Wolfgang Windl

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/426955/publications.pdf

Version: 2024-02-01

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	Progress, Challenges, and Opportunities in Two-Dimensional Materials Beyond Graphene. ACS Nano, 2013, 7, 2898-2926.	7.3	4,062
2	Cs₂AgBiX₆ (X = Br, Cl): New Visible Light Absorbing, Lead-Free Halide Perovskite Semiconductors. Chemistry of Materials, 2016, 28, 1348-1354.	3.2	1,077
3	Stability and Exfoliation of Germanane: A Germanium Graphane Analogue. ACS Nano, 2013, 7, 4414-4421.	7.3	910
4	Ab initiolattice dynamics of diamond. Physical Review B, 1993, 48, 3156-3163.	1.1	298
5	Ab initiocalculation of structural and lattice-dynamical properties of silicon carbide. Physical Review B, 1994, 50, 17054-17063.	1.1	213
6	First-Principles Study of Boron Diffusion in Silicon. Physical Review Letters, 1999, 83, 4345-4348.	2.9	206
7	Improving the stability and optical properties of germanane via one-step covalent methyl-termination. Nature Communications, 2014, 5, 3389.	5.8	201
8	Lattice stability, elastic constants and macroscopic moduli of NiTi martensites from first principles. Acta Materialia, 2008, 56, 6232-6245.	3.8	200
9	A comparative review of the aqueous corrosion of glasses, crystalline ceramics, and metals. Npj Materials Degradation, 2018, 2, .	2.6	150
10	Raman Spectroscopy, Photocatalytic Degradation, and Stabilization of Atomically Thin Chromium Tri-iodide. Nano Letters, 2018, 18, 4214-4219.	4.5	131
11	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
12	Ab initiolattice dynamics and charge fluctuations in alkaline-earth oxides. Physical Review B, 1994, 50, 3746-3753.	1.1	100
13	Second-order Raman spectra of diamond fromab initiophonon calculations. Physical Review B, 1993, 48, 3164-3170.	1.1	94
14	Atomic-resolution defect contrast in low angle annular dark-field STEM. Ultramicroscopy, 2012, 116, 47-55.	0.8	93
15	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
16	Ab initio modeling of boron clustering in silicon. Applied Physics Letters, 2000, 77, 2018-2020.	1.5	89
17	Structural evolution and kinetics in Cu-Zr metallic liquids from molecular dynamics simulations. Physical Review B, 2013, 88, .	1.1	85
18	Toward Siteâ€Specific Stamping of Graphene. Advanced Materials, 2009, 21, 1243-1246.	11.1	80

#	Article	IF	Citations
19	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
20	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
21	First-principles study of phosphorus diffusion in silicon: Interstitial- and vacancy-mediated diffusion mechanisms. Applied Physics Letters, 2003, 82, 1839-1841.	1.5	68
22	Tunable gaps and enhanced mobilities in strain-engineered silicane. Journal of Applied Physics, 2014, 115, .	1.1	68
23	Oxidation Resistance of Reactive Atoms in Graphene. Nano Letters, 2012, 12, 4651-4655.	4.5	64
24	Elastic anisotropy of Ni4Ti3 from first principles. Scripta Materialia, 2009, 60, 207-210.	2.6	61
25	Theory of strain and electronic structure ofSi1âˆ’yCyandSi1âˆ’xâˆ’yGexCyalloys. Physical Review B, 1998, 57, 2431-2442.	1.1	60
26	A first principles method to simulate electron mobilities in 2D materials. New Journal of Physics, 2014, 16, 105009.	1.2	60
27	Controlling the corrosion resistance of multi-principal element alloys. Scripta Materialia, 2020, 188, 96-101.	2.6	58
28	Second-order Raman spectra of SiC: Experimental and theoretical results fromab initiophonon calculations. Physical Review B, 1994, 49, 8764-8767.	1.1	56
29	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
30	Synthesis of 1T, 2H, and 6R Germanane Polytypes. Chemistry of Materials, 2018, 30, 1335-1343.	3.2	53
31	Recent Advances in Corrosion Science Applicable To Disposal of High-Level Nuclear Waste. Chemical Reviews, 2021, 121, 12327-12383.	23.0	52
32	Full First-Principles Theory of Spin Relaxation in Group-IV Materials. Physical Review Letters, 2012, 109, 166604.	2.9	51
33	Effect of stress on dopant and defect diffusion in Si: A general treatment. Physical Review B, 2001, 64, .	1.1	47
34	The application of approximate density functionals to complex systems. International Journal of Quantum Chemistry, 1998, 69, 327-340.	1.0	46
35	The Fermi surface geometrical origin of axis-dependent conduction polarity in layered materials. Nature Materials, 2019, 18, 568-572.	13.3	46
36	Electrochemical metrics for corrosion resistant alloys. Scientific Data, 2021, 8, 58.	2.4	46

#	Article	IF	Citations
37	Phonon-induced diamagnetic force and its effect on the lattice thermal conductivity. Nature Materials, 2015, 14, 601-606.	13.3	45
38	Carbon dependence of Raman mode frequencies inSi1â^'xâ^'yGexCyalloys. Physical Review B, 1996, 54, 12866-12872.	1.1	44
39	Expanded-volume phases of silicon: Zeolites without oxygen. Physical Review B, 1996, 53, 11288-11291.	1.1	42
40	First principles study of the structure and stability of carbynes. Carbon, 2009, 47, 367-383.	5.4	39
41	NaSn₂As₂: An Exfoliatable Layered van der Waals Zintl Phase. ACS Nano, 2016, 10, 9500-9508.	7.3	39
42	First-Principles Study of Defective and Nonstoichiometric Sr₂FeMoO₆. Chemistry of Materials, 2010, 22, 6092-6102.	3.2	37
43	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
44	Fast free-energy calculations for unstable high-temperature phases. Physical Review B, 2012, 86, .	1.1	35
45	Multiscale modeling of stress-mediated diffusion in silicon: Ab initio to continuum. Applied Physics Letters, 2001, 78, 201-203.	1.5	33
46	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
47	Ab initiomodeling and experimental study of Câ€“B interactions in Si. Applied Physics Letters, 2002, 80, 52-54.	1.5	32
48	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
49	Highly efficient transverse thermoelectric devices with Re₄Si₇ crystals. Energy and Environmental Science, 2021, 14, 4009-4017.	15.6	29
50	AbÂInitioIdentification of the Nitrogen Diffusion Mechanism in Silicon. Physical Review Letters, 2005, 95, 025901.	2.9	28
51	Microstructural evolution during multiaxial deformation of pseudoelastic NiTi studied by first-principles-based micromechanical modeling. Acta Materialia, 2009, 57, 3856-3867.	3.8	28
52	Probing carbonate in bone forming minerals on the nanometre scale. Acta Biomaterialia, 2015, 20, 129-139.	4.1	28
53	Electron-hole pair generation in SiC high-temperature alpha particle detectors. Applied Physics Letters, 2013, 103, .	1.5	27
54	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

#	Article	IF	Citations
55	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
56	Distribution and segregation of arsenic at theSiO2/Si interface. Journal of Applied Physics, 2008, 104, 023518.	1.1	25
57	Multi-Cell Monte Carlo Relaxation method for predicting phase stability of alloys. Scripta Materialia, 2017, 132, 9-12.	2.6	24
58	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
59	Understanding the efficacy of concentrated interstitial carbon in enhancing the pitting corrosion resistance of stainless steel. Acta Materialia, 2021, 221, 117433.	3.8	24
60	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. Physica Status Solidi (B): Basic Research, 2002, 233, 24-30.	0.7	21
61	Bond-order bond energy model for alloys. Acta Materialia, 2019, 179, 406-413.	3.8	21
62	Detailed arsenic concentration profiles at Si/SiO2 interfaces. Journal of Applied Physics, 2008, 104, 043507.	1.1	20
63	Native point defects in binary InP semiconductors. Journal of Materials Science, 2012, 47, 7482-7497.	1.7	20
64	Full ab initio calculation of second-order Raman spectra of semiconductors. International Journal of Quantum Chemistry, 1995, 56, 787-790.	1.0	19
65	Local electronic structure of LiFePO4 nanoparticles in aged Li-ion batteries. Acta Materialia, 2011, 59, 6917-6926.	3.8	19
66	Microscopic carbon distribution in Si1â^'yCyalloys: A Raman scattering study. Physical Review B, 1997, 56, 3648-3650.	1.1	18
67	First-Principles Modeling of Boron Clustering in Silicon. Physica Status Solidi (B): Basic Research, 2001, 226, 37-45.	0.7	18
68	An embedded atom method potential of beryllium. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 085001.	0.8	18
69	Effects of the local structure dependence of evaporation fields on field evaporation behavior. Applied Physics Letters, 2015, 107, .	1.5	18
70	The Chemical Design Principles for Axis-Dependent Conduction Polarity. Journal of the American Chemical Society, 2020, 142, 2812-2822.	6.6	18
71	A general model for thermal and electrical conductivity of binary metallic systems. Acta Materialia, 2017, 126, 272-279.	3.8	17
72	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

#	Article	IF	Citations
73	Layer- and gate-tunable spin-orbit coupling in a high-mobility few-layer semiconductor. Science Advances, 2021, 7, .	4.7	16
74	Structure and chemical analysis of aluminum wear debris: Experiments and ab initio simulations. Acta Materialia, 2007, 55, 6489-6498.	3.8	15
75	Atomic-Scale Engineering of the Electrostatic Landscape of Semiconductor Surfaces. Nano Letters, 2013, 13, 2418-2422.	4.5	15
76	Inâ€Situ Reactor Radiationâ€Induced Attenuation in Sapphire Optical Fibers. Journal of the American Ceramic Society, 2014, 97, 3883-3889.	1.9	15
77	Multi-cell Monte Carlo method for phase prediction. Npj Computational Materials, 2019, 5, .	3.5	15
78	Diffusion in silicon and the predictive power of ab-initio calculations. Physica Status Solidi (B): Basic Research, 2004, 241, 2313-2318.	0.7	14
79	Theoretical study of graphitic analogues of simple semiconductors. Modelling and Simulation in Materials Science and Engineering, 1999, 7, 929-938.	0.8	13
80	Low angle ADF STEM defect imaging. Microscopy and Microanalysis, 2012, 18, 676-677.	0.2	13
81	Fullerene and graphene formation from carbon nanotube fragments. Computational and Theoretical Chemistry, 2012, 987, 115-121.	1.1	13
82	Computationally Guided Discovery of Axis-Dependent Conduction Polarity in NaSnAs Crystals. Chemistry of Materials, 2021, 33, 946-951.	3.2	13
83	Ab initio modeling study of boron diffusion in silicon. Computational Materials Science, 2001, 21, 496-504.	1.4	11
84	Ca₂MnRuO₆: Magnetic Order Arising from Chemical Chaos. Chemistry of Materials, 2012, 24, 2757-2763.	3.2	11
85	Bond Synergy Model for Bond Energies in Alloy Oxides. Journal of the Electrochemical Society, 2020, 167, 141511.	1.3	11
86	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
87	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
88	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
89	Ab-Initio Calculations of the Energetics and Kinetics of Defects and Impurities in Silicon. ECS Transactions, 2006, 3, 171-182.	0.3	9
90	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

#	Article	IF	Citations
91	Self-trapping in B-doped amorphous Si: Intrinsic origin of low acceptor efficiency. Physical Review B, 2010, 81, .	1.1	9
92	Threeâ€dimensional imaging of shear bands in bulk metallic glass composites. Journal of Microscopy, 2016, 264, 304-310.	0.8	9
93	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
94	Static and dynamical properties of solid chlorine. Physical Review B, 1995, 51, 210-213.	1.1	8
95	Photoluminescence in Si1â^'xâ^'yGexCy alloys. Applied Physics Letters, 1997, 70, 2353-2355.	1.5	8
96	Influence of Surface Chemistry on Water Absorption in Functionalized Germanane. Chemistry of Materials, 2020, 32, 1537-1544.	3.2	8
97	Exploring the AgSb1â^'xBixI4 phase diagram: Thermochromism in layered CdCl2-type semiconductors. Journal of Solid State Chemistry, 2021, 297, 121997.	1.4	8
98	First principles calculation of polarization induced interfacial charges in GaN/AlN heterostructures. Applied Physics Letters, 2011, 98, .	1.5	7
99	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
100	Identification of Ge vacancies as electronic defects in methyl- and hydrogen-terminated germanane. Applied Physics Letters, 2018, 113, 061110.	1.5	7
101	Ab-Initio Calculation of Spectral Absorption Coefficients in Molten Fluoride Salts with Metal Impurities. Nuclear Technology, 2018, 204, 59-65.	0.7	7
102	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
103	A new understanding of near-threshold damage for 200 keV irradiation in silicon. Journal of Materials Science, 2005, 40, 3639-3650.	1.7	6
104	Concentration dependence of self-interstitial and boron diffusion in silicon. Applied Physics Letters, 2008, 92, .	1.5	6
105	Atomic-scale characterization of structural and electronic properties of Hf doped Î²-Ga2O3. Applied Physics Letters, 2021, 119, .	1.5	6
106	First-Principles Study of N Impurities in SiC Polytypes. Materials Research Society Symposia Proceedings, 1998, 510, 181.	0.1	5
107	Ab-Initio Pseudopotential Calculations of Boron Diffusion in Silicon. Materials Research Society Symposia Proceedings, 1999, 568, 91.	0.1	5
108	Predictive process simulation and stress-mediated diffusion in silicon. Computing in Science and Engineering, 2001, 3, 92-95.	1.2	5

#	Article	IF	Citations
109	Ferromagnetic Epitaxial Î¼-Fe2O3 on Î²-Ga2O3: A New Monoclinic Form of Fe2O3. Crystal Growth and Design, 2019, 19, 4205-4211.	1.4	5
110	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
111	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
112	Characterization of the Segregation of Arsenic at the Interface SiO₂/Si. Materials Research Society Symposia Proceedings, 2007, 994, 1.	0.1	4
113	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
114	Identification of turbostratic twisting in germanane. Journal of Materials Chemistry C, 2019, 7, 10092-10097.	2.7	4
115	Magnon drag effect in Fe-Co alloys. Journal of Applied Physics, 2019, 126, 125107.	1.1	4
116	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
117	Multiscale Modeling of Stress-Mediated Diffusion in Silicon - Volume Tensors. Materials Research Society Symposia Proceedings, 2001, 677, 941.	0.1	3
118	Theoretical Study of Boron Clustering in Silicon. Journal of Computational Electronics, 2005, 4, 203-219.	1.3	3
119	Synthesis, structural, and electronic properties of Sr_{1â^'x}Ca_xPdAs. Inorganic Chemistry Frontiers, 2020, 7, 2833-2839.	3.0	3
120	Firstâ€“Principles Investigation of the Ordered Si 4c compound. Materials Research Society Symposia Proceedings, 1998, 535, 299.	0.1	2
121	Investigation of the detailed structure of atomically sharp Ge/SiO/sub 2/ interfaces. , 2003, , .		2
122	Process-Induced Diffusion Phenomena in Advanced CMOS Technologies. Defect and Diffusion Forum, 2006, 258-260, 510-521.	0.4	2
123	Characterization of the pile-up of As at the SiO<inf>2</inf>/Si interface. , 2007, , .		2
124	Ab-Initio Modeling of Point Defects, Impurities and Diffusion in Silicon. ECS Transactions, 2008, 16, 89-96.	0.3	2
125	Advanced Extra Functionality CMOS-based Devices. Physica Status Solidi C: Current Topics in Solid State Physics, 2014, 11, 7-8.	0.8	2
126	Direct Observation of Defects in Hexagonal Boron Nitride Monolayers. Microscopy and Microanalysis, 2014, 20, 1738-1739.	0.2	2

#	Article	IF	Citations
127	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
128	Native point defects from stoichiometry-linked chemical potentials in cubic boron arsenide. Journal of Applied Physics, 2021, 129, 075703.	1.1	2
129	Lucky Number 13: A 13-Layer Polytype of the Alkyne Hydrogenation Catalyst CaGaGe. Inorganic Chemistry, 2021, 60, 14530-14534.	1.9	2
130	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
131	First-Principles Study of Point-Defect Production in Si and SiC. Materials Research Society Symposia Proceedings, 1997, 490, 41.	0.1	1
132	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
133	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
134	Energetics and Kinetics of Defects and Impurities in Silicon from Atomistic Calculations. Solid State Phenomena, 2005, 108-109, 125-132.	0.3	1
135	SiC Based Neutron Flux Monitors for Very High Temperature Nuclear Reactors. Materials Research Society Symposia Proceedings, 2006, 929, 1.	0.1	1
136	Characterization and Modeling of Atomically Sharp Perfect Si:Ge/SiO2 Interfaces. ECS Transactions, 2006, 3, 539-549.	0.3	1
137	Multiscale Simulations of The Elastic Properties of Polycrystalline Silicon. AIP Conference Proceedings, 2007, , .	0.3	1
138	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
139	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
140	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
141	Performance analysis and optimization of the RAMPAGE metal alloy potential generation software. , 2017, , .		1
142	Shear Banding in Bulk Metallic Glass Matrix Composites with Dendrite Reinforcements. Structural Integrity, 2019, , 338-340.	0.8	1
143	Atomistic-Simulation Based Modeling of Atom Probe Tomography. Microscopy and Microanalysis, 2019, 25, 284-285.	0.2	1
144	Process-Induced Diffusion Phenomena in Advanced CMOS Technologies. Defect and Diffusion Forum, 0, , 510-521.	0.4	1

#	Article	IF	Citations
145	Investigation of Nanostructured Germanium/Silicon Dioxide Interfaces. Journal of Computational and Theoretical Nanoscience, 2004, 1, 286-295.	0.4	1
146	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
147	Ab-Initio Modeling of C-B Interactions In Si. Materials Research Society Symposia Proceedings, 2001, 669, 1.	0.1	0
148	Multiscale simulation of diffusion, deactivation, and segregation of dopants - ab-initio to continuum. , 0, , .		0
149	Ab-Initio Pseudopotential Calculations of Phosphorus Diffusion in Silicon. Materials Research Society Symposia Proceedings, 2002, 717, 1.	0.1	0
150	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
151	Characterization of the origin of band states in the SiC/SiO₂ interface. , 2007, , .		0
152	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
153	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
154	Concentration-Dependence of Self-Interstitial and Boron Diffusion in Silicon. Materials Research Society Symposia Proceedings, 2008, 1070, 1.	0.1	0
155	First Principles Study of Boron in Amorphous Silicon. Materials Research Society Symposia Proceedings, 2008, 1070, 1.	0.1	0
156	Aberration-Corrected STEM Imaging and Spectroscopy of Single-Layered Materials. Microscopy and Microanalysis, 2011, 17, 1260-1261.	0.2	0
157	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
158	Full â€œAb-Initioâ€•Simulation of Field Evaporation of Samples with Grain Boundaries. Microscopy and Microanalysis, 2020, 26, 2878-2879.	0.2	0
159	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
160	Diffusion and Deactivation of As in Si: Combining Atomistic and Continuum Simulation Approaches. , 2007, , 13-16.		0
161	Ca₂Ga₄Ge₆ and Ca₃Ga₄Ge₆: Synthesis, Structure, and Electronic Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2022, 648, .	0.6	0
162	TRIM Modeling of Displacement Damage in SiC for Monoenergetic Neutrons. , 0, , 137-137-8.		0

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