Wolfgang Windl

List of Publications by Year
in descending order

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163	10,655	81743 39	31759 101
papers	citations	h-index	g-index

176	176	176	15905
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ca₂Ga₄Ge₆ and Ca₃Ga₄Ge₆: Synthesis, Structure, and Electronic Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2022, 648, .	0.6	0
2	Spatially Resolved Investigation of the Bandgap Variation across a Î²-(Al_xGa_{1â€“x})₂O₃/Î²-Ga₂O₃ Interface by STEMâ€“VEELS. ACS Applied Electronic Materials, 2022, 4, 585-591.	4.0	2
3	Cr_xPt_{1â€“x}Te₂ (x â‰ˆ 0.45): A Family of Air-Stable and Exfoliatable van der Waals Ferromagnets. ACS Nano, 2022, 16, 3852-3860.	7.3	9
4	Nonlinear Arrhenius behavior of self-diffusion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>Ti</mml:mi></mm and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Mo</mml:mi></mml:math>. Physical Review Materials, 2022, 6, .	0.9	1
5	Highly efficient transverse thermoelectric devices with Re₄Si₇ crystals. Energy and Environmental Science, 2021, 14, 4009-4017.	15.6	29
6	Layer- and gate-tunable spin-orbit coupling in a high-mobility few-layer semiconductor. Science Advances, 2021, 7, .	4.7	16
7	Synthesis and characterization of a new family of layered Pb_xSn_{4â^'x}As₃alloys. Journal of Materials Chemistry C, 2021, 9, 6477-6483.	2.7	5
8	Computationally Guided Discovery of Axis-Dependent Conduction Polarity in NaSnAs Crystals. Chemistry of Materials, 2021, 33, 946-951.	3.2	13
9	Electrochemical metrics for corrosion resistant alloys. Scientific Data, 2021, 8, 58.	2.4	46
10	Native point defects from stoichiometry-linked chemical potentials in cubic boron arsenide. Journal of Applied Physics, 2021, 129, 075703.	1.1	2
11	Exploring the AgSb1â^'xBixI4 phase diagram: Thermochromism in layered CdCl2-type semiconductors. Journal of Solid State Chemistry, 2021, 297, 121997.	1.4	8
12	Ga interstitial stability and its effect on the electronic properties of Î²-(AlxGa1-x)2O3 alloy. Microscopy and Microanalysis, 2021, 27, 2358-2359.	0.2	0
13	Recent Advances in Corrosion Science Applicable To Disposal of High-Level Nuclear Waste. Chemical Reviews, 2021, 121, 12327-12383.	23.0	52
14	Lucky Number 13: A 13-Layer Polytype of the Alkyne Hydrogenation Catalyst CaGaGe. Inorganic Chemistry, 2021, 60, 14530-14534.	1.9	2
15	Understanding the efficacy of concentrated interstitial carbon in enhancing the pitting corrosion resistance of stainless steel. Acta Materialia, 2021, 221, 117433.	3.8	24
16	Atomic-scale characterization of structural and electronic properties of Hf doped Î²-Ga2O3. Applied Physics Letters, 2021, 119, .	1.5	6
17	An integrated experimental and computational study of diffusion and atomic mobility of the aluminumâ€“magnesium system. Acta Materialia, 2020, 189, 214-231.	3.8	29
18	Controlling the corrosion resistance of multi-principal element alloys. Scripta Materialia, 2020, 188, 96-101.	2.6	58

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19	Full â€œAb-Initioâ€•Simulation of Field Evaporation of Samples with Grain Boundaries. Microscopy and Microanalysis, 2020, 26, 2878-2879.	0.2	0
20	Point Defect and Their Influence on the Atomic and Electronic Structure of Î²-(Al_xGa_{1-x})₂O₃ Alloys by STEM-EELS. Microscopy and Microanalysis, 2020, 26, 622-623.	0.2	2
21	Synthesis, structural, and electronic properties of Sr_{1â^'x}Ca_xPdAs. Inorganic Chemistry Frontiers, 2020, 7, 2833-2839.	3.0	3
22	Influence of Surface Chemistry on Water Absorption in Functionalized Germanane. Chemistry of Materials, 2020, 32, 1537-1544.	3.2	8
23	The Chemical Design Principles for Axis-Dependent Conduction Polarity. Journal of the American Chemical Society, 2020, 142, 2812-2822.	6.6	18
24	Bond Synergy Model for Bond Energies in Alloy Oxides. Journal of the Electrochemical Society, 2020, 167, 141511.	1.3	11
25	Shear Banding in Bulk Metallic Glass Matrix Composites with Dendrite Reinforcements. Structural Integrity, 2019, , 338-340.	0.8	1
26	Identification of turbostratic twisting in germanane. Journal of Materials Chemistry C, 2019, 7, 10092-10097.	2.7	4
27	Ferromagnetic Epitaxial Î¼-Fe2O3 on Î²-Ga2O3: A New Monoclinic Form of Fe2O3. Crystal Growth and Design, 2019, 19, 4205-4211.	1.4	5
28	Bond-order bond energy model for alloys. Acta Materialia, 2019, 179, 406-413.	3.8	21
29	Atomistic-Simulation Based Modeling of Atom Probe Tomography. Microscopy and Microanalysis, 2019, 25, 284-285.	0.2	1
30	Magnon drag effect in Fe-Co alloys. Journal of Applied Physics, 2019, 126, 125107.	1.1	4
31	The Fermi surface geometrical origin of axis-dependent conduction polarity in layered materials. Nature Materials, 2019, 18, 568-572.	13.3	46
32	Multi-cell Monte Carlo method for phase prediction. Npj Computational Materials, 2019, 5, .	3.5	15
33	Direct imaging of the nitrogen-rich edge in monolayer hexagonal boron nitride and its band structure tuning. Nanoscale, 2019, 11, 20676-20684.	2.8	10
34	Synthesis of 1T, 2H, and 6R Germanane Polytypes. Chemistry of Materials, 2018, 30, 1335-1343.	3.2	53
35	A comparative review of the aqueous corrosion of glasses, crystalline ceramics, and metals. Npj Materials Degradation, 2018, 2, .	2.6	150
36	Identification of Ge vacancies as electronic defects in methyl- and hydrogen-terminated germanane. Applied Physics Letters, 2018, 113, 061110.	1.5	7

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37	Raman Spectroscopy, Photocatalytic Degradation, and Stabilization of Atomically Thin Chromium Tri-iodide. Nano Letters, 2018, 18, 4214-4219.	4.5	131
38	Ab-Initio Calculation of Spectral Absorption Coefficients in Molten Fluoride Salts with Metal Impurities. Nuclear Technology, 2018, 204, 59-65.	0.7	7
39	Magnetic proximity effect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pt</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> bilayers. Physical Review Materials, 2018, 2, .	0.9	33
40	A general model for thermal and electrical conductivity of binary metallic systems. Acta Materialia, 2017, 126, 272-279.	3.8	17
41	Multi-Cell Monte Carlo Relaxation method for predicting phase stability of alloys. Scripta Materialia, 2017, 132, 9-12.	2.6	24
42	Three-dimensional imaging of individual point defects using selective detection angles in annular dark field scanning transmission electron microscopy. Ultramicroscopy, 2017, 172, 17-29.	0.8	24
43	Coupling Molecular Dynamics and Finite Element Simulations to Investigate the Nearest Neighbor Dependence of Field Evaporation. Microscopy and Microanalysis, 2017, 23, 646-647.	0.2	1
44	Performance analysis and optimization of the RAMPAGE metal alloy potential generation software. , 2017, , .		1
45	NaSn₂As₂: An Exfoliatable Layered van der Waals Zintl Phase. ACS Nano, 2016, 10, 9500-9508.	7.3	39
46	Threeâ€dimensional imaging of shear bands in bulk metallic glass composites. Journal of Microscopy, 2016, 264, 304-310.	0.8	9
47	Tailoring the Electronic Structure of Covalently Functionalized Germanane via the Interplay of Ligand Strain and Electronegativity. Chemistry of Materials, 2016, 28, 8071-8077.	3.2	71
48	Cs₂AgBiX₆ (X = Br, Cl): New Visible Light Absorbing, Lead-Free Halide Perovskite Semiconductors. Chemistry of Materials, 2016, 28, 1348-1354.	3.2	1,077
49	Super-X EDS Characterization of Chemical Segregation within a Superlattice Extrinsic Stacking Fault of a Ni- based Superalloy. Microscopy and Microanalysis, 2015, 21, 493-494.	0.2	4
50	Effects of the local structure dependence of evaporation fields on field evaporation behavior. Applied Physics Letters, 2015, 107, .	1.5	18
51	Probing Bonding Environments in Osmium-Based Double Perovskites Using Monochromated Dual Electron-Energy Loss Spectroscopy. Microscopy and Microanalysis, 2015, 21, 2365-2366.	0.2	0
52	Alpha spectroscopy for in-situ liquid radioisotope measurements. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2015, 780, 119-126.	0.7	7
53	Phonon-induced diamagnetic force and its effect on the lattice thermal conductivity. Nature Materials, 2015, 14, 601-606.	13.3	45
54	Probing carbonate in bone forming minerals on the nanometre scale. Acta Biomaterialia, 2015, 20, 129-139.	4.1	28

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55	Segregation and Î· phase formation along stacking faults during creep at intermediate temperatures in a Ni-based superalloy. Acta Materialia, 2015, 100, 19-31.	3.8	128
56	Reactor radiation-induced attenuation in fused silica optical fibers heated up to 1000 Â°C. Journal of Non-Crystalline Solids, 2015, 409, 88-94.	1.5	27
57	Inâ€Situ Reactor Radiationâ€Induced Attenuation in Sapphire Optical Fibers. Journal of the American Ceramic Society, 2014, 97, 3883-3889.	1.9	15
58	Advanced Extra Functionality CMOS-based Devices. Physica Status Solidi C: Current Topics in Solid State Physics, 2014, 11, 7-8.	0.8	2
59	Magnetic structure in epitaxially strained <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Sr</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">CrReO</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math>thin films by element-specific XAS and XMCD. Physical Review B, 2014, 89, .	1.1	16
60	Improving the stability and optical properties of germanane via one-step covalent methyl-termination. Nature Communications, 2014, 5, 3389.	5.8	201
61	A first principles method to simulate electron mobilities in 2D materials. New Journal of Physics, 2014, 16, 105009.	1.2	60
62	Tunable gaps and enhanced mobilities in strain-engineered silicane. Journal of Applied Physics, 2014, 115, .	1.1	68
63	Direct Observation of Defects in Hexagonal Boron Nitride Monolayers. Microscopy and Microanalysis, 2014, 20, 1738-1739.	0.2	2
64	Structural evolution and kinetics in Cu-Zr metallic liquids from molecular dynamics simulations. Physical Review B, 2013, 88, .	1.1	85
65	An embedded atom method potential of beryllium. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 085001.	0.8	18
66	Independent Ordering of Two Interpenetrating Magnetic Sublattices in the Double Perovskite Sr₂CoOsO₆. Journal of the American Chemical Society, 2013, 135, 18824-18830.	6.6	92
67	Electron-hole pair generation in SiC high-temperature alpha particle detectors. Applied Physics Letters, 2013, 103, .	1.5	27
68	Atomic-Scale Engineering of the Electrostatic Landscape of Semiconductor Surfaces. Nano Letters, 2013, 13, 2418-2422.	4.5	15
69	In-situ gamma radiation induced attenuation in silica optical fibers heated up to 600Â°C. Journal of Non-Crystalline Solids, 2013, 379, 192-200.	1.5	27
70	Stability and Exfoliation of Germanane: A Germanium Graphane Analogue. ACS Nano, 2013, 7, 4414-4421.	7.3	910
71	Progress, Challenges, and Opportunities in Two-Dimensional Materials Beyond Graphene. ACS Nano, 2013, 7, 2898-2926.	7.3	4,062
72	Low angle ADF STEM defect imaging. Microscopy and Microanalysis, 2012, 18, 676-677.	0.2	13

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73	Native point defects in binary InP semiconductors. Journal of Materials Science, 2012, 47, 7482-7497.	1.7	20
74	Ca₂MnRuO₆: Magnetic Order Arising from Chemical Chaos. Chemistry of Materials, 2012, 24, 2757-2763.	3.2	11
75	Oxidation Resistance of Reactive Atoms in Graphene. Nano Letters, 2012, 12, 4651-4655.	4.5	64
76	Fast free-energy calculations for unstable high-temperature phases. Physical Review B, 2012, 86, .	1.1	35
77	Fullerene and graphene formation from carbon nanotube fragments. Computational and Theoretical Chemistry, 2012, 987, 115-121.	1.1	13
78	Full First-Principles Theory of Spin Relaxation in Group-IV Materials. Physical Review Letters, 2012, 109, 166604.	2.9	51
79	Atomic-resolution defect contrast in low angle annular dark-field STEM. Ultramicroscopy, 2012, 116, 47-55.	0.8	93
80	Aberration-Corrected STEM Imaging and Spectroscopy of Single-Layered Materials. Microscopy and Microanalysis, 2011, 17, 1260-1261.	0.2	0
81	Local electronic structure of LiFePO4 nanoparticles in aged Li-ion batteries. Acta Materialia, 2011, 59, 6917-6926.	3.8	19
82	First principles calculation of polarization induced interfacial charges in GaN/AlN heterostructures. Applied Physics Letters, 2011, 98, .	1.5	7
83	Self-trapping in B-doped amorphous Si: Intrinsic origin of low acceptor efficiency. Physical Review B, 2010, 81, .	1.1	9
84	First-Principles Study of Defective and Nonstoichiometric Sr₂FeMoO₆. Chemistry of Materials, 2010, 22, 6092-6102.	3.2	37
85	Elastic anisotropy of Ni4Ti3 from first principles. Scripta Materialia, 2009, 60, 207-210.	2.6	61
86	Toward Siteâ€Specific Stamping of Graphene. Advanced Materials, 2009, 21, 1243-1246.	11.1	80
87	First principles study of the structure and stability of carbynes. Carbon, 2009, 47, 367-383.	5.4	39
88	Microstructural evolution during multiaxial deformation of pseudoelastic NiTi studied by first-principles-based micromechanical modeling. Acta Materialia, 2009, 57, 3856-3867.	3.8	28
89	Characterization of Open Volume Regions in a Simulated Cu-Zr Metallic Glass. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2008, 39, 1779-1785.	1.1	9
90	Lattice stability, elastic constants and macroscopic moduli of NiTi martensites from first principles. Acta Materialia, 2008, 56, 6232-6245.	3.8	200

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91	Charge of self-interstitials and boron-interstitial pairs as a function of doping concentration. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2008, 154-155, 198-201.	1.7	1
92	Detailed arsenic concentration profiles at Si/SiO2 interfaces. Journal of Applied Physics, 2008, 104, 043507.	1.1	20
93	Distribution and segregation of arsenic at theSiO2/Si interface. Journal of Applied Physics, 2008, 104, 023518.	1.1	25
94	Ab Initio Modeling of Contact Structure Formation of Carbon Nanotubes and Its Effect on Electron Transport. Materials Research Society Symposia Proceedings, 2008, 1081, 1.	0.1	0
95	Ab-Initio Modeling of Arsenic Pile-Up and Deactivation at the Si/SiO2 Interface. Materials Research Society Symposia Proceedings, 2008, 1070, 1.	0.1	0
96	Concentration-Dependence of Self-Interstitial and Boron Diffusion in Silicon. Materials Research Society Symposia Proceedings, 2008, 1070, 1.	0.1	0
97	First Principles Study of Boron in Amorphous Silicon. Materials Research Society Symposia Proceedings, 2008, 1070, 1.	0.1	0
98	Concentration dependence of self-interstitial and boron diffusion in silicon. Applied Physics Letters, 2008, 92, .	1.5	6
99	Ab-Initio Modeling of Point Defects, Impurities and Diffusion in Silicon. ECS Transactions, 2008, 16, 89-96.	0.3	2
100	Multiscale Simulations of The Elastic Properties of Polycrystalline Silicon. AIP Conference Proceedings, 2007, , .	0.3	1
101	Characterization of the origin of band states in the SiC/SiO₂ interface. , 2007, , .		0
102	Characterization of the Segregation of Arsenic at the Interface SiO₂/Si. Materials Research Society Symposia Proceedings, 2007, 994, 1.	0.1	4
103	Monte Carlo Modeling of Count Rates and Defects in a Silicon Carbide Detector Neutron Monitor System, Highlighting GT-MHR. Nuclear Technology, 2007, 159, 208-220.	0.7	1
104	Structure and chemical analysis of aluminum wear debris: Experiments and ab initio simulations. Acta Materialia, 2007, 55, 6489-6498.	3.8	15
105	Characterization of the pile-up of As at the SiO<inf>2</inf>/Si interface. , 2007, , .		2
106	Diffusion and Deactivation of As in Si: Combining Atomistic and Continuum Simulation Approaches. , 2007, , 13-16.		0
107	Ab-Initio Calculations of the Energetics and Kinetics of Defects and Impurities in Silicon. ECS Transactions, 2006, 3, 171-182.	0.3	9
108	SiC Based Neutron Flux Monitors for Very High Temperature Nuclear Reactors. Materials Research Society Symposia Proceedings, 2006, 929, 1.	0.1	1

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109	Process-Induced Diffusion Phenomena in Advanced CMOS Technologies. Defect and Diffusion Forum, 2006, 258-260, 510-521.	0.4	2
110	Characterization and Modeling of Atomically Sharp Perfect Si:Ge/SiO2 Interfaces. ECS Transactions, 2006, 3, 539-549.	0.3	1
111	Ab initio study of the effect of hydrogen and point defects on arsenic segregation at Si (100)/SiO2 interfaces. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 359-362.	1.7	0
112	Ab initio assisted process modeling for Si-based nanoelectronic devices. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 124-125, 62-71.	1.7	1
113	Theoretical Study of Boron Clustering in Silicon. Journal of Computational Electronics, 2005, 4, 203-219.	1.3	3
114	A new understanding of near-threshold damage for 200 keV irradiation in silicon. Journal of Materials Science, 2005, 40, 3639-3650.	1.7	6
115	Energetics and Kinetics of Defects and Impurities in Silicon from Atomistic Calculations. Solid State Phenomena, 2005, 108-109, 125-132.	0.3	1
116	Ab initio study of the effect of hydrogen and point defects on arsenic segregation at Si(100)â^•SiO2 interfaces. Applied Physics Letters, 2005, 86, 152106.	1.5	10
117	AbÂInitioIdentification of the Nitrogen Diffusion Mechanism in Silicon. Physical Review Letters, 2005, 95, 025901.	2.9	28
118	Simulation and Electron Energy-Loss Spectroscopy of Electron Beam Induced Point Defect Agglomerations in Silicon. Materials Research Society Symposia Proceedings, 2004, 810, 178.	0.1	1
119	Diffusion in silicon and the predictive power of ab-initio calculations. Physica Status Solidi (B): Basic Research, 2004, 241, 2313-2318.	0.7	14
120	Modeling and characterization of atomically sharp â€œperfectâ€•Ge/SiO2 interfaces. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 114-115, 156-161.	1.7	10
121	Investigation of Nanostructured Germanium/Silicon Dioxide Interfaces. Journal of Computational and Theoretical Nanoscience, 2004, 1, 286-295.	0.4	1
122	First-principles study of phosphorus diffusion in silicon: Interstitial- and vacancy-mediated diffusion mechanisms. Applied Physics Letters, 2003, 82, 1839-1841.	1.5	68
123	Investigation of the detailed structure of atomically sharp Ge/SiO/sub 2/ interfaces. , 2003, , .		2
124	Ab-Initio Pseudopotential Calculations of Phosphorus Diffusion in Silicon. Materials Research Society Symposia Proceedings, 2002, 717, 1.	0.1	0
125	Ab initiomodeling and experimental study of Câ€“B interactions in Si. Applied Physics Letters, 2002, 80, 52-54.	1.5	32
126	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. Physica Status Solidi (B): Basic Research, 2002, 233, 24-30.	0.7	21

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127	Ab initio modeling study of boron diffusion in silicon. Computational Materials Science, 2001, 21, 496-504.	1.4	11
128	Predictive process simulation and stress-mediated diffusion in silicon. Computing in Science and Engineering, 2001, 3, 92-95.	1.2	5
129	Ab-Initio Modeling of C-B Interactions In Si. Materials Research Society Symposia Proceedings, 2001, 669, 1.	0.1	0
130	Multiscale Modeling of Stress-Mediated Diffusion in Silicon - Volume Tensors. Materials Research Society Symposia Proceedings, 2001, 677, 941.	0.1	3
131	First-Principles Modeling of Boron Clustering in Silicon. Physica Status Solidi (B): Basic Research, 2001, 226, 37-45.	0.7	18
132	Multiscale modeling of stress-mediated diffusion in silicon: Ab initio to continuum. Applied Physics Letters, 2001, 78, 201-203.	1.5	33
133	Effect of stress on dopant and defect diffusion in Si: A general treatment. Physical Review B, 2001, 64, .	1.1	47
134	Ab initio modeling of boron clustering in silicon. Applied Physics Letters, 2000, 77, 2018-2020.	1.5	89
135	Theoretical study of graphitic analogues of simple semiconductors. Modelling and Simulation in Materials Science and Engineering, 1999, 7, 929-938.	0.8	13
136	First-Principles Study of Boron Diffusion in Silicon. Physical Review Letters, 1999, 83, 4345-4348.	2.9	206
137	Ab-Initio Pseudopotential Calculations of Boron Diffusion in Silicon. Materials Research Society Symposia Proceedings, 1999, 568, 91.	0.1	5
138	First-principles investigation of radiation induced defects in Si and SiC. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 61-65.	0.6	54
139	The application of approximate density functionals to complex systems. International Journal of Quantum Chemistry, 1998, 69, 327-340.	1.0	46
140	Theory of strain and electronic structure ofSi1â^'yCyandSi1â^'xâ^'yGexCyalloys. Physical Review B, 1998, 57, 2431-2442.	1.1	60
141	Firstâ€"Principles Investigation of the Ordered Si 4c compound. Materials Research Society Symposia Proceedings, 1998, 535, 299.	0.1	2
142	First-Principles Study of N Impurities in SiC Polytypes. Materials Research Society Symposia Proceedings, 1998, 510, 181.	0.1	5
143	Theoretical Calculation of the Vibrational modes in Ge₄₆ Clathrate and Related M_xGa_yGe_{46-y} Type Clathrates. Materials Research Society Symposia Proceedings, 1998, 545, 443.	0.1	4
144	Microscopic carbon distribution in Si1â^'yCyalloys: A Raman scattering study. Physical Review B, 1997, 56, 3648-3650.	1.1	18

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145	Photoluminescence in Si1â^'xâ^'yGexCy alloys. Applied Physics Letters, 1997, 70, 2353-2355.	1.5	8
146	Influence of The Local Microstructure on The Macroscopic Properties of Si_{1â€“xâ€“y}Ge_xC_y, Alloys. Materials Research Society Symposia Proceedings, 1997, 469, 443.	0.1	3
147	First-Principles Study of Point-Defect Production in Si and SiC. Materials Research Society Symposia Proceedings, 1997, 490, 41.	0.1	1
148	Carbon dependence of Raman mode frequencies inSi1â^'xâ^'yGexCyalloys. Physical Review B, 1996, 54, 12866-12872.	1.1	44
149	Contribution of quantum and thermal fluctuations to the elastic moduli and dielectric constants of covalent semiconductors. Physical Review B, 1996, 53, 7259-7266.	1.1	36
150	Expanded-volume phases of silicon: Zeolites without oxygen. Physical Review B, 1996, 53, 11288-11291.	1.1	42
151	Second-order Raman spectrum of AlSb fromabinitiophonon calculations and evidence for overbending in the LO phonon branch. Physical Review B, 1996, 54, 8580-8585.	1.1	6
152	Full ab initio calculation of second-order Raman spectra of semiconductors. International Journal of Quantum Chemistry, 1995, 56, 787-790.	1.0	19
153	Ab initio calculation of structural, lattice dynamical, and thermal properties of cubic silicon carbide. International Journal of Quantum Chemistry, 1995, 56, 801-817.	1.0	70
154	Static and dynamical properties of solid chlorine. Physical Review B, 1995, 51, 210-213.	1.1	8
155	Ab initiolattice dynamics and charge fluctuations in alkaline-earth oxides. Physical Review B, 1994, 50, 3746-3753.	1.1	100
156	Second-order Raman spectra of SiC: Experimental and theoretical results fromab initiophonon calculations. Physical Review B, 1994, 49, 8764-8767.	1.1	56
157	Ab initiocalculation of structural and lattice-dynamical properties of silicon carbide. Physical Review B, 1994, 50, 17054-17063.	1.1	213
158	Ab initiolattice dynamics of diamond. Physical Review B, 1993, 48, 3156-3163.	1.1	298
159	Second-order Raman spectra of diamond fromab initiophonon calculations. Physical Review B, 1993, 48, 3164-3170.	1.1	94
160	Multiscale simulation of diffusion, deactivation, and segregation of dopants - ab-initio to continuum. , 0, , .		0
161	Process-Induced Diffusion Phenomena in Advanced CMOS Technologies. Defect and Diffusion Forum, 0, , 510-521.	0.4	1
162	TRIM Modeling of Displacement Damage in SiC for Monoenergetic Neutrons. , 0, , 137-137-8.		0

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163	Freeâ€Energy Parameterization and Thermodynamics in Siâ€Geâ€Sn Alloys. Physica Status Solidi (B): Basic Research, 0, , .	0.7	0