Charles W Myles

List of Publications by Year
in descending order

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92	1,579	331670	361022
papers	citations	21 h-index	35 g-index

94	94	94	797
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Study of the Lattice Thermal Conductivity in Ge Framework Semiconductors. Physical Review Letters, 2001, 86, 2361-2364.	7.8	212
2	Structural and electronic properties of tin clathrate materials. Physical Review B, 2001, 64, .	3.2	61
3	Raman scattering study of stoichiometric Si and Ge type II clathrates. Journal of Applied Physics, 2002, 92, 7225-7230.	2.5	58
4	Theory of alloys. I. Embedded-cluster calculations of phonon spectra for a one-dimensional binary alloy. Physical Review B, 1979, 19, 4939-4951.	3.2	56
5	Framework Contraction in Na-Stuffed Si(cF136). Inorganic Chemistry, 2010, 49, 5338-5340.	4.0	52
6	Size dependence of the conduction-electron-spin-resonancegshift in a small sodium particle: Orthogonalized standing-wave calculations. Physical Review B, 1982, 26, 2414-2431.	3.2	47
7	Spectra of Ternary Alloys. Physical Review Letters, 1979, 42, 254-257.	7.8	45
8	Generalized embedded-atom format for semiconductors. Physical Review B, 1990, 41, 1247-1250.	3.2	45
9	Deep levels associated with (vacancy, impurity) pairs in covalent semiconductors. Physical Review B, 1984, 29, 6810-6823.	3.2	42
10	Electronic and vibrational properties of framework-substituted type-II silicon clathrates. Physical Review B, 2007, 75, .	3.2	42
11	Tight-binding view of alloy scattering in III-V ternary semiconducting alloys. Physical Review B, 1984, 29, 802-807.	3.2	33
12	Identification of defect centers in Hg1â^'xCdxTe using their energy level composition dependence. Journal of Applied Physics, 1985, 57, 5279-5286.	2.5	33
13	Molecular-dynamics study of the vacancy and vacancy-hydrogen interactions in silicon. Physical Review B, 1995, 52, 1718-1723.	3.2	33
14	Vibrational properties of tin clathrate materials. Physical Review B, 2002, 65, .	3.2	33
15	Dynamical two-point correlation functions in a high-temperature Heisenberg paramagnet. Physical Review B, 1974, 9, 4872-4881.	3.2	32
16	Rattling guest atoms in Si, Ge, and Sn-based type-II clathrate materials. Physica Status Solidi (B): Basic Research, 2003, 239, 26-34.	1.5	29
17	Prediction of Giant Thermoelectric Power Factor in Type-VIII Clathrate Si46. Scientific Reports, 2014, 4, 7028.	3.3	28
18	Theory of alloys. III. Embedded-cluster calculations of electronic spectra for a one-dimensional ternary alloy. Physical Review B, 1984, 30, 3283-3293.	3.2	26

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19	Type VIII Si based clathrates: prospects for a giant thermoelectric power factor. Physical Chemistry Chemical Physics, 2015, 17, 8850-8859.	2.8	23
20	Phonon dynamics in type-VIII silicon clathrates: Beyond the rattler concept. Physical Review B, 2017, 95, .	3.2	23
21	Dynamics of a system of randomly distributed spins with multipolar interactions: Application to dipolar systems. Physical Review B, 1976, 14, 1-12.	3.2	21
22	Theory of alloy broadening of deep levels in semiconductor alloys: Nitrogen inAlxGa1â^'xAs. Physical Review B, 1986, 34, 927-931.	3.2	21
23	Alloy broadening of impurity electronic spectra: One-dimensional tight-binding theory for a binary alloy. Physical Review B, 1982, 25, 3593-3607.	3.2	20
24	First-principles calculations of the vibrational and thermal properties of the type-I clathratesBa8Ga16SixGe30â^'xandSr8Ga16SixGe30â^'x. Physical Review B, 2008, 78, .	3.2	20
25	Prediction of a large number of electron pockets near the band edges in type-VIII clathrate Si₄₆and its physical properties from first principles. Journal of Physics Condensed Matter, 2013, 25, 475502.	1.8	19
26	Theory of alloys. II. Embedded-cluster calculations of phonon spectra for a one-dimensional ternary alloy. Physical Review B, 1983, 28, 4519-4534.	3.2	18
27	Electronic structure of theNa16Rb8Si136andK16Rb8Si136clathrates. Physical Review B, 2006, 74, .	3.2	18
28	Theoretical study of nuclear-spinâ€"lattice relaxation in solidH2. Physical Review B, 1975, 12, 1638-1648.	3.2	17
29	Thermal properties of guest-free Si136 and Ge136 clathrates: A first-principles study. Journal of Applied Physics, 2008, 104, 033535.	2.5	16
30	Vibrational spectra of one-dimensional mass-disordered quaternary alloys. Journal of Physics and Chemistry of Solids, 1981, 42, 1043-1050.	4.0	15
31	Alloy broadening of the deep electronic levels associated with the As vacancy inAlxGa1â^'xAs. Physical Review B, 1988, 38, 1210-1214.	3.2	15
32	Electronic structure of ternary semiconductor alloys: CPA calculations using sp3sâ^— bandstructures. Journal of Physics and Chemistry of Solids, 1987, 48, 1173-1184.	4.0	14
33	Avalanche breakdown inpâ€nAlGaAs/GaAs heterojunctions. Journal of Applied Physics, 1990, 67, 6917-6923.	2.5	14
34	Rattling â€œguestâ€•impurities in Si and Ge clathrate semiconductors. Physica B: Condensed Matter, 2007, 401-402, 695-698.	2.7	14
35	First principles calculations of the structural, electronic and vibrational properties of the clathrates Ba8Al16Ge30and Ba8Al16Si30. Journal of Physics Condensed Matter, 2008, 20, 415214.	1.8	14
36	Spectral density functions for aJ=1quadrupolar solid: Application to solidH2. Physical Review B, 1975, 11, 2339-2351.	3.2	13

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37	Theory of alloy broadening of impurity electronic spectra. Physical Review B, 1981, 24, 1137-1139.	3.2	13
38	Model for phonon-assisted indirect recombination at impurity sites in semiconductors: A test of impurity wave-function theories. Physical Review B, 1985, 32, 2685-2688.	3.2	13
39	Effect of alloy disorder on deep levels in Hg1â^'xCdxTe. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1986, 4, 2195-2199.	2.1	12
40	Phonon-assisted indirect recombination of bound excitons in N-doped GaP, including near-resonant processes. Physical Review B, 1988, 37, 1205-1217.	3.2	12
41	Semi-empirical tightbinding bandstructures for IIâ€“VI zincblende compounds. Journal of Physics and Chemistry of Solids, 1990, 51, 93-100.	4.0	12
42	Lockâ€on effect in pulsedâ€power semiconductor switches. Journal of Applied Physics, 1992, 71, 3036-3038.	2.5	12
43	Electronic, elastic, vibrational, and thermodynamic properties of type-VIII clathrates Ba8Ga16Sn30 and Ba8Al16Sn30 by first principles. Journal of Applied Physics, 2013, 114, 163509.	2.5	12
44	Alloy disorder effects on the electronic properties of III-V quaternary semiconductor alloys. Physical Review B, 1990, 41, 3582-3591.	3.2	11
45	Effects of lattice relaxation on deep levels in semiconductors. Physical Review B, 1991, 43, 2192-2200.	3.2	11
46	A first-principles lattice dynamical study of type-I, type-II, and type-VIII silicon clathrates. Journal of Materials Science, 2016, 51, 4538-4548.	3.7	11
47	High-temperature nuclear-magnetic-resonance line shapes in dense paramagnetic insulators. Physical Review B, 1975, 11, 3225-3237.	3.2	10
48	Quadrupolar exchange effects on the dynamics of high-temperature paramagnets. Physical Review B, 1979, 19, 1331-1344.	3.2	10
49	Electronic properties of the quaternary semiconductor alloyGaSb1â^'xâ^'yAsxPy: Coherent-potential approximation. Physical Review B, 1987, 35, 2532-2535.	3.2	10
50	Effects of alloy disorder on Schottky-barrier heights. Physical Review B, 1987, 35, 9758-9765.	3.2	10
51	Charge state splittings of deep levels in Hg1â^'xCdxTe. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1988, 6, 2675-2680.	2.1	10
52	Deep levels produced by triplet vacancyâ€impurity complexes in GaP. Journal of Applied Physics, 1989, 65, 4273-4278.	2.5	10
53	Structural, electronic, phonon and thermodynamic properties of hypothetical type-VIII clathrates Ba8Si46 and Ba8Al16Si30 investigated by first principles. Journal of Alloys and Compounds, 2014, 587, 474-480.	5.5	10
54	Semiempirical formalism for the calculation of deep-level wave functions inkspace. Physical Review B, 1986, 33, 8234-8237.	3.2	9

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55	Molecular-dynamics study of defect formation ina-Si:H. Physical Review B, 1995, 51, 1671-1679.	3.2	9
56	Dynamical spin correlation functions in a system of randomly distributed spins with râ^'n interactions. AIP Conference Proceedings, 1975, , .	0.4	7
57	Interaction of nuclear spins with phonons in a dense paramagnetic insulator. Physical Review B, 1975, 11, 3238-3250.	3.2	7
58	Shape dependence of the conduction-electron spin-resonancegshift in a small sodium particle. Physical Review B, 1982, 26, 2648-2651.	3.2	7
59	Theory of alloy broadening of deep levels in semiconductor alloys: Effects of second-neighbor disorder. Physical Review B, 1988, 38, 10533-10541.	3.2	7
60	Electronic properties of Hg1â^'xâ^'yCdxZnyTe. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1989, 7, 321-325.	2.1	7
61	Defect identification in semiconductor alloys using deep level composition dependence. II. Application to GaAs1â^'xPx. Journal of Applied Physics, 1990, 67, 7351-7358.	2.5	7
62	Molecular-dynamics approach to lattice-relaxation effects on deep levels in semiconductors. Physical Review B, 1991, 43, 9947-9950.	3.2	7
63	Alloy broadening of impurity electronic spectra: One-dimensional-model calculations for a ternary alloy. Physical Review B, 1985, 32, 3416-3421.	3.2	6
64	Deep levels associated with vacancyâ€impurity complexes in GaAs. Applied Physics Letters, 1987, 51, 2034-2036.	3.3	6
65	Deep-level wave functions including lattice-relaxation effects. Physical Review B, 1993, 47, 4281-4288.	3.2	6
66	Density-functional investigation of Na₁₆A₈Ge₁₃₆(A = Rb,Cs) clathrates. Journal of Physics Condensed Matter, 2007, 19, 466206.	1.8	6
67	Effect of Guest Atom Composition on the Structural and Vibrational Properties of the Type II Clathrate-Based Materials AxSi136, AxGe136 and AxSn136 (A = Na, K, Rb, Cs; 0 â‰ x â‰ 24). Materials, 2016, 9, 691.	2.9	6
68	Simulation of Current Filaments in Photoconductive Semiconductor Switches. , 2005, , .		5
69	Diagrammatic derivation ofT1for solidH2. Physical Review B, 1976, 13, 3199-3202.	3.2	4
70	Coherent potential approximation for quaternary alloys: Application to phonon spectra in one dimension. Journal of Physics and Chemistry of Solids, 1985, 46, 1305-1319.	4.0	4
71	Chemical trends for deep levels associated with vacancy-impurity complexes in semiconductors. Physical Review B, 1989, 40, 6222-6235.	3.2	4
72	Effect of Deep Level Impact Ionization on Avalanche Breakdown in Semiconductor p-n Junctions. Physica Status Solidi A, 2000, 181, 219-229.	1.7	4

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73	Higher-Order Acoustic-Paramagnetic-Resonance Transitions of Magnetic Impurities in Dielectrics. Physical Review B, 1973, 8, 2049-2059.	3.2	3
74	Incoherent neutron scattering from solid mixtures of orthohydrogen and parahydrogen. Physical Review B, 1976, 13, 2636-2640.	3.2	3
75	Spin dynamics in anisotropic paramagnets. Physical Review B, 1977, 15, 5326-5349.	3.2	3
76	Coherent potential approximation calculations for electronic spectra of one-dimensional quaternary alloys. Journal of Physics and Chemistry of Solids, 1987, 48, 329-340.	4.0	3
77	Deep levels associated with triplet impurity complexes in GaP. Physical Review B, 1989, 40, 10425-10429.	3.2	3
78	Semiempirical total-energy functional for silicon-hydrogen interactions in solids. Physical Review B, 1993, 48, 17086-17091.	3.2	3
79	First-Principles Analysis of Vibrational Properties of Type II SiGe Alloy Clathrates. Nanomaterials, 2019, 9, 723.	4.1	3
80	Theory of Higher-Order Acoustic Paramagnetic-Resonance Transitions of Magnetic Ions in Dielectrics. Physical Review Letters, 1972, 28, 1620-1622.	7.8	2
81	Incoherent neutron scattering from solid mixtures of orthohydrogen and parahydrogen. Physical Review B, 1977, 15, 3279-3280.	3.2	2
82	Crystal- and magnetic-field effects on nuclear-spinâ€”lattice relaxation in solidH2. Physical Review B, 1978, 18, 6230-6244.	3.2	2
83	Theory of time-resolved luminescence of bound excitons in semiconductor alloys. Physical Review B, 1989, 39, 6216-6219.	3.2	2
84	Effect of alloy disorder on the deep levels produced by the anion vacancy inGaAs1â^'xPx. Physical Review B, 1989, 40, 11947-11950.	3.2	2
85	Deep levels including lattice relaxation: first- and second-neighbor effects. Journal of Physics and Chemistry of Solids, 2000, 61, 1855-1864.	4.0	2
86	Lattice Relaxation Effects on Deep Levels: Molecular Dynamics Calculations. Materials Science Forum, 1992, 83-87, 505-510.	0.3	1
87	Large supercell molecular dynamics study of defect formation in hydrogenated amorphous silicon. Journal of Physics and Chemistry of Solids, 2002, 63, 1691-1698.	4.0	1
88	First Principles Study of the Vibrational and Thermal Properties of Sn-Based Type II Clathrates, CsxSn136 (0 â‰¤ x â‰¤ 24) and Rb24Ga24Sn112. Inorganics, 2019, 7, 74.	2.7	1
89	Electronic Property and Negative Thermal Expansion Behavior of Si136-xGex (x = 8, 32, 40, 104) Clathrate Solid Solution from First Principles. Nanomaterials, 2019, 9, 851.	4.1	1
90	First-Principles Investigation on Type-II Aluminum-Substituted Ternary and Quaternary Clathrate Semiconductors R8Al8Si128 (R = Cs, Rb), Cs8Na16Al24Si112. Applied Sciences (Switzerland), 2019, 9, 125.	2.5	1

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91	Ultrasonic attenuation in a quadrupolar solid. Physical Review B, 1976, 13, 3645-3654.	3.2	0
92	IncoherentJ=1â†'0neutron scattering from solidH2. Physical Review B, 1981, 23, 4741-4748.	3.2	0