Gyaneshwar P Srivastava

List of Publications by Year
in descending order

242 papers	4,308 citations	136950 32 h-index	161849 54 g-index
247 all docs	247 docs citations	247 times ranked	2951 citing authors

#	Article	IF	Citations
1	Atomic structure and ordering in semiconductor alloys. Physical Review B, 1985, 31, 2561-2564.	3.2	360
2	Theory of semiconductor surface reconstruction. Reports on Progress in Physics, 1997, 60, 561-613.	20.1	134
3	Dimensionality and size effects in simple metals. Physical Review B, 1986, 34, 8246-8257.	3.2	116
4	First-principles studies of ground-state and dynamical properties of MgS, MgSe, and MgTe in the rocksalt, zinc blende, wurtzite, and nickel arsenide phases. Physical Review B, 2006, 73, .	3.2	114
5	Electronic properties of twin boundaries and twinning superlattices in diamond-type and zinc-blende-type semiconductors. Physical Review B, 1993, 48, 17181-17193.	3.2	102
6	Adsorption of group-V elements on IIIâ€“V (1 1 0) surfaces. Surface Science Reports, 1996, 25, 141-223.	7.2	97
7	First-principles studies of structural, electronic, and dynamical properties ofBechalcogenides. Physical Review B, 2004, 70, .	3.2	95
8	Photoelectron spectroscopy of solids and their surfaces. Reports on Progress in Physics, 1980, 43, 1357-1414.	20.1	78
9	Geometry and electronic band structure of an ordered monolayer deposition of Bi on III-V(110) semiconductor surfaces. Physical Review B, 1995, 51, 2334-2346.	3.2	76
10	Structural, elastic, electronic, and phonon properties of zinc-blende and wurtzite BeO. Journal of Applied Physics, 2009, 105, .	2.5	66
11	Optical properties of twinning superlattices in diamond-type and zinc-blende-type semiconductors. Physical Review B, 1995, 52, 14078-14085.	3.2	60
12	III-V(110) surface dynamics from anab initiofrozen-phonon approach. Physical Review B, 1995, 52, 2001-2007.	3.2	59
13	Phonons in zinc-blende and wurtzite phases of GaN, AlN, and BN with the adiabatic bond-charge model. Physical Review B, 2000, 62, 5028-5035.	3.2	56
14	The electronic structure of cleaved indium phosphide (110) surfaces: experiment and theory. Journal of Physics C: Solid State Physics, 1983, 16, 3627-3640.	1.5	51
15	A comparative study of dissociative adsorption of NH3, PH3, and AsH3 on Si(001)â€“(2Ã—1). Journal of Chemical Physics, 2001, 114, 9549-9556.	3.0	51
16	Theoretical evidence concerning mixed dimer growth on the surface. Journal of Physics Condensed Matter, 1996, 8, 6641-6651.	1.8	50
17	Structural and dynamical properties of zinc-blende GaN, AlN, BN, and their (110) surfaces. Physical Review B, 2005, 71, .	3.2	49
18	Atomic geometries of InP(110)-Sb(1 ML) and GaAs(110)-Sb(1 ML). Physical Review B, 1992, 46, 7300-7303.	3.2	48

#	Article	IF	Citations
19	Theory of the lattice thermal conductivity in bulk and films of GaN. Physical Review B, 2010, 81, .	3.2	47
20	Thermal conductivity of single crystal and ceramic AlN. Journal of Applied Physics, 2008, 103, .	2.5	43
21	Theoretical studies of atomic vibrations on theSi(001)(2Ã—1)surface. Physical Review B, 1997, 56, 4656-4664.	3.2	41
22	Dissociative adsorption ofNH3onSi(001)â^'(2Ã—1). Physical Review B, 1998, 58, 7944-7949.	3.2	40
23	Surface phonons on InP(110) with the adiabatic bond-charge model. Physical Review B, 1996, 53, 15675-15681.	3.2	39
24	Calculation of lattice thermal conductivity of Ge from 4 to 900 K. Philosophical Magazine and Journal, 1976, 34, 795-809.	1.7	38
25	Dimer length variation for different reconstructions of Si, Ge, and mixed Si-Ge dimers on Si(001) and Ge(001) substrates. Physical Review B, 1999, 60, 1488-1491.	3.2	38
26	Angle resolved photoelectron spectroscopy-the cleaved (110) surface of indium phosphide. Journal of Physics C: Solid State Physics, 1980, 13, 1581-1591.	1.5	36
27	Atomic geometry and bonding on the GaAs(001)-Î²2(2Ã—4) surface fromab initiopseudopotential calculations. Physical Review B, 1996, 53, 12589-12592.	3.2	34
28	Dissociative adsorption ofSi2H6on the Si(001) surface. Physical Review B, 2000, 61, 10216-10222.	3.2	34
29	Simple approach to self-energy corrections in semiconductors and insulators. Physical Review B, 1993, 48, 4388-4397.	3.2	33
30	Bi covered Si(111) surface revisited. Journal of Physics Condensed Matter, 2003, 15, 2441-2447.	1.8	33
31	Hypersonic Modes in Nanophononic Semiconductors. Physical Review Letters, 2008, 101, 105502.	7.8	33
32	Phonon conductivity in graphene. Journal of Applied Physics, 2012, 112, .	2.5	33
33	Ab initioinvestigation of BCS-type superconductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">LuNi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">C</mml:mi></mml:math>-type superconductors. Physical Review B, 2015, 92, .	3.2	33
34	Temperature dependence of the thermal conductivity of different forms of diamond. Journal of Applied Physics, 2007, 101, 123507.	2.5	32
35	Phonons and superconductivity in fcc and dhcp lanthanum. Physical Review B, 2010, 81, .	3.2	32
36	The influence of adsorbed layers in controlling Schottky barriers. Journal of Physics C: Solid State Physics, 1981, 14, L191-L194.	1.5	30

#	ARTICLE	IF	CITATIONS
37	Structure and electronic states ofInAs(001)â˜(2Ã—4)surfaces. Physical Review B, 2000, 62, 15778-15787.	3.2	30
38	Electronic, elastic and phonon properties of the rock-salt LaSb and YSb. Journal of Physics Condensed Matter, 2007, 19, 156207.	1.8	30
39	Electronic and phonon properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>B</mml:mtext><mml:mi>X</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn	3.2	30
40	Electronic Structure of a Neutral Phosphorus Vacancy in GaP and InP. Physica Status Solidi (B): Basic Research, 1979, 93, 761-765.	1.5	29
41	Electronic structure, phonons and electronâ€“phonon interaction in MgXNi3(X = B, C and N). Journal of Physics Condensed Matter, 2006, 18, 11089-11101.	1.8	29
42	Quenching of local magnetic moment in oxygen adsorbed graphene nanoribbons. Journal of Chemical Physics, 2008, 128, 201101.	3.0	29
43	The Electronic Band Structure of SnS. Physica Status Solidi (B): Basic Research, 1980, 101, K31.	1.5	28
44	Structure and stability of the Si(001)c(4Ã—4)-Sb surface. Physical Review B, 1998, 57, R12701-R12704.	3.2	28
45	Angle-resolved photo-emission from the cleaved (110) surface of cadmium telluride. Journal of Physics C: Solid State Physics, 1986, 19, 1259-1271.	1.5	26
46	Theoretical study of the anharmonic decay of nonequilibrium LO phonons in semiconductor structures. Physical Review B, 1994, 50, 14179-14186.	3.2	25
47	Atomic geometry, electronic structure, and vibrational properties of the Ge(001)(2Ã—1) surface. Physical Review B, 1998, 57, 4649-4655.	3.2	25
48	Adsorption of partially and fully dissociatedH2Smolecules on the Si(001) and Ge(001) surfaces. Physical Review B, 1999, 60, 5497-5505.	3.2	25
49	Lattice dynamics of silicon nanostructures. Nanotechnology, 2006, 17, 3288-3298.	2.6	25
50	Role of generalized-gradient approximation in structural and electronic properties of bulk and surface ofÎ²-GaN and GaAs. Physical Review B, 1999, 59, 3008-3014.	3.2	24
51	The equilibrium geometry and electronic structure of Bi nanolines on clean and hydrogenated Si(001) surfaces. Nanotechnology, 2005, 16, 2427-2435.	2.6	24
52	Ground state, phonon spectrum, and superconducting properties of the nonoxide perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CdCNi</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review B, 2008, 78, .	3.2	23
53	Nonlocal Pseudopotential Calculations for Two Isoelectronic Series: Geâ€GaAsâ€ZnSe and Îµâ€Snâ€InSbâ€CdTe. Physica Status Solidi (B): Basic Research, 1982, 112, 581-597.	1.5	22
54	An ab initio pseudopotential calculation of ground-state and excited-state properties of gallium nitride. Journal of Physics Condensed Matter, 1994, 6, 8781-8794.	1.8	22

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55	Comparative study of Sb bonding on group-IV semiconductor (001) substrates. Physical Review B, 1997, 56, 9221-9223.	3.2	22
56	Coupling-constant dependence of the density functional correlation energy. Journal of Chemical Physics, 1998, 109, 5212-5220.	3.0	22
57	Ab initio surface reaction energetics of SiH4 and Si2H6 on Si(001)-(2Ã—2). Journal of Chemical Physics, 2005, 123, 174703.	3.0	22
58	Electronic structure and total energy of Si, Ge and Î±-Sn by the self-consistent local pseudopotential method. Journal of Physics C: Solid State Physics, 1982, 15, 707-719.	1.5	21
59	Atomic geometry, electronic states and bonding at the GaP(11)-Sb(1 ML) interface. Journal of Physics Condensed Matter, 1993, 5, 4695-4710.	1.8	21
60	Structure and energetics of segregated and nonsegregated Ge(001)/Si(2Ã—1). Physical Review B, 1998, 57, 8794-8796.	3.2	20
61	Thermoelectric properties of p-type (Bi2Te3)x(Sb2Te3)1â^'x single crystals doped with 3â€‰wt. % Te. Journal of Applied Physics, 2013, 113, .	2.5	20
62	Atomic geometry and electronic structure of a monolayer of Sb on (110) GaAs and InP. Physical Review B, 1993, 47, 16616-16619.	3.2	19
63	Phonon dispersion on a GaAs(110) surface studied using the adiabatic bond charge model. Journal of Physics Condensed Matter, 1996, 8, 1345-1358.	1.8	19
64	Theoretical studies of the initial stages of Zn adsorption onGaAs(001)â^'(2Ã—4). Physical Review B, 2000, 62, 13623-13630.	3.2	19
65	Specific heat calculations of III-N bulk materials. Physica Status Solidi C: Current Topics in Solid State Physics, 2006, 3, 1495-1498.	0.8	19
66	The anharmonic phonon decay rate in group-III nitrides. Journal of Physics Condensed Matter, 2009, 21, 174205.	1.8	19
67	Electrons, phonons and superconductivity in rocksalt and tungstenâ€“carbide phases of CrC. Journal of Physics Condensed Matter, 2012, 24, 455704.	1.8	19
68	Effects of spin-orbit coupling on the electron-phonon superconductivity in the cubic Laves-phase compounds <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaIr</mml:mi><mml:mn>2</mml:mn></mml:msub></mm and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaRh</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2017, 96, .	3.2	19
69	A microscopic study of Landau level states in quantum wires. Semiconductor Science and Technology, 1994, 9, 1305-1315.	2.0	18
70	Atomic geometry, electronic structure, and vibrational properties of the AlSb(110) and GaSb(110) surfaces. Physical Review B, 1999, 59, 4925-4932.	3.2	18
71	Self-organized Bi lines on the Si(001) surface:â€ƒA theoretical study. Physical Review B, 2002, 66, .	3.2	18
72	Lifetime of nonequilibrium zone-center longitudinal optical phonons in zinc-blende materials. Applied Physics Letters, 2002, 81, 3395-3397.	3.3	18

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73	Tunability of the piezoelectric fields in strained III-V semiconductors. Applied Physics Letters, 2009, 95, 041912.	3.3	18
74	Tuning phonon properties in thermoelectric materials. Reports on Progress in Physics, 2015, 78, 026501.	20.1	18
75	Derivation and calculation of complementary variational principles for the lattice thermal conductivity. Journal of Physics C: Solid State Physics, 1976, 9, 3037-3053.	1.5	17
76	Comparativeab initiopseudopotential studies of group V overlayers on Si(001). Journal of Physics Condensed Matter, 1998, 10, 7751-7768.	1.8	17
77	Electronic structure, phonons, and electron-phonon interaction in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mo</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review B, 2010, 82, .	3.2	17
78	Evolution of thermal properties from graphene to graphite. Applied Physics Letters, 2014, 104, 031903.	3.3	17
79	Phonon dispersion in the (110) direction: a testing ground for phenomenological models of germanium. Journal of Physics C: Solid State Physics, 1988, 21, 5087-5106.	1.5	16
80	Adsorption and desorption of S on and off Si(001) studied by ab initio density functional theory. Journal of Applied Physics, 1998, 84, 6070-6075.	2.5	16
81	Theory of Thermal Conduction in Nonmetals. MRS Bulletin, 2001, 26, 445-450.	3.5	16
82	Lattice dynamics of ultrasmall silicon nanostructures. Applied Physics Letters, 2005, 87, 231906.	3.3	16
83	Ab initiocalculation of phonons for bulk TiC and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>TiC</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>001</mml:m Physical Review B, 2009, 80, .	3.2	16
84	Ordering of lowest conduction-band states in (GaAs)n/(AlAs)m[111] superlattices. Physical Review B, 1992, 46, 15150-15155.	3.2	15
85	Ab initiostudy of atomic geometry, electronic states, and bonding for H2S adsorption on III-V semiconductor (110)-(1Å—1)surfaces. Physical Review B, 1998, 57, 4486-4492.	3.2	15
86	Phonons and superconductivity in the cubic perovskite Cr3RhN. Journal of Applied Physics, 2012, 112, .	2.5	15
87	A comparative ab initio study of superconductivity in the body centered tetragonal YC2 and LaC2. Journal of Applied Physics, 2015, 117, .	2.5	15
88	Electron-phonon superconductivity in the filled skutterudites <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LaRu</mml:mi><mml:mn>4</mml:mn></mml:mathvariant="normal">P</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:mrow><mml:mo>,</mml:mo><mml:mo>Â</mml:mo><, and <mml:math xmlns:mml="http://www.w3.or. Physical Review B, 2017, 95, .	3.2	14
89	Investigating the normal state and superconducting state properties of orthorhombic and hexagonal ZrRuP: A first-principles study. Physical Review B, 2019, 100, .	3.2	14
90	The electronic structure of cleaved silicon (111) surfaces following adsorption of aluminium. Journal of Physics C: Solid State Physics, 1980, 13, L369-L374.	1.5	13

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91	Self-consistent pseudopotential calculation for the electronic structure of Ge. Physical Review B, 1982, 25, 2815-2820.	3.2	13
92	The atomic geometry of the ZnSe (110) surface: determination by total-energy methods. Journal of Physics C: Solid State Physics, 1986, 19, 5987-5994.	1.5	12
93	Phonons on II-VI (110) semiconductor surfaces. Physical Review B, 2000, 62, 15797-15805.	3.2	12
94	Phononic gaps in thin semiconductor superlattices. Journal of Applied Physics, 2010, 107, 043504.	2.5	12
95	Electron-phonon superconductivity in the ternary phosphides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ba</mml:mi><mml:msub><mml:mi>M</mml:mi><mml:mn mathvariant="normal">P</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math><mml:math		

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109	Title is missing!. Journal of Physics C: Solid State Physics, 1975, 8, 4147-4156.	1.5	10
110	Ordering of conduction band states in (GaAs)n(AlAs)n[001] and [110] superlattices. Semiconductor Science and Technology, 1992, 7, 648-653.	2.0	10
111	Ab initioinvestigation of Bi-covered GaSb(110) surfaces. Physical Review B, 2000, 61, 2688-2698.	3.2	10
112	Electronic structure of a stepped semiconductor surface: Density functional theory ofSi(114)â˜'(2Ã—1). Physical Review B, 2004, 69, .	3.2	10
113	First-principles study of electronic and dynamical properties of AuAl2. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 3027-3030.	0.8	10
114	Theoretical examination of superconductivity in the cubic antiperovskite Cr3GaN under pressure. Journal of Applied Physics, 2013, 114, 053905.	2.5	10
115	Anharmonic effects in the thermoelectric properties of PbTe. Journal of Applied Physics, 2014, 116, .	2.5	10
116	Theoretical investigation of superconductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrPd</mml:mi><mml:mn>2</mml:mn></mml xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrPd</mml:mi><mml:mn>2</mml:mn></mml and<mml:math xmlns:mml="http://www.w3.org/1998. Physical Review B, 2016, 93, .	3.2	10
117	Surface phonons on the NbC(001) and TaC(001) surfaces. Physical Review B, 2012, 85, .	3.2	9
118	Physical properties of the body-centred tetragonal. Philosophical Magazine, 2017, 97, 1866-1883.	1.6	9
119	Derivation and calculation of a sequence of lowerâ€bound results for lattice thermal conductivity. Physica Status Solidi (B): Basic Research, 1976, 77, 131-140.	1.5	8
120	Electronic structure of [113]-grown (GaAs)m(AlAs)nsuperlattices. Physical Review B, 1994, 49, 10749-10752.	3.2	8
121	Surface morphology effects on the optical phonon modes in InAsxSb1â€“x epilayers on GaAs(001). Physica Status Solidi (B): Basic Research, 2006, 243, R19-R21.	1.5	8
122	Energetic stability, equilibrium geometry, and electronic properties of Bi-inducedSi(001)â˜'(2Ã—n)surfaces. Physical Review B, 2006, 74, .	3.2	8
123	Ground state, phonon spectrum, and superconducting properties of the cubic inverse perovskiteSc3AlN. Physical Review B, 2010, 81, .	3.2	8
124	Electronâ€“phonon interaction and superconductivity in the borocarbide superconductor. Philosophical Magazine, 2017, 97, 2669-2688.	1.6	8
125	Electronic structure of natural self-organized PbS-Bi2S3twinning superlattices. Physical Review B, 1997, 55, 9286-9289.	3.2	7
126	Vibrational properties of Ge- and Sb-adsorbed Si(001) surfaces. Physical Review B, 1998, 58, 10754-10760.	3.2	7

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127	STM images and energetics of the bi-covered (<FONT FACE=Symbol>Ã–3 Ã— <FONT) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	1.4	7
128	Ab initiocalculation of the ground-state properties of CoSi2. Journal of Physics Condensed Matter, 2005, 17, 7127-7132.	1.8	7
129	Gradual changes in electronic properties from graphene to graphite: first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 495503.	1.8	7
130	Theoretical investigation of superconductivity in ternary silicide NaAlSi with layered diamond-like structure. Philosophical Magazine, 2016, 96, 1006-1019.	1.6	7
131	The effect of spin orbit interaction on the physical properties of LaTSi3 (T = Ir, Pd, and Rh): First-principles calculations. Journal of Applied Physics, 2017, 121, 193904.	2.5	7
132	Control of thermal conductivity with species mass in transition-metal dichalcogenides. Journal of Applied Physics, 2018, 123, .	2.5	7
133	Temperature-dependent Raman linewidths in transition-metal dichalcogenides. Physical Review B, 2018, 98, .	3.2	7
134	Lower and Upper Bounds on the Threeâ€Phonon Uâ€Resistances in Ge. Physica Status Solidi (B): Basic Research, 1973, 56, K39.	1.5	6
135	On the Boundary Scattering of Phonons. Canadian Journal of Physics, 1973, 51, 223-225.	1.1	6
136	Improvement of variational bounds on lattice thermal conductivity by scaling and Ritz procedures. Journal of Physics C: Solid State Physics, 1977, 10, 1843-1854.	1.5	6
137	Diagonal and nondiagonal Peierls contribution to the thermal conductivity of anharmonic crystals. Physical Review B, 1981, 23, 4273-4275.	3.2	6
138	Nature of the lowest conduction band in thin GaAs/AlAs (110) superlattices. Semiconductor Science and Technology, 1990, 5, 269-273.	2.0	6
139	Chemisorption of aluminium on GaAs(110). Journal of Physics Condensed Matter, 1993, 5, 9025-9036.	1.8	6
140	Geometry and electronic band structure of GaAs(110)-Bi (1 ML). Physical Review B, 1993, 48, 8450-8453.	3.2	6
141	Direct optical transitions in indirect semiconductors: The case of Ge twinning superlattices. Physical Review B, 1995, 52, 1474-1476.	3.2	6
142	Atomic vibrations in thin(GaAs)n(AlAs)nsuperlattices. Physical Review B, 1997, 56, 13387-13392.	3.2	6
143	Calculation of atomic geometry, electronic states, and bonding for the S-deposited InP(110) surface. Physical Review B, 1997, 56, 1928-1935.	3.2	6
144	Calculation of phonon dispersion on the ZnSe(110) surface. Physical Review B, 1998, 57, 3791-3794.	3.2	6

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145	Iron silicide wires patterned by Bi nanolines on the H/Si(001) surface: Spin density functional calculations. Physical Review B, 2008, 78, .	3.2	6
146	Quantitative study of the enhancement of the thermal conductivity of AlN ceramics by nanoscale processing. Journal of Physics Condensed Matter, 2009, 21, 174207.	1.8	6
147	Study of synthesis and photocatalytic performance of the monoclinic/cubic heterophase junction of rare earth doped zirconia. Journal of Physics and Chemistry of Solids, 2021, 159, 110286.	4.0	6
148	Effect of polarizability on the vibrational and thermal properties of rare gas solids. Canadian Journal of Physics, 1978, 56, 849-858.	1.1	5
149	Self-consistent non-local pseudopotential calculations for the ground-state properties of Î±-Sn. Journal of Physics C: Solid State Physics, 1983, 16, 1649-1657.	1.5	5
150	Atomic Structure of the GaAs(001)-Î²2(2 Ã— 4) Surface. Surface Review and Letters, 1998, 05, 219-222.	1.1	5
151	Adsorption of Te on Ge(001): Density-functional calculations. Physical Review B, 2003, 67, .	3.2	5
152	The lattice dynamics of rectangular silicon nanowires. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 2617-2620.	0.8	5
153	Ab initioinvestigations of phonon anomalies and superconductivity in the rock-salt YS. Philosophical Magazine, 2007, 87, 4109-4118.	1.6	5
154	Ab initio investigations of the phonon anomaly and superconductivity in fcc La. Journal of Applied Physics, 2008, 104, 063916.	2.5	5
155	Anab initiostudy of electronic and structural properties of Mn in a GaAs environment. Journal of Physics Condensed Matter, 2009, 21, 485504.	1.8	5
156	Theory of Thermal Conductivity of Micro- and Nano-structured Materials. Materials Research Society Symposia Proceedings, 2009, 1172, 83.	0.1	5
157	Progressive structural and electronic properties of nano-structured carbon atomic chains. Journal of Applied Physics, 2013, 113, 193704.	2.5	5
158	Three-phonon scattering processes and thermal conductivity in IV-chalocogenides. Journal of Physics Condensed Matter, 2015, 27, 335801.	1.8	5
159	Extension of the modified effective medium approach to nanocomposites with anisotropic thermal conductivities. Physical Review B, 2018, 98, .	3.2	5
160	Physical properties of hexagonal BaPtAs with noncentrosymmetric SrPtSb-type and centrosymmetric YPtAs-type crystal structures: Effects of spin-orbit coupling. Physical Review B, 2019, 100, .	3.2	5
161	Theoretical investigation of superconductivity in the non-centrosymmetric SrPtGe₃ and CaPtSi₃ compounds. Philosophical Magazine, 2019, 99, 198-223.	1.6	5
162	Temperature dependence of the bounds on thermal resistance due to U-process. Physica Status Solidi (B): Basic Research, 1971, 47, 669-677.	1.5	4

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163	Electronic Charge Densities for Two Isoelectronic Series: Geâ€GaAsâ€ZnSe and Î±â€Snâ€InSbâ€CdTe. Physica Status Solidi (B): Basic Research, 1981, 103, K85.	1.5	4
164	Reply to â€˜â€˜Comment on â€˜Atomic structure and ordering in semiconductor alloysâ€™ â€™â€™. Physical Review B, 1987, 36, 2902-2905.	3.2	4
165	Structure of Zn adsorption on GaAs(001)-(2Ã—4). Applied Physics Letters, 2000, 76, 3735-3737.	3.3	4
166	Effect of hydrogenation on the adsorption ofGeonSi(001). Physical Review B, 2001, 64, .	3.2	4
167	Origin of superconductivity in layered centrosymmetric LaNiGa2. Applied Physics Letters, 2014, 104, .	3.3	4
168	Mode confinement, interface mass-smudging, and sample length effects on phonon transport in thin nanocomposite superlattices. Journal of Physics Condensed Matter, 2019, 31, 055303.	1.8	4
169	Separate Contributions of Longitudinal and Transverse Phonons towards the Thermal Conductivity of Ge in the Ziman Limit. Physical Review B, 1973, 7, 897-898.	3.2	3
170	Self-consistent pseudopotential calculations of the equilibrium bulk properties of diamond-type semiconductors. Journal of Physics C: Solid State Physics, 1982, 15, L739-L742.	1.5	3
171	Disorder effects on tunneling through one-dimensional double-barrier quantum-well structures: A coherent-potential approximation. Physical Review B, 1993, 47, 4372-4378.	3.2	3
172	Microscopic calculation of valence-band states in semiconductor structures in the presence of a magnetic field. Physical Review B, 1996, 54, 14623-14632.	3.2	3
173	Atomic Structure of a Monolayer of Ge on Si(001)(2 Ã— 1). Surface Review and Letters, 1998, 05, 97-100.	1.1	3
174	Electronic and vibrational properties of the As:InP(110) and Sb:InP(110) surfaces. Physical Review B, 2001, 65, .	3.2	3
175	Structural, electronic, and dynamical properties of Si(110) capped with a monolayer of GaAs. Physical Review B, 2002, 66, .	3.2	3
176	Geometry and phonon structure of the SiC(110) surface. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 3023-3026.	0.8	3
177	Atomic vibrations on theÎ±â€™Sn(001)(2Ã—1)surface investigated by a linear response scheme and an adiabatic bond-charge model. Physical Review B, 2005, 72, .	3.2	3
178	Reply to Comment on â€˜Bi nanolines on Si(001): registry with the substrateâ€™. Nanotechnology, 2006, 17, 1803-1805.	2.6	3
179	Atomic and electronic structure of S-terminated GaAs(001) surface. Journal of Applied Physics, 2010, 108, 063713.	2.5	3
180	Ab initioinvestigation of the electronic properties of graphene on InAs(111)A. Journal of Physics Condensed Matter, 2012, 24, 485004.	1.8	3

#	Article	IF	Citations
181	Size and dimensionality dependent phonon conductivity in nanocomposites. Journal of Physics Condensed Matter, 2016, 28, 145304.	1.8	3
182	Lattice thermal conduction in ultra-thin nanocomposites. Journal of Applied Physics, 2016, 119, 244309.	2.5	3
183	Electronâ€“phonon interaction and superconductivity in the. Philosophical Magazine, 2017, 97, 128-143.	1.6	3
184	Ab initio investigation of electron-phonon interaction in LaSn3 and CaSn3. Philosophical Magazine Letters, 2018, 98, 375-391.	1.2	3
185	Atomic and electronic structures of Sn covered W(110) surface. European Physical Journal B, 2020, 93, 1.	1.5	3
186	Effect of interface density, quality and period on the lattice thermal conductivity of nanocomposite materials. Journal of Applied Physics, 2020, 127, .	2.5	3
187	First-principles calculations of physical properties and superconductivity of orthorhombic Mo2BC and Nb2BN. Journal of Applied Physics, 2021, 130, 153902.	2.5	3
188	Enhancement of high entropy oxide (La0.2Nd0.2Sm0.2Gd0.2Y0.2)2Zr2O7 mechanical and photocatalytic properties via Eu doping. Journal of Materials Science, 2022, 57, 7863.	3.7	3
189	On the bounds on the threeâ€phonon Uâ€resistances. Physica Status Solidi (B): Basic Research, 1972, 50, K121.	1.5	2
190	On the use of the variational n-parameter trial function in the calculation of the lattice thermal conductivity. Journal of Physics C: Solid State Physics, 1976, 9, L11-L13.	1.5	2
191	A note on the nature of the phonon collision operator. Journal of Physics C: Solid State Physics, 1977, 10, L63-L66.	1.5	2
192	Role of optical phonons in the highâ€temperature lattice thermal conductivity of semiconductors. Physica Status Solidi (B): Basic Research, 1978, 90, K125.	1.5	2
193	The derivation of pseudoatom information in germanium from total-energy calculations. Journal of Physics Condensed Matter, 1992, 4, 1947-1958.	1.8	2
194	Intersubband absorption line broadening in In0.53Ga0.47As/In0.52Al0.48As quantum wells: A pseudopotential calculation. Solid State Communications, 1992, 81, 841-843.	1.9	2
195	Electronic properties of (111) twin boundaries and twinning superlattices in lead sulfide. Physical Review B, 1995, 52, 13734-13737.	3.2	2
196	In-plane magnetic field studies of InAs/GaSb superlattices. Physical Review B, 1997, 55, 5177-5183.	3.2	2
197	Ab initio Determination of Structural and Dynamical Properties of Mg2Sn. AIP Conference Proceedings, 2007, , .	0.4	2
198	Structure of theGaP(001)â˜'4Ã—2-Insurface investigated with LEED, STM, photoelectron spectroscopy, andab initiocalculations. Physical Review B, 2008, 78, .	3.2	2

#	Article	IF	Citations
199	Density-functional calculations for self-assembled Bi-nanolines on the InAs(100) surface. Journal of Applied Physics, 2009, 106, .	2.5	2
200	A Detailed Theoretical Study of the Thermal Conductivity of Bi₂(Te_{0.85}Se_{0.15})₃ Single Crystals. Materials Research Society Symposia Proceedings, 2012, 1404, 60.	0.1	2
201	Atomic and electronic structure of rigid carbon atomic chains. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 1738-1743.	1.8	2
202	Anisotropic Thermal Conduction in Transition Metal Dichalcogenide Nanocomposites with Rough Interfaces. Nanomaterials, 2018, 8, 1054.	4.1	2
203	Dirac and Weyl Semimetals in Sn_{1â^'x}In_xTe. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000362.	2.4	2
204	Tunable Thermal Transport Characteristics of Nanocomposites. Nanomaterials, 2020, 10, 673.	4.1	2
205	Probing the electronâ€“phonon interaction in superconductivity for KSn2 using the Migdal-Eliashberg theory and linear-response theory. Philosophical Magazine Letters, 2020, 100, 33-54.	1.2	2
206	Hypercircle Approach and Complementary Variational Principles for Lattice Thermal Conductivity. Physica Status Solidi (B): Basic Research, 1977, 80, 657-660.	1.5	1
207	Electronic and optic properties of crystalline and amorphous Si. Physica Status Solidi (B): Basic Research, 1978, 85, K121.	1.5	1
208	Report on a Kellar plan course in first-year university physics. Physics Education, 1989, 24, 295-299.	0.5	1
209	Atomic relaxation and electronic states in ultrathin Ge/ZnSe superlattices. Semiconductor Science and Technology, 1993, 8, 67-72.	2.0	1
210	Electronic-structure calculations of self-organized PbS-Bi2S3â^'(Ag2S)(113) twinning superlattices. Physical Review B, 1998, 57, 4557-4565.	3.2	1
211	Phonons on GaN(110). Applied Physics Letters, 2002, 80, 3322-3324.	3.3	1
212	Structural and dynamical properties of the Ge(001)/Sb(2Ã—1) surface. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 3031-3034.	0.8	1
213	Phonon spectrum and density of states on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ga</mml:mi><mml:mi mathvariant="normal">As</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>001</mml:mn><mml:mo>)</mml:mo></mml:mrow></mml:mrow Physical Review B, 2007, 76, .	3.2	1
214	Theoretical modelling of surface phonons. Open Physics, 2009, 7, .	1.7	1
215	Formation of nanoscale gold chain on a Si(110) surface: A density functional investigation. Journal of Applied Physics, 2011, 110, .	2.5	1
216	Energy Band Gap Modification of Graphene Deposited on a Multilayer Hexagonal Boron Nitride Substrate. Materials Research Society Symposia Proceedings, 2012, 1407, 45.	0.1	1

#	Article	IF	Citations
217	An Extensive Theoretical Study of the Phonon Conductivity and Thermoelectric Properties of SiGe Alloys. Materials Research Society Symposia Proceedings, 2012, 1404, 19.	0.1	1
218	Tuning phonon properties to enhance the thermoelectric figure of merit. , 2014, , .		1
219	Tunable Electronic Properties of Lateral Monolayer Transition Metal Dichalcogenide Superlattice Nanoribbons. Nanomaterials, 2021, 11, 534.	4.1	1
220	Solid foundations. Physics World, 1994, 7, 63-65.	0.0	0
221	Electronic structure of (GaAs)m(AlAs)nsuperlattices grown in the [211] direction. Physical Review B, 1995, 52, 7830-7833.	3.2	0
222	Atomic vibrations in thin [111] superlattices. Journal of Physics Condensed Matter, 1998, 10, 2829-2843.	1.8	0
223	Characterization of theGe(001)/Siâˆ'(2Ã—1)surface using lattice dynamics. Physical Review B, 1999, 60, 10648-10651.	3.2	0
224	Adsorption of C2H2-C2O3 on Si(001). Brazilian Journal of Physics, 2004, 34, 563-564.	1.4	0
225	Ab initio determination of structural and dynamical properties of the InP(110)-S interface. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 3035-3038.	0.8	0
226	Structure, Electronic Properties and Zone Centre Phonon Modes on the BeS(110) Surface. AIP Conference Proceedings, 2007, , .	0.4	0
227	Structural and electronic properties of zinc blende BeTe and ist (110) surface. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 595-597.	0.8	0
228	Ground state properties of zinc-blende and wurtzite phases of MgS. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 598-600.	0.8	0
229	Atomic Theory Of Phononic Gaps In Nano-patterned Semiconductors. , 2009, , .		0
230	Anharmonic Lifetime of Phonons in Nanophononic Semiconductors. Materials Research Society Symposia Proceedings, 2009, 1172, 26.	0.1	0
231	Theory of phonon conductivity of semiconductor superlattices. Materials Research Society Symposia Proceedings, 2011, 1347, 1.	0.1	0
232	The role of three-phonon Normal processes in the thermal conductivity of graphene. Materials Research Society Symposia Proceedings, 2012, 1404, 66.	0.1	0
233	Using steric constraints to template an organic array on Si(111)â€7â€‰Ã—â€‰7. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 647-652.	1.8	0
234	Atomic and Electronic Structure of Multilayer Graphene on a Monolayer Hexagonal Boron Nitride. Materials Research Society Symposia Proceedings, 2013, 1549, 65-70.	0.1	0

#	Article	IF	Citations
235	Detailed Theoretical Investigation and Comparison of the Thermal Conductivities of n- and p-type Bi2Te3 Based Alloys. Materials Research Society Symposia Proceedings, 2013, 1543, 1.	0.1	0
236	A Theoretical study of the Thermoelectric Transport Coefficients of n-type PbTe. Materials Research Society Symposia Proceedings, 2014, 1661, 7.	0.1	0
237	Effect of Tensile Strain on Thermal Properties of Graphene. Materials Research Society Symposia Proceedings, 2014, 1661, 1.	0.1	0
238	First-principles calculations of physical properties and superconductivity of orthorhombic ScRuSi and ZrRhSi. Physical Review B, 2020, 102, .	3.2	0
239	The effect of spinâ€“orbit interaction on superconductivity in the filled skutterudites MPt₄Ge₁₂(M=Ba, Sr and Th). Philosophical Magazine, 2020, 100, 2735-2758.	1.6	0
240	Atomic vibrations in thin [111] (GaAs)n(A1As)n superlattices. Journal of Physics Condensed Matter, 1998, 10, 7701-7701.	1.8	0
241	Anharmonic, dimensionality and size effects in phonon transport (2017 J. Phys.: Condens. Matter 29) Tj ETQq1 1 0.784314 rgBT /Ove	1.8	0
242	Phonon Dispersion Curves for Rubidium Fluoride. Journal of the Physical Society of Japan, 1975, 38, 1785-1785.	1.6	0