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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	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
2	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
3	First-Principles Analysis of Vibrational Properties of Type II SiGe Alloy Clathrates. Nanomaterials, 2019, 9, 723.	4.1	3
4	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
5	Phonon dynamics in type-VIII silicon clathrates: Beyond the rattler concept. Physical Review B, 2017, 95, .	3.2	23
6	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
7	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
8	Type VIII Si based clathrates: prospects for a giant thermoelectric power factor. Physical Chemistry Chemical Physics, 2015, 17, 8850-8859.	2.8	23
9	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
10	Prediction of Giant Thermoelectric Power Factor in Type-VIII Clathrate Si46. Scientific Reports, 2014, 4, 7028.	3.3	28
11	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
12	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
13	Framework Contraction in Na-Stuffed Si(cF136). Inorganic Chemistry, 2010, 49, 5338-5340.	4.0	52
14	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
15	First-principles calculations of the vibrational and thermal properties of the type-I clathratesBa8Ga16SixGe30â^'xandSr8Ga16SixGe30â^'x. Physical Review B, 2008, 78, .	3.2	20
16	Thermal properties of guest-free Si136 and Ge136 clathrates: A first-principles study. Journal of Applied Physics, 2008, 104, 033535.	2.5	16
17	Density-functional investigation of Na₁₆A₈Ge₁₃₆(A = Rb,Cs) clathrates. Journal of Physics Condensed Matter, 2007, 19, 466206.	1.8	6
18	Electronic and vibrational properties of framework-substituted type-II silicon clathrates. Physical Review B, 2007, 75, .	3.2	42

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19	Rattling â€œguestâ€•impurities in Si and Ge clathrate semiconductors. Physica B: Condensed Matter, 2007, 401-402, 695-698.	2.7	14
20	Electronic structure of theNa16Rb8Si136andK16Rb8Si136clathrates. Physical Review B, 2006, 74, .	3.2	18
21	Simulation of Current Filaments in Photoconductive Semiconductor Switches. , 2005, , .		5
22	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
23	Vibrational properties of tin clathrate materials. Physical Review B, 2002, 65, .	3.2	33
24	Raman scattering study of stoichiometric Si and Ge type II clathrates. Journal of Applied Physics, 2002, 92, 7225-7230.	2.5	58
25	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
26	Structural and electronic properties of tin clathrate materials. Physical Review B, 2001, 64, .	3.2	61
27	Theoretical Study of the Lattice Thermal Conductivity in Ge Framework Semiconductors. Physical Review Letters, 2001, 86, 2361-2364.	7.8	212
28	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
29	Deep levels including lattice relaxation: first- and second-neighbor effects. Journal of Physics and Chemistry of Solids, 2000, 61, 1855-1864.	4.0	2
30	Molecular-dynamics study of defect formation ina-Si:H. Physical Review B, 1995, 51, 1671-1679.	3.2	9
31	Molecular-dynamics study of the vacancy and vacancy-hydrogen interactions in silicon. Physical Review B, 1995, 52, 1718-1723.	3.2	33
32	Semiempirical total-energy functional for silicon-hydrogen interactions in solids. Physical Review B, 1993, 48, 17086-17091.	3.2	3
33	Deep-level wave functions including lattice-relaxation effects. Physical Review B, 1993, 47, 4281-4288.	3.2	6
34	Lattice Relaxation Effects on Deep Levels: Molecular Dynamics Calculations. Materials Science Forum, 1992, 83-87, 505-510.	0.3	1
35	Lockâ€on effect in pulsedâ€power semiconductor switches. Journal of Applied Physics, 1992, 71, 3036-3038.	2.5	12
36	Effects of lattice relaxation on deep levels in semiconductors. Physical Review B, 1991, 43, 2192-2200.	3.2	11

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37	Molecular-dynamics approach to lattice-relaxation effects on deep levels in semiconductors. Physical Review B, 1991, 43, 9947-9950.	3.2	7
38	Semi-empirical tightbinding bandstructures for IIâ€“VI zincblende compounds. Journal of Physics and Chemistry of Solids, 1990, 51, 93-100.	4.0	12
39	Alloy disorder effects on the electronic properties of III-V quaternary semiconductor alloys. Physical Review B, 1990, 41, 3582-3591.	3.2	11
40	Generalized embedded-atom format for semiconductors. Physical Review B, 1990, 41, 1247-1250.	3.2	45
41	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
42	Avalanche breakdown inpâ€nAlGaAs/GaAs heterojunctions. Journal of Applied Physics, 1990, 67, 6917-6923.	2.5	14
43	Deep levels produced by triplet vacancyâ€impurity complexes in GaP. Journal of Applied Physics, 1989, 65, 4273-4278.	2.5	10
44	Theory of time-resolved luminescence of bound excitons in semiconductor alloys. Physical Review B, 1989, 39, 6216-6219.	3.2	2
45	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
46	Deep levels associated with triplet impurity complexes in GaP. Physical Review B, 1989, 40, 10425-10429.	3.2	3
47	Electronic properties of Hg1â^'xâ^'yCdxZnyTe. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1989, 7, 321-325.	2.1	7
48	Chemical trends for deep levels associated with vacancy-impurity complexes in semiconductors. Physical Review B, 1989, 40, 6222-6235.	3.2	4
49	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
50	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
51	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
52	Alloy broadening of the deep electronic levels associated with the As vacancy inAlxGa1â^'xAs. Physical Review B, 1988, 38, 1210-1214.	3.2	15
53	Electronic properties of the quaternary semiconductor alloyGaSb1â^'xâ^'yAsxPy: Coherent-potential approximation. Physical Review B, 1987, 35, 2532-2535.	3.2	10
54	Deep levels associated with vacancyâ€impurity complexes in GaAs. Applied Physics Letters, 1987, 51, 2034-2036.	3.3	6

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55	Effects of alloy disorder on Schottky-barrier heights. Physical Review B, 1987, 35, 9758-9765.	3.2	10
56	Electronic structure of ternary semiconductor alloys: CPA calculations using sp3sâˆ— bandstructures. Journal of Physics and Chemistry of Solids, 1987, 48, 1173-1184.	4.0	14
57	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
58	Theory of alloy broadening of deep levels in semiconductor alloys: Nitrogen inAlxGa1â^'xAs. Physical Review B, 1986, 34, 927-931.	3.2	21
59	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
60	Semiempirical formalism for the calculation of deep-level wave functions inkspace. Physical Review B, 1986, 33, 8234-8237.	3.2	9
61	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
62	Alloy broadening of impurity electronic spectra: One-dimensional-model calculations for a ternary alloy. Physical Review B, 1985, 32, 3416-3421.	3.2	6
63	Identification of defect centers in Hg1â^'xCdxTe using their energy level composition dependence. Journal of Applied Physics, 1985, 57, 5279-5286.	2.5	33
64	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
65	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
66	Tight-binding view of alloy scattering in III-V ternary semiconducting alloys. Physical Review B, 1984, 29, 802-807.	3.2	33
67	Deep levels associated with (vacancy, impurity) pairs in covalent semiconductors. Physical Review B, 1984, 29, 6810-6823.	3.2	42
68	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
69	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
70	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
71	Shape dependence of the conduction-electron spin-resonancegshift in a small sodium particle. Physical Review B, 1982, 26, 2648-2651.	3.2	7
72	Vibrational spectra of one-dimensional mass-disordered quaternary alloys. Journal of Physics and Chemistry of Solids, 1981, 42, 1043-1050.	4.0	15

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73	Theory of alloy broadening of impurity electronic spectra. Physical Review B, 1981, 24, 1137-1139.	3.2	13
74	IncoherentJ=1â†'0neutron scattering from solidH2. Physical Review B, 1981, 23, 4741-4748.	3.2	0
75	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
76	Spectra of Ternary Alloys. Physical Review Letters, 1979, 42, 254-257.	7.8	45
77	Quadrupolar exchange effects on the dynamics of high-temperature paramagnets. Physical Review B, 1979, 19, 1331-1344.	3.2	10
78	Crystal- and magnetic-field effects on nuclear-spinâ€"lattice relaxation in solidH2. Physical Review B, 1978, 18, 6230-6244.	3.2	2
79	Incoherent neutron scattering from solid mixtures of orthohydrogen and parahydrogen. Physical Review B, 1977, 15, 3279-3280.	3.2	2
80	Spin dynamics in anisotropic paramagnets. Physical Review B, 1977, 15, 5326-5349.	3.2	3
81	Ultrasonic attenuation in a quadrupolar solid. Physical Review B, 1976, 13, 3645-3654.	3.2	0
82	Incoherent neutron scattering from solid mixtures of orthohydrogen and parahydrogen. Physical Review B, 1976, 13, 2636-2640.	3.2	3
83	Diagrammatic derivation ofT1for solidH2. Physical Review B, 1976, 13, 3199-3202.	3.2	4
84	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
85	Dynamical spin correlation functions in a system of randomly distributed spins with râ^'n interactions. AIP Conference Proceedings, 1975, , .	0.4	7
86	Interaction of nuclear spins with phonons in a dense paramagnetic insulator. Physical Review B, 1975, 11, 3238-3250.	3.2	7
87	Theoretical study of nuclear-spinâ€"lattice relaxation in solidH2. Physical Review B, 1975, 12, 1638-1648.	3.2	17
88	Spectral density functions for aJ=1quadrupolar solid: Application to solidH2. Physical Review B, 1975, 11, 2339-2351.	3.2	13
89	High-temperature nuclear-magnetic-resonance line shapes in dense paramagnetic insulators. Physical Review B, 1975, 11, 3225-3237.	3.2	10
90	Dynamical two-point correlation functions in a high-temperature Heisenberg paramagnet. Physical Review B, 1974, 9, 4872-4881.	3.2	32

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91	Higher-Order Acoustic-Paramagnetic-Resonance Transitions of Magnetic Impurities in Dielectrics. Physical Review B, 1973, 8, 2049-2059.	3.2	3
92	Theory of Higher-Order Acoustic Paramagnetic-Resonance Transitions of Magnetic Ions in Dielectrics. Physical Review Letters, 1972, 28, 1620-1622.	7.8	2