface reconstructions: geometries, chemical bonding and optical properties. Applied Surface Science, 2002, 190, 264-268.	6.1	25
133	First-principles investigations of the dielectric properties of polypropylene/metal-oxide interfaces. Physical Review B, 2009, 80, .	3.2	25
134	Electronic Control over Attachment and Self-Assembly of Alkyne Groups on Gold. ACS Nano, 2012, 6, 9267-9275.	14.6	25
135	Oxidization stability of atomically precise graphene nanoribbons. Physical Review Materials, 2018, 2, .	2.4	25
136	Curly-Packed Structure Polymers for High-Temperature Capacitive Energy Storage. Chemistry of Materials, 2022, 34, 2333-2341.	6.7	25
137	Si diffusion in GaAs and Si-induced interdiffusion in GaAs/AlAs superlattices. Physical Review B, 1994, 49, 2985-2988.	3.2	24
138	Step-induced optical anisotropy of Si(111):H surfaces. Physical Review B, 2000, 61, 7604-7608.	3.2	24
139	Structure and energetics of Ga-rich GaAs() surfaces. Surface Science, 2002, 507-510, 406-410.	1.9	24
140	Implementation of ultrasoft pseudopotentials in large-scale grid-based electronic structure calculations. Physical Review B, 2007, 76, .	3.2	23
141	First-principles methodology for quantum transport in multiterminal junctions. Journal of Chemical Physics, 2009, 131, 164105.	3.0	23
142	Self-Organized and Cu-Coordinated Surface Linear Polymerization. Scientific Reports, 2013, 3, 2102.	3.3	23
143	Real-space multigrid methods for large-scale electronic structure problems. International Journal of Quantum Chemistry, 1997, 65, 531-543.	2.0	22
144	Band gap control of small bundles of carbon nanotubes using applied electric fields: A density functional theory study. Applied Physics Letters, 2010, 97, 063113.	3.3	22

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145	Angle Resolved Photoemission Spectroscopy of the InP(001) surface. Applied Surface Science, 2000, 166, 224-230.	6.1	21
146	The electronic structure of deep SP-bonded acceptor impurities in semiconductors. Solid State Communications, 1981, 37, 705-708.	1.9	19
147	Local density pseudopotential calculations for molecules: O2 and Mo2O2S2(S2)2â^'2. Journal of Chemical Physics, 1984, 81, 3987-3995.	3.0	19
148	AsGa-XIcomplexes as models for theEL2 center in GaAs. Physical Review B, 1993, 47, 1667-1670.	3.2	18
149	Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. Advanced Theory and Simulations, 2019, 2, 1800172.	2.8	18
150	Direct writing of heterostructures in single atomically precise graphene nanoribbons. Physical Review Materials, 2019, 3, .	2.4	18
151	N-Type Doping and Diffusion of Impurities in Diamond. Materials Research Society Symposia Proceedings, 1989, 162, 315.	0.1	17
152	Disappearance of grain boundaries in sintering. Applied Physics Letters, 1991, 58, 595-597.	3.3	17
153	(001) Surfaces of GaP and InP: structural motifs, electronic states and optical signatures. Applied Surface Science, 2000, 166, 179-184.	6.1	17
154	Structural and electronic properties of arsenic chalcogenide molecules. Physical Review B, 1989, 39, 10831-10838.	3.2	16
155	Pressure and Strain Effects on Diffusion. Materials Research Society Symposia Proceedings, 1989, 163, 523.	0.1	16
156	Chemical and strain effects on Boron-doped Si(100). Physical Review B, 1999, 59, 4813-4821.	3.2	16
157	Segregation effects at vacancies inAlxGa1â^'xNandSixGe1â^'xalloys. Physical Review B, 1999, 59, 1567-1570.	3.2	16
158	Understanding and enhancing polarization in complex materials. Computing in Science and Engineering, 2004, 6, 12-21.	1.2	16
159	Insights into the Morphotropic Phase Boundary in Ferroelectric Polymers from the Molecular Perspective. Journal of Physical Chemistry C, 2019, 123, 8727-8730.	3.1	16
160	ZERO AND FINITE TEMPERATURE STUDY OF SINGLE FULLERENE CAGES AND CARBON â€œONIONSâ€•â€" GEOMETRY AND SHAPE. Modern Physics Letters B, 1993, 07, 1883-1895.	1.9	15
161	Large-Scale Applications of Real-Space Multigrid Methods to Surfaces, Nanotubes, and Quantum Transport. Physica Status Solidi (B): Basic Research, 2000, 217, 685-701.	1.5	15
162	Atomic indium nanowires on Si(111): the (4 Ã— 1)â€"(8 Ã— 2) phase transition studied with reflectance anisotropy spectroscopy. Applied Surface Science, 2004, 234, 302-306.	6.1	15

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163	Effects of end group functionalization and level alignment on electron transport in molecular devices. Journal of Chemical Physics, 2008, 128, 024708.	3.0	15
164	Doping-Dependent Negative Differential Resistance in Hybrid Organic/Inorganic Siâˆ’Porphyrinâˆ’Si Junctions. ACS Nano, 2008, 2, 1517-1522.	14.6	15
165	Simulated annealing strategies for molecular dynamics. Computer Physics Communications, 1991, 66, 177-180.	7.5	14
166	Atomic structure of Al-GaAs(110) interfaces. Physical Review Letters, 1992, 69, 486-489.	7.8	14
167	Native Defects in Wurtzite GaN And AlN. Materials Research Society Symposia Proceedings, 1994, 339, 693.	0.1	14
168	Theoretical bounds for multiwalled carbon nanotube growth. Chemical Physics Letters, 1998, 296, 471-476.	2.6	14
169	Theoretical Investigations of Carbon Nanotube Growth. Molecular Simulation, 2000, 25, 1-12.	2.0	14
170	Calculation of surface optical properties: from qualitative understanding to quantitative predictions. Thin Solid Films, 2004, 455-456, 764-771.	1.8	14
171	Step edge-mediated assembly of periodic arrays of long graphene nanoribbons on Au(111). Chemical Communications, 2019, 55, 11848-11851.	4.1	14
172	Electronic structures of cluster compounds of molybdenum sulfide (MoS42-, Mo3S92-) and nickel molybdenum sulfide (Ni(MoS4)22-) by XPS studies. Inorganic Chemistry, 1987, 26, 1422-1425.	4.0	13
173	Oxidation- and organic-molecule-induced changes of the Si surface optical anisotropy:ab initiopredictions. Journal of Physics Condensed Matter, 2004, 16, S4323-S4334.	1.8	13
174	Hydrogenation effect on the structural transition of C60. Chemical Physics Letters, 2005, 403, 359-362.	2.6	13
175	Electron transport in multiterminal molecular devices: A density functional theory study. Physical Review B, 2010, 81, .	3.2	13
176	Local manifestations of thickness-dependent topology and edge states in the topological magnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>MnBi</mml:mi><mml:mn>2</mml:mn></mr Physical Review B, 2022, 105, .	3.2	12
177	The effective-mass nature of deep-level point-defect states in semiconductors. Solid State Communications, 1980, 33, 1045-1049.	1.9	11
178	Charge transport in DNA nanowires connected to carbon nanotubes. Physical Review B, 2015, 92, .	3.2	11
179	On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. Chemical Science, 2021, 12, 15637-15644.	7.4	11
180	The wetted solidâ€"A generalization of the Plateau problem and its implications for sintered materials. Journal of Mathematical Physics, 1990, 31, 610-615.	1.1	10

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181	Shapes of wetted solids and sinters. Physical Review B, 1991, 43, 8113-8122.	3.2	10
182	Interfacial Segregation and Electrodiffusion of Dopants inAlN/GaNSuperlattices. Physical Review Letters, 2006, 96, 185501.	7.8	10
183	Theory of interfaces and surfaces in wide-gap nitrides. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1997, 15, 1144.	1.6	9
184	Atomistic simulations of aromatic polyurea and polyamide for capacitive energy storage. Physical Review B, 2015, 92, .	3.2	9
185	Large-Scale Phonon Calculations Using the Real-Space Multigrid Method. Journal of Chemical Theory and Computation, 2019, 15, 6859-6864.	5.3	9
186	Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. Npj Computational Materials, 2019, 5, .	8.7	9
187	Comparison of the electronic properties of bis(disulfido)dioxidi-.mu.-sulfidodimolybdate(2-) and bis(disulfido)disulfidodi-.mu.-sulfidodimolybdate(2-). Inorganic Chemistry, 1986, 25, 3876-3879.	4.0	8
188	Efficient techniques for computer simulations of heteroepitaxial growth. Applied Physics Letters, 1990, 56, 1971-1973.	3.3	8
189	Ab initiosimulations of H2in Li-doped carbon nanotube systems. Journal of Physics Condensed Matter, 2007, 19, 086226.	1.8	8
190	Insights into prion protein function from atomistic simulations. Prion, 2010, 4, 13-19.	1.8	8
191	Doping Properties of Amphoteric C, Si, and Ge Impurities in GaN and AlN. Acta Physica Polonica A, 1996, 90, 735-738.	0.5	8
192	EdmondsetÂal.Reply:. Physical Review Letters, 2005, 94, .	7.8	7
193	Properties of wurtzite w-MnN and of w-MnN inclusions in (Ga,Mn)N. Applied Physics Letters, 2006, 88, 092502.	3.3	7
194	First-principles simulations of PVDF copolymers with high dielectric energy density: PVDF-HFP and PVDF-BTFE. Physical Review B, 2016, 94, .	3.2	7
195	Quantum molecular dynamics simulations of fullerenes and graphitic microtubules. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 74-78.	1.0	5
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