Jerry Bernholc

List of Publications by Year
in descending order

258 papers	19,170 citations	15001 68 h-index	13635 134 g-index
265 all docs	265 docs citations	265 times ranked	14274 citing authors

#	Article	IF	Citations
1	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></ Physical Review B, 2022, 105, .	1.1	12
2	Curly-Packed Structure Polymers for High-Temperature Capacitive Energy Storage. Chemistry of Materials, 2022, 34, 2333-2341.	3.2	25
3	Relaxor ferroelectric polymer exhibits ultrahigh electromechanical coupling at low electric field. Science, 2022, 375, 1418-1422.	6.0	74
4	Ab initio simulations of metal contacts for graphene-based devices. Journal of Applied Physics, 2022, 131, 214301.	1.1	2
5	Study of Anharmonicity in Zirconium Hydrides Using Inelastic Neutron Scattering and Ab-Initio Computer Modeling. Inorganics, 2021, 9, 29.	1.2	3
6	High-temperature polymers with record-high breakdown strength enabled by rationally designed chain-packing behavior in blends. Matter, 2021, 4, 2448-2459.	5.0	100
7	Morphology-induced dielectric enhancement in polymer nanocomposites. Nanoscale, 2021, 13, 10933-10942.	2.8	27
8	On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations. Chemical Science, 2021, 12, 15637-15644.	3.7	11
9	High-entropy polymer produces a giant electrocaloric effect at low fields. Nature, 2021, 600, 664-669.	13.7	121
10	Structural Insight in the Interfacial Effect in Ferroelectric Polymer Nanocomposites. Advanced Materials, 2020, 32, e2005431.	11.1	84
11	Chirality-induced relaxor properties in ferroelectric polymers. Nature Materials, 2020, 19, 1169-1174.	13.3	93
12	Mesh independence of the generalized Davidson algorithm. Journal of Computational Physics, 2020, 409, 109322.	1.9	3
13	Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence. ACS Nano, 2020, 14, 5090-5098.	7.3	27
14	Large-Scale Phonon Calculations Using the Real-Space Multigrid Method. Journal of Chemical Theory and Computation, 2019, 15, 6859-6864.	2.3	9
15	Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons. Npj Computational Materials, 2019, 5, .	3.5	9
16	Step edge-mediated assembly of periodic arrays of long graphene nanoribbons on Au(111). Chemical Communications, 2019, 55, 11848-11851.	2.2	14
17	Insights into the Morphotropic Phase Boundary in Ferroelectric Polymers from the Molecular Perspective. Journal of Physical Chemistry C, 2019, 123, 8727-8730.	1.5	16
18	Design of Atomically Precise Nanoscale Negative Differential Resistance Devices. Advanced Theory and Simulations, 2019, 2, 1800172.	1.3	18

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19	Direct writing of heterostructures in single atomically precise graphene nanoribbons. Physical Review Materials, 2019, 3, .	0.9	18
20	Ferroelectric polymers exhibiting behaviour reminiscent of a morphotropic phase boundary. Nature, 2018, 562, 96-100.	13.7	200
21	Oxidization stability of atomically precise graphene nanoribbons. Physical Review Materials, 2018, 2, .	0.9	25
22	Binding of Copper and Cisplatin to Atox1 Is Mediated by Glutathione through the Formation of Metalâ€“Sulfur Clusters. Biochemistry, 2017, 56, 3129-3141.	1.2	27
23	Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons. Nature Communications, 2017, 8, 14815.	5.8	58
24	Selective sensing of ethylene and glucose using carbon-nanotube-based sensors: an ab initio investigation. Nanoscale, 2017, 9, 1687-1698.	2.8	33
25	Generating high dielectric constant blends from lower dielectric constant dipolar polymers using nanostructure engineering. Nano Energy, 2017, 32, 73-79.	8.2	89
26	Seamless Staircase Electrical Contact to Semiconducting Graphene Nanoribbons. Nano Letters, 2017, 17, 6241-6247.	4.5	64
27	Enhancement of the dielectric response in polymer nanocomposites with low dielectric constant fillers. Nanoscale, 2017, 9, 10992-10997.	2.8	216
28	Point Defects and Impurities in Silicon Carbide and Group III-Nitrides â˜†. , 2017, , .		0
29	First-principles simulations of PVDF copolymers with high dielectric energy density: PVDF-HFP and PVDF-BTFE. Physical Review B, 2016, 94, .	1.1	7
30	Mechanisms of NH3 and NO2 detection in carbon-nanotube-based sensors: An ab initio investigation. Carbon, 2016, 101, 177-183.	5.4	56
31	Atomistic simulations of aromatic polyurea and polyamide for capacitive energy storage. Physical Review B, 2015, 92, .	1.1	9
32	Charge transport in DNA nanowires connected to carbon nanotubes. Physical Review B, 2015, 92, .	1.1	11
33	Enzymatic Mechanism of Copper-Containing Nitrite Reductase. Biochemistry, 2015, 54, 1233-1242.	1.2	58
34	Optimizing nanostructure to achieve high dielectric response with low loss in strongly dipolar polymers. Nano Energy, 2015, 16, 227-234.	8.2	44
35	Self-Organized and Cu-Coordinated Surface Linear Polymerization. Scientific Reports, 2013, 3, 2102.	1.6	23
36	Theory of nitrogen doping of carbon nanoribbons: Edge effects. Journal of Chemical Physics, 2012, 136, 014702.	1.2	26

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37	Electronic Control over Attachment and Self-Assembly of Alkyne Groups on Gold. ACS Nano, 2012, 6, 9267-9275.	7.3	25
38	Supramolecular Self-Assembly of Ï€-Conjugated Hydrocarbons via 2D Cooperative CHÍ€ Interaction. ACS Nano, 2012, 6, 566-572.	7.3	63
39	Electric Field Induced Phase Transitions in Polymers: A Novel Mechanism for High Speed Energy Storage. Physical Review Letters, 2012, 108, 087802.	2.9	43
40	Mechanism of copper(II)-induced misfolding of Parkinson's disease protein. Scientific Reports, 2011, 1, 11.	1.6	71
41	Polarization effects and phase equilibria in high-energy-density polyvinylidene-fluoride-based polymers. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 553-557.	0.3	3
42	Electron transport in multiterminal molecular devices: A density functional theory study. Physical Review B, 2010, 81, .	1.1	13
43	Band gap control of small bundles of carbon nanotubes using applied electric fields: A density functional theory study. Applied Physics Letters, 2010, 97, 063113.	1.5	22
44	Insights into prion protein function from atomistic simulations. Prion, 2010, 4, 13-19.	0.9	8
45	Properties of High-Performance Capacitor Materials and Nanoscale Electronic Devices. , 2010, , .		0
46	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.	2.9	63
47	Negative Differential Resistance in C₆₀-Based Electronic Devices. ACS Nano, 2010, 4, 7205-7210.	7.3	52
48	First-principles investigations of the dielectric properties of polypropylene/metal-oxide interfaces. Physical Review B, 2009, 80, .	1.1	25
49	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.	3.3	35
50	First-principles methodology for quantum transport in multiterminal junctions. Journal of Chemical Physics, 2009, 131, 164105.	1.2	23
51	Electronic Properties of High-Performance Capacitor Materials and Nanoscale Multiterminal Devices. , 2009, , .		0
52	Theoretical Approach to Polarization Effects in Semiconductors. , 2008, , 2-25.		0
53	Effects of end group functionalization and level alignment on electron transport in molecular devices. Journal of Chemical Physics, 2008, 128, 024708.	1.2	15
54	Edge States and Optical Transition Energies in Carbon Nanoribbons. Physical Review Letters, 2008, 101, 246803.	2.9	40

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55	Multiscale Simulations of High Performance Capacitors and Nanoelectronic Devices. , 2008, , .		0
56	Doping-Dependent Negative Differential Resistance in Hybrid Organic/Inorganic Siâˆ’Porphyrinâˆ’Si Junctions. ACS Nano, 2008, 2, 1517-1522.	7.3	15
57	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.	1.2	42
58	Recent developments and applications of the real-space multigrid method. Journal of Physics Condensed Matter, 2008, 20, 294205.	0.7	63
59	Equivalence of dipole correction and Coulomb cutoff techniques in supercell calculations. Physical Review B, 2008, 77, .	1.1	34
60	Ab initiosimulations of H2in Li-doped carbon nanotube systems. Journal of Physics Condensed Matter, 2007, 19, 086226.	0.7	8
61	Implementation of ultrasoft pseudopotentials in large-scale grid-based electronic structure calculations. Physical Review B, 2007, 76, .	1.1	23
62	Atomic scale design of nanostructures. Molecular Physics, 2007, 105, 147-156.	0.8	4
63	Phase Equilibria in High Energy Density PVDF-Based Polymers. Physical Review Letters, 2007, 99, 047801.	2.9	77
64	Multiscale Simulations of High Performance Capacitors and Nanoelectronic Devices. , 2007, , .		1
65	Multiscale Simulations of Quantum Structures. , 2006, , .		1
66	Density functional theory studies of quantum transport in molecular systems. International Journal of Quantum Chemistry, 2006, 106, 3334-3342.	1.0	4
67	Resonant coupling and negative differential resistance in metal/ferrocenyl alkanethiolate/STM structures. Physical Review B, 2006, 74, .	1.1	32
68	Properties of wurtzite w-MnN and of w-MnN inclusions in (Ga,Mn)N. Applied Physics Letters, 2006, 88, 092502.	1.5	7
69	Interfacial Segregation and Electrodiffusion of Dopants inAlN/GaNSuperlattices. Physical Review Letters, 2006, 96, 185501.	2.9	10
70	Hydrogenation effect on the structural transition of C60. Chemical Physics Letters, 2005, 403, 359-362.	1.2	13
71	Optical Absorption of Water: Coulomb Effects versus Hydrogen Bonding. Physical Review Letters, 2005, 94, 037404.	2.9	123
72	Theory of Electronic Structure and Magnetic Interactions in (Ga,Mn)N and (Ga,Mn)As. AIP Conference Proceedings, 2005, , .	0.3	0

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73	Collective polarization effects inÎ²-polyvinylidene fluoride and its copolymers with tri- and tetrafluoroethylene. Physical Review B, 2005, 72, .	1.1	87
74	Fermi-level effects on the electronic structure and magnetic couplings in (Ga,Mn)N. Physical Review B, 2005, 72, .	1.1	28
75	EdmondsetÂal.Reply:. Physical Review Letters, 2005, 94, .	2.9	7
76	Electron transport in molecular systems. Journal of Physics: Conference Series, 2005, 16, 283-286.	0.3	2
77	Nonequilibrium Quantum Transport Properties of Organic Molecules on Silicon. Physical Review Letters, 2005, 95, 206805.	2.9	65
78	Carbon Nanotubeâ^'Metal Cluster Composites:Â A New Road to Chemical Sensors?. Nano Letters, 2005, 5, 847-851.	4.5	209
79	Oxidation- and organic-molecule-induced changes of the Si surface optical anisotropy:ab initiopredictions. Journal of Physics Condensed Matter, 2004, 16, S4323-S4334.	0.7	13
80	Ab InitioStudies of Polarization and Piezoelectricity in Vinylidene Fluoride and BN-Based Polymers. Physical Review Letters, 2004, 92, 115504.	2.9	116
81	Large-Scale Quantum-Mechanical Simulations of Nanoscale Devices and New Materials. , 2004, , .		0
82	Understanding and enhancing polarization in complex materials. Computing in Science and Engineering, 2004, 6, 12-21.	1.2	16
83	Calculation of surface optical properties: from qualitative understanding to quantitative predictions. Thin Solid Films, 2004, 455-456, 764-771.	0.8	14
84	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.	3.1	15
85	Mn Interstitial Diffusion in(Ga,Mn)As. Physical Review Letters, 2004, 92, 037201.	2.9	476
86	Gallium-rich reconstructions on GaAs(001). Physica Status Solidi (B): Basic Research, 2003, 240, 91-98.	0.7	27
87	Spontaneous polarization and piezoelectricity in boron nitride nanotubes. Physical Review B, 2003, 67, .	1.1	211
88	First-Principle Study of Molecular Springs under Shear Deformation. Journal of Physical Chemistry A, 2003, 107, 1377-1383.	1.1	2
89	Nanowire-induced optical anisotropy of the Si(111)-In surface. Physical Review B, 2003, 68, .	1.1	30
90	Cycloaddition reaction versus dimer cleavage at theSi(001):C5H8interface. Physical Review B, 2003, 68, .	1.1	26

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91	Response to â€œComment on â€˜Intrinsic electron transport properties of carbon nanotube Y junctionsâ€™â€Šâ€•[Appl. Phys. Lett. 83, 1674 (2003)]. Applied Physics Letters, 2003, 83, 1676-1677.	1.5	3
92	Surface Segregation of Ge at SiGe(001) by Concerted Exchange Pathways. Physical Review Letters, 2002, 88, 166101.	2.9	30
93	Interplay of surface reconstruction and surface electric fields in the optical anisotropy of GaAs(001). Physical Review B, 2002, 66, .	1.1	31
94	Intrinsic electron transport properties of carbon nanotube Y-junctions. Applied Physics Letters, 2002, 81, 5234-5236.	1.5	74
95	Mechanical Properties and Electronic Transport in Carbon Nanotubes. , 2002, , 195-203.		0
96	Field Emission Properties of BN/C and BN@C Hybrid Nanotubes. Materials Research Society Symposia Proceedings, 2002, 739, 571.	0.1	0
97	Electronic and field emission properties of boron nitride/carbon nanotube superlattices. Applied Physics Letters, 2002, 81, 46-48.	1.5	118
98	Ultimate strength of carbon nanotubes: A theoretical study. Physical Review B, 2002, 65, .	1.1	239
99	Mechanical and Electrical Properties of Nanotubes. Annual Review of Materials Research, 2002, 32, 347-375.	4.3	343
100	Structure and energetics of Ga-rich GaAs() surfaces. Surface Science, 2002, 507-510, 406-410.	0.8	24
101	Ab InitioInvestigations of Lithium Diffusion in Carbon Nanotube Systems. Physical Review Letters, 2002, 88, 075506.	2.9	254
102	ATOMIC TRANSFORMATIONS, STRENGTH, PLASTICITY, AND ELECTRON TRANSPORT IN STRAINED CARBON NANOTUBES. , 2002, , 357-376.		0
103	Ab Initio Simulations of the Si (100) Surface: Steps and Melting. , 2002, , 135-145.		0
104	GaAs(001) surface reconstructions: geometries, chemical bonding and optical properties. Applied Surface Science, 2002, 190, 264-268.	3.1	25
105	Terrace and step contributions to the optical anisotropy of Si(001) surfaces. Physical Review B, 2001, 63, .	1.1	61
106	Point Defects and Impurities in Silicon Carbide and Group III-Nitrides. , 2001, , 7131-7139.		0
107	Quantum Transport in Nanotube-Based Structures. Materials Research Society Symposia Proceedings, 2001, 706, 1.	0.1	0
108	Li Uptake in Carbon Nanotube Systems: A First Principles Investigation. Materials Research Society Symposia Proceedings, 2001, 706, 1.	0.1	0

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109	GaAs(001): Surface Structure and Optical Properties. Physica Status Solidi A, 2001, 188, 1401-1409.	1.7	53
110	O(N)real-space method forab initioquantum transport calculations: Application to carbon nanotubeâ€“metal contacts. Physical Review B, 2001, 64, .	1.1	115
111	Structural and electronic properties of carbon nanotube tapers. Physical Review B, 2001, 64, .	1.1	45
112	GaAs(001): Surface Structure and Optical Properties. , 2001, 188, 1401.		1
113	Terrace and step contributions to the surface optical anisotropy of Si(001). Springer Proceedings in Physics, 2001, , 299-300.	0.1	0
114	Materials Science Needs and Is Getting Quantitative Methods. Physics Today, 2000, 53, 75-76.	0.3	1
115	Calculating buckyballs and nanotubes. Physics Today, 2000, 53, 76-77.	0.3	0
116	Large-Scale Applications of Real-Space Multigrid Methods to Surfaces, Nanotubes, and Quantum Transport. Physica Status Solidi (B): Basic Research, 2000, 217, 685-701.	0.7	15
117	Mechanical properties, defects and electronic behavior of carbon nanotubes. Carbon, 2000, 38, 1703-1711.	5.4	162
118	(001) Surfaces of GaP and InP: structural motifs, electronic states and optical signatures. Applied Surface Science, 2000, 166, 179-184.	3.1	17
119	Angle Resolved Photoemission Spectroscopy of the InP(001) surface. Applied Surface Science, 2000, 166, 224-230.	3.1	21
120	Ab initiophonon dispersions of wurtzite AlN, GaN, and InN. Physical Review B, 2000, 61, 6720-6725.	1.1	253
121	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
122	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.	1.1	87
123	Optical Anisotropy of theSiC(001)-(3Ã—2)Surface: Evidence for the Two-Adlayer Asymmetric-Dimer Model. Physical Review Letters, 2000, 85, 4381-4384.	2.9	37
124	Towards grid-basedO(N)density-functional theory methods: Optimized nonorthogonal orbitals and multigrid acceleration. Physical Review B, 2000, 62, 1713-1722.	1.1	220
125	Step-induced optical anisotropy of Si(111):H surfaces. Physical Review B, 2000, 61, 7604-7608.	1.1	24
126	Theoretical STM signatures and transport properties of native defects in carbon nanotubes. Physical Review B, 2000, 61, 14194-14203.	1.1	96

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127	Surface segregation and interface stability of AlN/GaN, GaN/InN, and AlN/InN {0001} epitaxial systems. Physical Review B, 2000, 61, 10820-10826.	1.1	26
128	Theoretical Investigations of Carbon Nanotube Growth. Molecular Simulation, 2000, 25, 1-12.	0.9	14
129	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
130	Defect energetics and impurity incorporation mechanisms at the arsenic-passivated Si(100) surface. Physical Review B, 1999, 60, 8178-8184.	1.1	2
131	Surface sensitivity of impurity incorporation: Mg at GaN (0001) surfaces. Physical Review B, 1999, 59, 9771-9774.	1.1	56
132	(2Ã—4)GaP(001) surface: Atomic structure and optical anisotropy. Physical Review B, 1999, 60, 2488-2494.	1.1	58
133	Chemical and strain effects on Boron-doped Si(100). Physical Review B, 1999, 59, 4813-4821.	1.1	16
134	Segregation effects at vacancies inAlxGa1â^'xNandSixGe1â^'xalloys. Physical Review B, 1999, 59, 1567-1570.	1.1	16
135	Ad-dimers on Strained Carbon Nanotubes: A New Route for Quantum Dot Formation?. Physical Review Letters, 1999, 83, 4132-4135.	2.9	104
136	Structural fingerprints in the reflectance anisotropy spectra ofInP(001)(2Ã—4)surfaces. Physical Review B, 1999, 59, 2234-2239.	1.1	43
137	SELF-ENERGY EFFECTS IN THE OPTICAL ANISOTROPY OF GaP(001). Surface Review and Letters, 1999, 06, 1159-1165.	0.5	25
138	Mechanical deformations and coherent transport in carbon nanotubes. Physical Review B, 1999, 60, R16338-R16341.	1.1	137
139	Computational Materials Science: The Era of Applied Quantum Mechanics. Physics Today, 1999, 52, 30-35.	0.3	45
140	Formation of Nanotube-Based Quantum Dots With Strain and Addimers. Materials Research Society Symposia Proceedings, 1999, 593, 149.	0.1	0
141	Atomic Transformations and Quantum Transport in Carbon Nanotubes. Materials Research Society Symposia Proceedings, 1999, 593, 547.	0.1	0
142	Theoretical bounds for multiwalled carbon nanotube growth. Chemical Physics Letters, 1998, 296, 471-476.	1.2	14
143	Theory of growth and mechanical properties of nanotubes. Applied Physics A: Materials Science and Processing, 1998, 67, 39-46.	1.1	124
144	Brittle and Ductile Behavior in Carbon Nanotubes. Physical Review Letters, 1998, 81, 4656-4659.	2.9	475

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145	Mechanism of strain release in carbon nanotubes. Physical Review B, 1998, 57, R4277-R4280.	1.1	441
146	Chemical Trends in Impurity Incorporation into Si(100). Physical Review Letters, 1998, 81, 1642-1645.	2.9	36
147	Lip-Lip Interactions and the Growth of Multiwalled Carbon Nanotubes. Physical Review Letters, 1998, 80, 313-316.	2.9	91
148	Consistent methodology for calculating surface and interface energies. Physical Review B, 1998, 57, 7281-7291.	1.1	161
149	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
150	Strain effects on the interface properties of nitride semiconductors. Physical Review B, 1997, 55, R7323-R7326.	1.1	101
151	Doping properties of C, Si, and Ge impurities in GaN and AlN. Physical Review B, 1997, 56, 9496-9505.	1.1	233
152	Theory of surface morphology of wurtzite GaN (0001) surfaces. Physical Review B, 1997, 56, R12725-R12728.	1.1	100
153	Theory of Interfaces and Surfaces of Wide-Gap Nitrides. Materials Research Society Symposia Proceedings, 1997, 482, 904.	0.1	2
154	Polarization field effects on the electron-hole recombination dynamics in In0.2Ga0.8N/In1â^'xGaxN multiple quantum wells. Applied Physics Letters, 1997, 71, 3135-3137.	1.5	125
155	Kinetics of metal-catalyzed growth of single-walled carbon nanotubes. Physical Review B, 1997, 55, R6097-R6100.	1.1	142
156	High strain rate fracture and C-chain unraveling in carbon nanotubes. Computational Materials Science, 1997, 8, 341-348.	1.4	475
157	Nanotubes. Current Opinion in Solid State and Materials Science, 1997, 2, 706-715.	5.6	61
158	Real-space multigrid methods for large-scale electronic structure problems. International Journal of Quantum Chemistry, 1997, 65, 531-543.	1.0	22
159	Structural flexibility of carbon nanotubes. Journal of Chemical Physics, 1996, 104, 2089-2092.	1.2	1,115
160	Nanomechanics of Carbon Tubes: Instabilities beyond Linear Response. Physical Review Letters, 1996, 76, 2511-2514.	2.9	2,450
161	Theory of Defects, Doping, Surfaces and Interfaces in Wide Gap Nitrides. Materials Research Society Symposia Proceedings, 1996, 423, 465.	0.1	1
162	Theory of Interfaces in Wide-Gap Nitrides. Materials Research Society Symposia Proceedings, 1996, 449, 893.	0.1	4

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163	Structural mechanics of carbon nanotubes: From continuum elasticity to atomistic fracture. Journal of Computer-Aided Materials Design, 1996, 3, 173-182.	0.7	53
164	Real-space multigrid-based approach to large-scale electronic structure calculations. Physical Review B, 1996, 54, 14362-14375.	1.1	341
165	Amphoteric properties of substitutional carbon impurity in GaN and AlN. Applied Physics Letters, 1996, 69, 233-235.	1.5	106
166	Doping Properties of Amphoteric C, Si, and Ge Impurities in GaN and AlN. Acta Physica Polonica A, 1996, 90, 735-738.	0.2	8
167	(Negative) Electron Affinity of AlN and AlGaN Alloys. Materials Research Society Symposia Proceedings, 1995, 395, 777.	0.1	31
168	Simulations of SI(100) Growth: Step Flow and Low Temperature Growth. Materials Research Society Symposia Proceedings, 1995, 399, 511.	0.1	1
169	Electronic Structure Calculations on a Real-Space Mesh with Multigrid Acceleration. Materials Research Society Symposia Proceedings, 1995, 408, 145.	0.1	0
170	Growth of carbon nanotubes: a molecular dynamics study. Chemical Physics Letters, 1995, 236, 150-155.	1.2	54
171	Ab initio studies of single-height Si(001) steps. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1995, 30, 167-173.	1.7	5
172	Fluorine-Based Mechanisms for Atomic-Layer-Epitaxial Growth on Diamond (110). Physical Review Letters, 1995, 74, 4875-4878.	2.9	4
173	Ab InitioStudies of the Diffusion Barriers at Single-Height Si(100) Steps. Physical Review Letters, 1995, 75, 101-104.	2.9	107
174	Native defects in gallium nitride. Physical Review B, 1995, 51, 17255-17258.	1.1	444
175	Surface structures and electron affinities of bare and hydrogenated diamond C(100) surfaces. Physical Review B, 1995, 51, 5291-5296.	1.1	89
176	Large-scale electronic-structure calculations with multigrid acceleration. Physical Review B, 1995, 52, R5471-R5474.	1.1	208
177	Towards the Identification of the Dominant Donor in GaN. Physical Review Letters, 1995, 75, 296-299.	2.9	295
178	Theory of carbon nanotube growth. Physical Review B, 1995, 52, 14850-14858.	1.1	106
179	Impurity-Enhanced Disordering in Superlattices. Materials Science Forum, 1994, 143-147, 593-598.	0.3	1
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181	Si diffusion in GaAs and Si-induced interdiffusion in GaAs/AlAs superlattices. Physical Review B, 1994, 49, 2985-2988.	1.1	24
182	Structural defects and the shape of large fullerenes. Chemical Physics Letters, 1994, 219, 473-478.	1.2	59
183	Growth Energetics of Carbon Nanotubes. Physical Review Letters, 1994, 73, 2468-2471.	2.9	103
184	Negative-electron-affinity effects on the diamond (100) surface. Physical Review B, 1994, 50, 5803-5806.	1.1	369
185	Structural transformations, reactions, and electronic properties of fullerenes, onions, and buckytubes. Computational Materials Science, 1994, 2, 547-556.	1.4	1
186	Native Defects in Wurtzite GaN And AlN. Materials Research Society Symposia Proceedings, 1994, 339, 693.	0.1	14
187	Molecular Dynamics Studies of Nanotube Growth in a Carbon ARC. Materials Research Society Symposia Proceedings, 1994, 359, 235.	0.1	0
188	Impurity incorporation and doping of diamond. Physica B: Condensed Matter, 1993, 185, 144-149.	1.3	45
189	Structure and energetics of single and multilayer fullerene cages. Physical Review Letters, 1993, 70, 3023-3026.	2.9	105
190	Quantum molecular dynamics simulations of fullerenes and graphitic microtubules. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 74-78.	1.0	5
191	Atomic structure and doping of microtubules. Physical Review B, 1993, 47, 1708-1711.	1.1	168
192	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.	1.0	15
193	Reactivity, stability, and formation of fullerenes. Physical Review B, 1993, 48, 5724-5727.	1.1	26
194	AsGa-XIcomplexes as models for theEL2 center in GaAs. Physical Review B, 1993, 47, 1667-1670.	1.1	18
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