Joerg Neugebauer

List of Publications by Year
in descending order

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440	37,340	3525 90	3647 180
papers	citations	h-index	g-index

468	468	468	25428
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Defect phases â€“ thermodynamics and impact on material properties. International Materials Reviews, 2022, 67, 89-117.	9.4	17
2	MEAM interatomic potentials of Ni, Re, and Niâ€“ReÂalloys for atomistic fracture simulations. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 015002.	0.8	2
3	Origins of the hydrogen signal in atom probe tomography: case studies of alkali and noble metals. New Journal of Physics, 2022, 24, 013008.	1.2	10
4	Unveiling nonmonotonic chemical trends in the solubility of H in complex Fe-Cr-Mn carbides by means of ab initio based approaches. Physical Review Materials, 2022, 6, .	0.9	1
5	Limitations of empirical supercell extrapolation for calculations of point defects in bulk, at surfaces, and in two-dimensional materials. Physical Review B, 2022, 105, .	1.1	6
6	Workflow Engineering in Materials Design within the BATTERY 2030+ Project. Advanced Energy Materials, 2022, 12, .	10.2	18
7	Ab initio calculation of the magnetic Gibbs free energy of materials using magnetically constrained supercells. Physical Review B, 2022, 105, .	1.1	2
8	Ab initio investigations of point and complex defect structures in B2-FeAl. Physical Review Materials, 2022, 6, .	0.9	3
9	Controlled Doping of Electrocatalysts through Engineering Impurities. Advanced Materials, 2022, 34, e2203030.	11.1	12
10	Approximating the impact of nuclear quantum effects on thermodynamic properties of crystalline solids by temperature remapping. Physical Review B, 2022, 105, .	1.1	2
11	Ab initio study of the structural response to magnetic disorder and van der Waals interactions in FeSe. Physical Review B, 2021, 103, .	1.1	3
12	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. Npj Computational Materials, 2021, 7, .	3.5	17
13	A fully automated approach to calculate the melting temperature of elemental crystals. Computational Materials Science, 2021, 187, 110065.	1.4	18
14	Efficient electronic passivation scheme for computing low-symmetry compound semiconductor surfaces in density-functional theory slab calculations. Physical Review Materials, 2021, 5, .	0.9	0
15	Finite-size correction for slab supercell calculations of materials with spontaneous polarization. Npj Computational Materials, 2021, 7, .	3.5	14
16	A Combined Experimental and First-Principles Based Assessment of Finite-Temperature Thermodynamic Properties of Intermetallic Al3Sc. Materials, 2021, 14, 1837.	1.3	5
17	Dielectric Properties of Nanoconfined Water: A Canonical Thermopotentiostat Approach. Physical Review Letters, 2021, 126, 136803.	2.9	42
18	Impact of Water Coadsorption on the Electrode Potential of H-Pt(1 1 1)-Liquid Water Interfaces. Physical Review Letters, 2021, 126, 166802.	2.9	21

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19	B2 ordering in body-centered-cubic AlNbTiV refractory high-entropy alloys. Physical Review Materials, 2021, 5, .	0.9	14
20	Finite-temperature interplay of structural stability, chemical complexity, and elastic properties of bcc multicomponent alloys from ab initio trained machine-learning potentials. Physical Review Materials, 2021, 5, .	0.9	9
21	Segmentation of Static and Dynamic Atomic-Resolution Microscopy Data Sets with Unsupervised Machine Learning Using Local Symmetry Descriptors. Microscopy and Microanalysis, 2021, , 1-11.	0.2	1
22	Revealing atomic-scale vacancy-solute interaction in nickel. Scripta Materialia, 2021, 203, 114036.	2.6	7
23	Impact of magnetic transition on Mn diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-iron: Correlative state-of-the-art theoretical and experimental study. Physical Review B, 2021, 104, .	1.1	3
24	Atomic scale configuration of planar defects in the Nb-rich C14 Laves phase NbFe2. Acta Materialia, 2020, 183, 362-376.	3.8	29
25	Atomic relaxation around defects in magnetically disordered materials computed by atomic spin constraints within an efficient Lagrange formalism. Physical Review B, 2020, 102, .	1.1	15
26	Anharmonic free energy of lattice vibrations in fcc crystals from a mean-field bond. Physical Review B, 2020, 102, .	1.1	6
27	Segregation-assisted spinodal and transient spinodal phase separation at grain boundaries. Npj Computational Materials, 2020, 6, .	3.5	29
28	Mechanism of collective interstitial ordering in Feâ€“C alloys. Nature Materials, 2020, 19, 849-854.	13.3	32
29	Interplay of Chemistry and Faceting at Grain Boundaries in a Model Al Alloy. Physical Review Letters, 2020, 124, 106102.	2.9	25
30	Phonons in magnetically disordered materials: Magnetic versus phononic time scales. Physical Review B, 2020, 101, .	1.1	8
31	Generalized dipole correction for charged surfaces in the repeated-slab approach. Physical Review B, 2020, 102, .	1.1	20
32	Impact of magnetism on the phase stability of rare-earth based hard magnetic materials. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 68, 101731.	0.7	6
33	AbÂinitio Description of Bond Breaking in Large Electric Fields. Physical Review Letters, 2020, 124, 176801.	2.9	24
34	Performance of the standard exchange-correlation functionals in predicting melting properties fully from first principles: Application to Al and magnetic Ni. Physical Review B, 2020, 101, .	1.1	15
35	Correlation analysis of strongly fluctuating atomic volumes, charges, and stresses in body-centered cubic refractory high-entropy alloys. Physical Review Materials, 2020, 4, .	0.9	17
36	Role of magnetic ordering for the design of quinary TWIP-TRIP high entropy alloys. Physical Review Materials, 2020, 4, .	0.9	18

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37	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	0.9	24
38	Phase diagram of grain boundary facet and line junctions in silicon. Physical Review Materials, 2020, 4, .	0.9	1
39	Titelbild: Discovery of Elusive K₄O₆, a Compound Stabilized by Configurational Entropy of Polarons (Angew. Chem. 1/2019). Angewandte Chemie, 2019, 131, 1-1.	1.6	49
40	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	3.5	79
41	Ab Initiobased method to study structural phase transitions in dynamically unstable crystals, with new insights on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math>to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï‰</mml:mi></mml:math>transformation in Uranium. Physical Review B, 2019, 100, .	1.1	12
42	Deciphering Charge Transfer and Electronic Polarization Effects at Gold Nanocatalysts on Reduced Titania Support. Journal of Physical Chemistry C, 2019, 123, 5495-5506.	1.5	12
43	Invar effects in FeNiCo medium entropy alloys: From an Invar treasure map to alloy design. Intermetallics, 2019, 111, 106520.	1.8	34
44	Impact of lattice relaxations on phase transitions in a high-entropy alloy studied by machine-learning potentials. Npj Computational Materials, 2019, 5, .	3.5	110
45	Role of hole confinement in the recombination properties of InGaN quantum structures. Scientific Reports, 2019, 9, 9047.	1.6	6
46	Elasticity of Phases in Fe-Al-Ti Superalloys: Impact of Atomic Order and Anti-Phase Boundaries. Crystals, 2019, 9, 299.	1.0	11
47	pyiron: An integrated development environment for computational materials science. Computational Materials Science, 2019, 163, 24-36.	1.4	64
48	Thermodynamics of grain boundary segregation, interfacial spinodal and their relevance for nucleation during solid-solid phase transitions. Acta Materialia, 2019, 168, 109-120.	3.8	56
49	The Basics of Electronic Structure Theory for Periodic Systems. Frontiers in Chemistry, 2019, 7, 106.	1.8	57
50	Imaging individual solute atoms at crystalline imperfections in metals. New Journal of Physics, 2019, 21, 123020.	1.2	26
51	Phonon Lifetimes throughout the Brillouin Zone at Elevated Temperatures from Experiment andAbÂInitio. Physical Review Letters, 2019, 123, 235501.	2.9	20
52	Ultrastrong Mediumâ€Entropy Singleâ€Phase Alloys Designed via Severe Lattice Distortion. Advanced Materials, 2019, 31, e1807142.	11.1	301
53	Transferability of interatomic potentials for molybdenum and silicon. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 025007.	0.8	17
54	Discovery of Elusive K₄O₆, a Compound Stabilized by Configurational Entropy of Polarons. Angewandte Chemie, 2019, 131, 155-159.	1.6	2

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55	Discovery of Elusive K₄O₆, a Compound Stabilized by Configurational Entropy of Polarons. Angewandte Chemie - International Edition, 2019, 58, 149-153.	7.2	9
56	Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams. Physical Review Materials, 2019, 3, .	0.9	18
57	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. Physical Review Materials, 2019, 3, .	0.9	30
58	Impact of local electrostatic field rearrangement on field ionization. Journal Physics D: Applied Physics, 2018, 51, 105601.	1.3	20
59	Selective Solvent-Induced Stabilization of Polar Oxide Surfaces in an Electrochemical Environment. Physical Review Letters, 2018, 120, 066101.	2.9	20
60	Calculating free energies of point defects from ab initio. Computational Materials Science, 2018, 148, 249-259.	1.4	47
61	Temperature-dependent phonon spectra of magnetic random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	19
62	Ab initio simulation of hydrogen-induced decohesion in cementite-containing microstructures. Acta Materialia, 2018, 150, 53-58.	3.8	40
63	Advanced data mining in field ion microscopy. Materials Characterization, 2018, 146, 307-318.	1.9	10
64	Impact of Co and Fe Doping on the Martensitic Transformation and the Magnetic Properties in Niâ€Mnâ€Based Heusler Alloys. Physica Status Solidi (B): Basic Research, 2018, 255, 1700455.	0.7	14
65	Atomistic modelling of light-element co-segregation at structural defects in iron. Procedia Structural Integrity, 2018, 13, 1099-1104.	0.3	3
66	A machine learning approach to model solute grain boundary segregation. Npj Computational Materials, 2018, 4, .	3.5	89
67	Origin of the Low Magnetic Moment in Fe2AlTi: An Ab Initio Study. Materials, 2018, 11, 1732.	1.3	19
68	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	1.1	61
69	Anomalous Phonon Lifetime Shortening in Paramagnetic CrN Caused by Spin-Lattice Coupling: A Combined Spin and AbÂInitio Molecular Dynamics Study. Physical Review Letters, 2018, 121, 125902.	2.9	53
70	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. Entropy, 2018, 20, 655.	1.1	69
71	First-principles calculations for charged defects at surfaces, interfaces, and two-dimensional materials in the presence of electric fields. Physical Review B, 2018, 97, .	1.1	71
72	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. Physical Review B, 2018, 97, .	1.1	45

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73	Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries. Physical Review Letters, 2018, 121, 015702.	2.9	65
74	Modeling of Phase Equilibria in Ni-H: Bridging the Atomistic with the Continuum Scale. Metals, 2018, 8, 280.	1.0	4
75	First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion. Physical Review Letters, 2018, 120, 246801.	2.9	71
76	The prognostic relevance of lymph node ratio in patients with oral squamous cell carcinoma treated with neoadjuvant therapy regimen and radical surgery. Journal of Cranio-Maxillo-Facial Surgery, 2018, 46, 1659-1663.	0.7	8
77	Elastically frustrated rehybridization: Origin of chemical order and compositional limits in InGaN quantum wells. Physical Review Materials, 2018, 2, .	0.9	36
78	Tetragonal fcc-Fe induced by Îº -carbide precipitates: Atomic scale insights from correlative electron microscopy, atom probe tomography, and density functional theory. Physical Review Materials, 2018, 2, .	0.9	14
79	Impact of asymmetric martensite and austenite nucleation and growth behavior on the phase stability and hysteresis of freestanding shape-memory nanoparticles. Physical Review Materials, 2018, 2, .	0.9	14
80	Migration mechanisms of a faceted grain boundary. Physical Review Materials, 2018, 2, .	0.9	14
81	Precipitate-induced nonlinearities of diffusion along grain boundaries in Al-based alloys. Physical Review Materials, 2018, 2, .	0.9	13
82	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>{</mml:mo><mml:mn>110</mml:mn><mml:mo>}</mm planar faults in strained bcc metals: Origins and implications of a commonly observed artifact of classical potentials. Physical Review Materials, 2018, 2, .	0.9	17
83	GBÂcode: A grain boundary generation code. Journal of Open Source Software, 2018, 3, 900.	2.0	17
84	Modelling of grain boundary dynamics using amplitude equations. Continuum Mechanics and Thermodynamics, 2017, 29, 895-911.	1.4	8
85	Fermi-level pinning and intrinsic surface states of Al1â^'xInxN(101Â¯) surfaces. Applied Physics Letters, 2017, 110, .	1.5	5
86	Atomistic Modelingâ€Based Design of Novel Materials. Advanced Engineering Materials, 2017, 19, 1600688.	1.6	14
87	Atomic structures of twin boundaries in hexagonal close-packed metallic crystals with particular focus on Mg. Npj Computational Materials, 2017, 3, .	3.5	28
88	Ab initio modelling of solute segregation energies to a general grain boundary. Acta Materialia, 2017, 132, 138-148.	3.8	42
89	Hydrogen behaviour at twist {110} grain boundaries in Î± -Fe. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160402.	1.6	12
90	100 years publicâ€“private partnership in metallurgical and materials science research. Materials Today, 2017, 20, 335-337.	8.3	0

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91	Ab initioexplanation of disorder and off-stoichiometry in Fe-Mn-Al-C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î</mml:mi></mml:math>carbides. Physical Review B, 2017, 95, .	1.1	29
92	Low-temperature features in the heat capacity of unary metals and intermetallics for the example of bulk aluminum and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Al</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:m mathvariant="normal">Sc</mml:mi></mml:math>. Physical Review B, 2017, 95, .	1.1	12
93	Operando Phonon Studies of the Protonation Mechanism in Highly Active Hydrogen Evolution Reaction Pentlandite Catalysts. Journal of the American Chemical Society, 2017, 139, 14360-14363.	6.6	53
94	High Fidelity Reconstruction of Experimental Field Ion Microscopy Data by Atomic Relaxation Simulations. Microscopy and Microanalysis, 2017, 23, 642-643.	0.2	5
95	A rare-earth free magnesium alloy with improved intrinsic ductility. Scientific Reports, 2017, 7, 10458.	1.6	129
96	Accurate electronic free energies of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi mathvariant="italic">d</mml:mi><mml:mo>,</mml:mo><mml:mn>4</mml:mn><mml:mi mathvariant="italic">d</mml:mi></mml:mrow></mml:math> , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>5</mml:mn><mml:mi mathvariant="italic">d</mml:mi></mml:mrow></mml:math> transition metals at high temperatures. Ph	1.1	70
97	Magnetic properties of the CrMnFeCoNi high-entropy alloy. Physical Review B, 2017, 96, .	1.1	124
98	Efficient approach to compute melting properties fully from ab initio with application to Cu. Physical Review B, 2017, 96, .	1.1	53
99	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. Acta Materialia, 2017, 136, 262-270.	3.8	275
100	Adsorption and desorption of hydrogen at nonpolar <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>GaN</mml:mi><mml:mo>(</mml:mo><mml:mn>1</mml:mn><mml: surfaces: Kinetics and impact on surface vibrational and electronic properties. Physical Review B, 2017, 95, .	1.1	15
101	Origin of Structural Modulations in Ultrathin Fe Films on Cu(001). Physical Review Letters, 2017, 118, 236101.	2.9	5
102	Confined chemical and structural states at dislocations in Fe-9wt%Mn steels: A correlative TEM-atom probe study combined with multiscale modelling. Acta Materialia, 2017, 124, 305-315.	3.8	73
103	Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. Acta Materialia, 2017, 123, 90-101.	3.8	161
104	The Role of Î-Carbides as Hydrogen Traps in High-Mn Steels. Metals, 2017, 7, 264.	1.0	27
105	Thermomechanical response of NiTi shape-memory nanoprecipitates in TiV alloys. Physical Review Materials, 2017, 1, .	0.9	23
106	First-principles calculation of the elastic dipole tensor of a point defect: Application to hydrogen inÎ±-zirconium. Physical Review B, 2016, 94, .	1.1	24
107	From electronic structure to phase diagrams: A bottom-up approach to understand the stability of titaniumâ€“transition metal alloys. Acta Materialia, 2016, 113, 311-319.	3.8	58
108	A QM/MM approach for low-symmetry defects in metals. Computational Materials Science, 2016, 118, 259-268.	1.4	14

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109	Changes in volume during the four monthsâ€™ remodelling period of iliac crest grafts in reconstruction of the alveolar ridge. British Journal of Oral and Maxillofacial Surgery, 2016, 54, 751-756.	0.4	17
110	Ab initio-guided design of twinning-induced plasticity steels. MRS Bulletin, 2016, 41, 320-325.	1.7	25
111	Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires. Acta Materialia, 2016, 111, 321-334.	3.8	35
112	Functional adaptation of crustacean exoskeletal elements through structural and compositional diversity: a combined experimental and theoretical study. Bioinspiration and Biomimetics, 2016, 11, 055006.	1.5	35
113	Interplay between interstitial displacement and displacive lattice transformations. Physical Review B, 2016, 94, .	1.1	10
114	The impact of carbon and oxygen in alpha-titanium:ab initiostudy of solution enthalpies and grain boundary segregation. Journal of Physics Condensed Matter, 2016, 28, 385001.	0.7	12
115	Nonlinear elastic effects in phase field crystal and amplitude equations: Comparison toab initiosimulations of bcc metals and graphene. Physical Review B, 2016, 93, .	1.1	18
116	AbÂinitioPrediction of Martensitic and Intermartensitic Phase Boundaries in Ni-Mn-Ga. Physical Review Letters, 2016, 116, 025503.	2.9	57
117	Deformationâ€Induced Martensite: A New Paradigm for Exceptional Steels. Advanced Materials, 2016, 28, 7753-7757.	11.1	61
118	Electron and chemical reservoir corrections for point-defect formation energies. Physical Review B, 2016, 93, .	1.1	50
119	First-principles investigation of hydrogen interaction with TiC precipitates in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-Fe. Physical Review B, 2016, 93, .	1.1	117
120	Impact of local magnetism on stacking fault energies: A first-principles investigation for fcc iron. Physical Review B, 2016, 93, .	1.1	37
121	Strong impact of lattice vibrations on electronic and magnetic properties of paramagnetic Fe revealed by disordered local moments molecular dynamics. Physical Review B, 2016, 93, .	1.1	43
122	Scale bridging description of coherent phase equilibria in the presence of surfaces and interfaces. Physical Review B, 2016, 94, .	1.1	10
123	Atomistic migration mechanisms of atomically flat, stepped, and kinked grain boundaries. Physical Review B, 2016, 94, .	1.1	33
124	Combined atom probe tomography and density functional theory investigation of the Al off-stoichiometry of Îº-carbides in an austenitic Feâ€“Mnâ€“Alâ€“C low density steel. Acta Materialia, 2016, 106, 229-238.	3.8	97
125	Quaternary Al-Cu-Mg-Si Q Phase: Sample Preparation, Heat Capacity Measurement and First-Principles Calculations. Journal of Phase Equilibria and Diffusion, 2016, 37, 119-126.	0.5	12
126	The structure and dynamics of chitin nanofibrils in an aqueous environment revealed by molecular dynamics simulations. RSC Advances, 2016, 6, 30710-30721.	1.7	21

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127	Multiscale modeling of hydrogen enhanced homogeneous dislocation nucleation. Acta Materialia, 2016, 107, 144-151.	3.8	24
128	Impact of magnetic fluctuations on lattice excitations in fcc nickel. Journal of Physics Condensed Matter, 2016, 28, 076002.	0.7	15
129	Ab Initio Determined Phase Diagram of Clean and Solvated Muscovite Mica Surfaces. Langmuir, 2016, 32, 1027-1033.	1.6	9
130	Influence of magnetic excitations on the phase stability of metals and steels. Current Opinion in Solid State and Materials Science, 2016, 20, 77-84.	5.6	31
131	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. Acta Materialia, 2016, 102, 241-250.	3.8	17
132	Importance of coordination number and bond length in titanium revealed by electronic structure investigations. Physica Status Solidi (B): Basic Research, 2015, 252, 1907-1924.	0.7	27
133	Improved method of calculatingab initiohigh-temperature thermodynamic properties with application to ZrC. Physical Review B, 2015, 91, .	1.1	86
134	Role of biaxial strain and microscopic ordering for structural and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">In</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi>Ga</mml:mi><mml:mrow><mml:mn>1</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>. Physical Review B, 2015, 92, .	1.1	6
135	Development and application of a Ni-Ti interatomic potential with high predictive accuracy of the martensitic phase transition. Physical Review B, 2015, 92, .	1.1	187
136	Mechanisms and kinetics of the migration of grain boundaries containing extended defects. Physical Review B, 2015, 92, .	1.1	24
137	Difference in linear polarization of biaxially strained <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">I</mml:mi><mml:msub><mml:mi mathvariant="normal">n</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">G</mml:mi><mml:msub><mml:mi	1.1	3
138	Publisher's Note: From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium [Phys. Rev. B92, 064107 (2015)]. Physical Review B, 2015, 92, .	1.1	0
139	Comparison of Design and Torque Measurements of Various Manual Wrenches. International Journal of Oral and Maxillofacial Implants, 2015, 30, 526-533.	0.6	10
140	Effects of various chair-side surface treatment methods on dental restorative materials with respect to contact angles and surface roughness. Dental Materials Journal, 2015, 34, 796-813.	0.8	41
141	Design and discovery of materials guided by theory and computation. Npj Computational Materials, 2015, 1, .	3.5	33
142	Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases. New Journal of Physics, 2015, 17, 093004.	1.2	15
143	Ab initioâ€based bulk and surface thermodynamics of InGaN alloys: Investigating the effects of strain and surface polarity. Physica Status Solidi (B): Basic Research, 2015, 252, 855-865.	0.7	16
144	Interplay of strain and interdiffusion in Heusler alloy bilayers. Physica Status Solidi - Rapid Research Letters, 2015, 9, 321-325.	1.2	5

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145	Rapid theory-guided prototyping of ductile Mg alloys: from binary to multi-component materials. New Journal of Physics, 2015, 17, 093009.	1.2	35
146	Understanding Anharmonicity in fcc Materials: From its Origin toabÂinitioStrategies beyond the Quasiharmonic Approximation. Physical Review Letters, 2015, 114, 195901.	2.9	115
147	Random phase approximation up to the melting point: Impact of anharmonicity and nonlocal many-body effects on the thermodynamics of Au. Physical Review B, 2015, 91, .	1.1	18
148	Multiscale description of dislocation induced nano-hydrides. Acta Materialia, 2015, 89, 50-59.	3.8	29
149	Identification of bulk oxide defects in an electrochemical environment. Faraday Discussions, 2015, 180, 97-112.	1.6	24
150	A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron. Acta Materialia, 2015, 90, 69-76.	3.8	73
151	From wetting to melting along grain boundaries using phase field and sharp interface methods. Computational Materials Science, 2015, 108, 293-300.	1.4	5
152	Ab initio study of compositional trends in solid solution strengthening in metals with low Peierls stresses. Acta Materialia, 2015, 98, 367-376.	3.8	23
153	From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium. Physical Review B, 2015, 92, .	1.1	26
154	Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one. Acta Materialia, 2015, 100, 90-97.	3.8	389
155	Structural transformations among austenite, ferrite and cementite in Feâ€“C alloys: A unified theory based on ab initio simulations. Acta Materialia, 2015, 99, 281-289.	3.8	59
156	Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation. Acta Materialia, 2015, 85, 53-66.	3.8	47
157	Connecting semiconductor defect chemistry with electrochemistry: Impact of the electrolyte on the formation and concentration of point defects in ZnO. Surface Science, 2015, 631, 190-195.	0.8	9
158	Ordering phenomena and formation of nanostructures in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">In</mml:mi></mml:mrow><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">Ga</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:msub></mml:math>layers coherently grown on GaN(0001). Physical Review B, 2014, 90, .	1.1	20
159	Structural stability and thermodynamics of CrN magnetic phases fromab initiocalculations and experiment. Physical Review B, 2014, 90, .	1.1	95
160	Macroscopic elastic properties of textured ZrN-AlN polycrystalline aggregates: Fromab initiocalculations to grain-scale interactions. Physical Review B, 2014, 90, .	1.1	34
161	Origin of the unusually strong luminescence of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>a</mml:mi></mml:math>-type screw dislocations in GaN. Physical Review B, 2014, 90, .	1.1	19
162	Influence of short-range forces on melting along grain boundaries. Physical Review B, 2014, 89, .	1.1	6

#	Article	IF	Citations
163	Negatively Charged Ions on Mg(0001) Surfaces: Appearance and Origin of Attractive Adsorbate-Adsorbate Interactions. Physical Review Letters, 2014, 113, 136102.	2.9	21
164	Ab initiostudy of H-vacancy interactions in fcc metals: Implications for the formation of superabundant vacancies. Physical Review B, 2014, 89, .	1.1	104
165	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	16.4	1,967
166	Influence of the dislocation core on the glide of the Â½ã€ˆ111ã€‰{110} edge dislocation in bcc-iron: An embedded atom method study. Computational Materials Science, 2014, 87, 274-282.	1.4	16
167	Breakdown of the Arrhenius Law in Describing Vacancy Formation Energies: The Importance of Local Anharmonicity Revealed byAb initioThermodynamics. Physical Review X, 2014, 4, .	2.8	92
168	Ab initio based study of finite-temperature structural, elastic and thermodynamic properties of FeTi. Intermetallics, 2014, 45, 11-17.	1.8	16
169	Extending the Concept of Defect Chemistry from Semiconductor Physics to Electrochemistry. Physical Review Applied, 2014, 1, .	1.5	62
170	Understanding and controlling indium incorporation and surface segregation on In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N surfaces: Anab initioapproach. Physical Review B, 2014, 89, .	1.1	47
171	Scale bridging between atomistic and mesoscale modelling: applications of amplitude equation descriptions. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 034001.	0.8	5
172	Ab initiostudy of point defects in NiTi-based alloys. Physical Review B, 2014, 89, .	1.1	28
173	Separating strain from composition in unit cell parameter maps obtained from aberration corrected high resolution transmission electron microscopy imaging. Journal of Applied Physics, 2014, 115, 033113.	1.1	10
174	Phase-field modeling of grain-boundary premelting using obstacle potentials. Physical Review E, 2014, 90, 012401.	0.8	24
175	Reliability evaluation of thermophysical properties from first-principles calculations. Journal of Physics Condensed Matter, 2014, 26, 335401.	0.7	9
176	A generalized plane-wave formulation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mi mathvariant="bold">k</mml:mi><mml:mo>Â·</mml:mo><mml:mi mathvariant="bold">p</mml:mi></mml:mrow></mml:math> formalism and continuum-elasticity approach to elastic and electronic properties of semiconductor nanostructures. Computational Mate	1.4	31
177	Ab Initio Predicted Impact of Pt on Phase Stabilities in Ni-Mn-Ga Heusler Alloys. Journal of Phase Equilibria and Diffusion, 2014, 35, 695-700.	0.5	11
178	Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment. Physical Review Letters, 2014, 113, 165503.	2.9	93
179	Ab Initio Based Understanding of the Segregation and Diffusion Mechanisms of Hydrogen in Steels. Jom, 2014, 66, 1399-1405.	0.9	64
180	Ductility improvement of Mg alloys by solid solution: Ab initio modeling, synthesis and mechanical properties. Acta Materialia, 2014, 70, 92-104.	3.8	250

#	Article	IF	Citations
181	Perspectives on point defect thermodynamics. Physica Status Solidi (B): Basic Research, 2014, 251, 97-129.	0.7	58
182	Impact of nanodiffusion on the stacking fault energy in high-strength steels. Acta Materialia, 2014, 75, 147-155.	3.8	69
183	Designing Heusler nanoprecipitates by elastic misfit stabilization in Feâ€“Mn maraging steels. Acta Materialia, 2014, 76, 94-105.	3.8	65
184	Role of the mesoscale in migration kinetics of flat grain boundaries. Physical Review B, 2014, 89, .	1.1	41
185	Impact of <scp>M</scp>n on the solution enthalpy of hydrogen in austenitic <scp>F</scp>eâ€<scp>M</scp>n alloys: A firstâ€principles study. Journal of Computational Chemistry, 2014, 35, 2239-2244.	1.5	8
186	Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite. Acta Materialia, 2013, 61, 1773-1784.	3.8	43
187	Polarization effects due to thickness fluctuations in nonpolar InGaN/GaN quantum wells. Applied Physics Letters, 2013, 103, 073115.	1.5	9
188	Hidden surface states at non-polar GaN (101Â¯) facets: Intrinsic pinning of nanowires. Applied Physics Letters, 2013, 103, .	1.5	45
189	Ab initiostudy of thermodynamic, electronic, magnetic, structural, and elastic properties of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>N allotropes. Physical Review B, 2013, 88, .	1.1	19
190	Interplay between Coulomb interaction and quantum-confined Stark-effect in polar and nonpolar wurtzite InN/GaN quantum dots. European Physical Journal B, 2013, 86, 1.	0.6	16
191	Density functional theory in materials science. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 438-448.	6.2	102
192	Ab Initio Based conformational study of the crystalline Î±â€chitin. Biopolymers, 2013, 99, 22-34.	1.2	27
193	Basal and non-basal dislocation slip in Mgâ€“Y. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 576, 61-68.	2.6	206
194	Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals. Journal of the Mechanical Behavior of Biomedical Materials, 2013, 20, 296-304.	1.5	32
195	CHAPTER 9. Multiâ€scale Modelling of a Biological Material: The Arthropod Exoskeleton. RSC Smart Materials, 2013, , 197-218.	0.1	2
196	Dangling-bond defect in a-Si:H: Characterization of network and strain effects by first-principles calculation of the EPR parameters. Physical Review B, 2013, 87, .	1.1	15
197	Ab initioand atomistic study of generalized stacking fault energies in Mg and Mgâ€“Y alloys. New Journal of Physics, 2013, 15, 043020.	1.2	97
198	Thermodynamic modeling of chromium: strong and weak magnetic coupling. Journal of Physics Condensed Matter, 2013, 25, 425401.	0.7	18

#	Article	IF	Citations
199	Band offsets at zincblende-wurtzite GaAs nanowire sidewall surfaces. Applied Physics Letters, 2013, 103, .	1.5	28
200	Ab initioidentified design principles of solid-solution strengthening in Al. Science and Technology of Advanced Materials, 2013, 14, 025001.	2.8	11
201	Blocking Growth by an Electrically Active Subsurface Layer: The Effect of Si as an Antisurfactant in the Growth of GaN. Physical Review Letters, 2013, 110, 036103.	2.9	66
202	GaN(0001) surface states: Experimental and theoretical fingerprints to identify surface reconstructions. Physical Review B, 2013, 88, .	1.1	37
203	Interfacial Structure and Chemistry of GaN on Ge(111). Physical Review Letters, 2013, 111, 256101.	2.9	5
204	Self-consistent Scale-bridging Approach to Compute the Elasticity of Multi-phase Polycrystalline Materials. Materials Research Society Symposia Proceedings, 2013, 1524, 301.	0.1	28
205	Strong dipole coupling in nonpolar nitride quantum dots due to Coulomb effects. Applied Physics Letters, 2012, 100, .	1.5	19
206	Reconstructions and electronic structure of (112Â¯2) and (112Â¯2Â¯) semipolar AlN surfaces. Journal of Applied Physics, 2012, 112, 033510.	1.1	7
207	Solution enthalpy of hydrogen in fourth row elements: Systematic trends derived from first principles. Physical Review B, 2012, 85, .	1.1	13
208	Theory-Guided Materials Design of Multi-Phase Ti-Nb Alloys with Bone-Matching Elastic Properties. Materials, 2012, 5, 1853-1872.	1.3	70
209	Combined ab initio, experimental, and CALPHAD approach for an improved thermodynamic evaluation of the Mgâ€“Si system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2012, 37, 77-86.	0.7	19
210	The dangling-bond defect in amorphous silicon: Statistical random versus kinetically driven defect geometries. Journal of Non-Crystalline Solids, 2012, 358, 2063-2066.	1.5	14
211	Advancing density functional theory to finite temperatures: methods and applications in steel design. Journal of Physics Condensed Matter, 2012, 24, 053202.	0.7	75
212	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. Physical Review B, 2012, 85, .	1.1	157
213	Trends in the elastic response of binary early transition metal nitrides. Physical Review B, 2012, 85, .	1.1	136
214	Ab initioEPR parameters for dangling-bond defect complexes in silicon: Effect of Jahn-Teller distortion. Physical Review B, 2012, 85, .	1.1	14
215	Vacancy formation energies in fcc metals: Influence of exchange-correlation functionals and correction schemes. Physical Review B, 2012, 85, .	1.1	85
216	Ab Initioâ€Based Prediction of Phase Diagrams: Application to Magnetic Shape Memory Alloys. Advanced Engineering Materials, 2012, 14, 547-561.	1.6	37

#	Article	IF	Citations
217	A flexible, plane-wave based multiband $${mathbf{k}cdotmathbf{p}}$$ model. Optical and Quantum Electronics, 2012, 44, 183-188.	1.5	24
218	First-principles study of the thermodynamic and elastic properties of eutectic Feâ€“Ti alloys. Acta Materialia, 2012, 60, 1594-1602.	3.8	36
219	The relation between ductility and stacking fault energies in Mg and Mgâ€“Y alloys. Acta Materialia, 2012, 60, 3011-3021.	3.8	481
220	<scp>CBCT</scp> device dependency on the transfer accuracy from computerâ€aided implantology procedures. Clinical Oral Implants Research, 2012, 23, 1089-1097.	1.9	18
221	Ab initiobased determination of thermodynamic properties of cementite including vibronic, magnetic, and electronic excitations. Physical Review B, 2011, 84, .	1.1	57
222	A flexible, plane-wave-based formulation of continuum elasticity and multiband k·p models. , 2011, , .		1
223	Combined multifrequency EPR and DFT study of dangling bonds in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>a</mml:mi></mml:math>-Si:H. Physical Review B, 2011, 84, .	1.1	31
224	Temperature-driven phase transitions from first principles including all relevant excitations: The fcc-to-bcc transition in Ca. Physical Review B, 2011, 84, .	1.1	52
225	Chitin in the Exoskeletons of Arthropoda: From Ancient Design to Novel Materials Science. Topics in Geobiology, 2011, , 35-60.	0.6	34
226	First-principles study on the interaction of H interstitials with grain boundaries in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>- and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>-Fe. Physical Review B, 2011, 84, .	1.1	211
227	Growth process, characterization, and modeling of electronic properties of coupled InAsSbP nanostructures. Journal of Applied Physics, 2011, 110, 043708.	1.1	14
228	Ab initiostudy of electron paramagnetic resonance hyperfine structure of the silicon dangling bond: Role of the local environment. Physical Review B, 2011, 83, .	1.1	7
229	Designing shape-memory Heusler alloys from first-principles. Applied Physics Letters, 2011, 99, .	1.5	91
230	Anisotropic mechanical behavior of ultrafine eutectic TiFe cast under non-equilibrium conditions. Intermetallics, 2011, 19, 327-335.	1.8	27
231	Prevalence of pathologic findings in the maxillary sinus in cone-beam computerized tomography. Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics, 2011, 111, 634-640.	1.6	106
232	Orientational ordering of interstitial atoms and martensite formation in dilute Fe-based solid solutions. Physical Review B, 2011, 83, .	1.1	36
233	Strain-induced effects on the electronic structure and N K-edge ELNES of wurtzite A1N and AlxGa1â^'xN. Journal of Physics: Conference Series, 2011, 326, 012016.	0.3	1
234	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors. , 2011, , 213-239.		7

#	Article	IF	Citations
235	Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. European Physical Journal Plus, 2011, 126, 1.	1.2	22
236	Electrostatic interactions between charged defects in supercells. Physica Status Solidi (B): Basic Research, 2011, 248, 1067-1076.	0.7	395
237	Formation energies of point defects at finite temperatures. Physica Status Solidi (B): Basic Research, 2011, 248, 1295-1308.	0.7	56
238	Theoretical modeling of growth processes, extended defects, and electronic properties of IIIâ€nitride semiconductor nanostructures. Physica Status Solidi (B): Basic Research, 2011, 248, 1837-1852.	0.7	3
239	Determining the Elasticity of Materials Employing Quantumâ€mechanical Approaches: From the Electronic Ground State to the Limits of Materials Stability. Steel Research International, 2011, 82, 86-100.	1.0	27
240	The object-oriented DFT program library S/PHI/nX. Computer Physics Communications, 2011, 182, 543-554.	3.0	77
241	Hydrogen-enhanced local plasticity at dilute bulk H concentrations: The role of Hâ€“H interactions and the formation of local hydrides. Acta Materialia, 2011, 59, 2969-2980.	3.8	132
242	First-principles investigation of the effect of carbon on the stacking fault energy of Feâ€“C alloys. Acta Materialia, 2011, 59, 3041-3048.	3.8	103
243	In situ scanning tunneling microscopy study of selective dissolution of Au3Cu and Cu3Au (001). Electrochimica Acta, 2011, 56, 1694-1700.	2.6	19
244	Robustness and optimal use of design principles of arthropod exoskeletons studied by ab initio-based multiscale simulations. Journal of the Mechanical Behavior of Biomedical Materials, 2011, 4, 129-145.	1.5	91
245	The influence of additions of Al and Si on the lattice stability of fcc and hcp Feâ€“Mn random alloys. Journal of Physics Condensed Matter, 2011, 23, 246003.	0.7	17
246	Role of spin quantization in determining the thermodynamic properties of magnetic transition metals. Physical Review B, 2011, 83, .	1.1	45
247	Construction and performance of fully numerical optimum atomic basis sets. Physical Review B, 2011, 84, .	1.1	2
248	Quasiparticle band offsets of semiconductor heterojunctions from a generalized marker method. Physical Review B, 2011, 84, .	1.1	12
249	Ab initiostudy of pressure stabilized NiTi allotropes: Pressure-induced transformations and hysteresis loops. Physical Review B, 2011, 84, .	1.1	34
250	A density functional theory based estimation of the anharmonic contributions to the free energy of a polypeptide helix. Journal of Chemical Physics, 2011, 135, 084122.	1.2	1
251	Electronic structure of 1/6ã€202Â¯3ã€‰ partial dislocations in wurtzite GaN. Journal of Applied Physics, 2011, 109, .	1.1	16
252	CAD/CAM-produced surgical guides: Optimizing the treatment workflow. International Journal of Computerized Dentistry, 2011, 14, 93-103.	0.2	5

#	Article	IF	Citations
253	Using Ab Initio Calculations in Designing bcc MgLiâ€“X Alloys for Ultraâ€Lightweight Applications. Advanced Engineering Materials, 2010, 12, 1198-1205.	1.6	20
254	Revealing the Design Principles of Highâ€Performance Biological Composites Using Ab initio and Multiscale Simulations: The Example of Lobster Cuticle. Advanced Materials, 2010, 22, 519-526.	11.1	285
255	Ab Initio Guided Design of bcc Ternary Mgâ€“Liâ€“X (Xâ€‰=â€‰Ca, Al, Si, Zn, Cu) Alloys for Ultraâ€Lightweight Applications. Advanced Engineering Materials, 2010, 12, 572-576.	1.6	21
256	Ab initio study of thermodynamic, structural, and elastic properties of Mg-substituted crystalline calcite. Acta Biomaterialia, 2010, 6, 4506-4512.	4.1	44
257	Plane-wave implementation of the real-space formalism and continuum elasticity theory. Computer Physics Communications, 2010, 181, 765-771.	3.0	28
258	Rescaled Monte Carlo approach for magnetic systems:Ab initiothermodynamics of bcc iron. Physical Review B, 2010, 81, .	1.1	57
259	Ab initiostudy of the solubility and kinetics of hydrogen in austenitic high Mn steels. Physical Review B, 2010, 81, .	1.1	35
260	Native and hydrogen-containing point defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mg</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msu A density functional theory study. Physical Review B, 2010, 81, .	1.1	24
261	Computer-aided manufacturing technologies for guided implant placement. Expert Review of Medical Devices, 2010, 7, 113-129.	1.4	42
262	L21-ordered Feâ€“Alâ€“Ti alloys. Intermetallics, 2010, 18, 1360-1364.	1.8	21
263	Combined ab initio and experimental study of structural and elastic properties of Fe3Al-based ternaries. Intermetallics, 2010, 18, 1310-1315.	1.8	37
264	Ab initio study of the anomalous volume-composition dependence in Feâ€“Al alloys. Intermetallics, 2010, 18, 1316-1321.	1.8	37
265	Thermodynamic properties of cementite (). Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 129-133.	0.7	72
266	Comparison of cone-beam computerized tomography and intraoral radiographs for determination of the periodontal ligament in a variable phantom. Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics, 2010, 109, e95-e101.	1.6	32
267	Salivary calculus diagnosis with 3-dimensional cone-beam computed tomography. Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics, 2010, 110, 94-100.	1.6	37
268	Hydrogen adsorption on polar ZnO(0001)-Zn: Extending equilibrium surface phase diagrams to kinetically stabilized structures. Physical Review B, 2010, 82, .	1.1	58
269	Generation and performance of special quasirandom structures for studying the elastic properties of random alloys: Application to Al-Ti. Physical Review B, 2010, 81, .	1.1	145
270	First-principles study of the thermodynamics of hydrogen-vacancy interaction in fcc iron. Physical Review B, 2010, 82, .	1.1	106

#	Article	IF	Citations
271	Evaluation of maxillary sinus anatomy by cone-beam CT prior to sinus floor elevation. International Journal of Oral and Maxillofacial Implants, 2010, 25, 258-65.	0.6	65
272	Enhancing nitrogen solubility in GaAs and InAs by surface kinetics: Anab initiostudy. Physical Review B, 2009, 79, .	1.1	19
273	Large anisotropic adatom kinetics on nonpolar GaN surfaces: Consequences for surface morphologies and nanowire growth. Physical Review B, 2009, 79, .	1.1	172
274	Temperature Stabilized Surface Reconstructions at Polar ZnO(0001). Physical Review Letters, 2009, 103, 065502.	2.9	118
275	Interplay between long-range elastic and short-range chemical interactions in Fe-C martensite formation. Physical Review B, 2009, 79, .	1.1	45
276	Polarization-induced charge carrier separation in polar and nonpolar grown GaN quantum dots. Journal of Applied Physics, 2009, 106, .	1.1	28
277	Experimental immediate loading of dental implants in conjunction with grafting procedures. Journal of Biomedical Materials Research - Part B Applied Biomaterials, 2009, 91B, 604-612.	1.6	3
278	Periâ€Implant Bone Organization under Immediate Loading Conditions: Collagen Fiber Orientation and Mineral Density Analyses in the Minipig Model. Clinical Implant Dentistry and Related Research, 2009, 11, 41-51.	1.6	22
279	Accuracy of a newly developed integrated system for dental implant planning. Clinical Oral Implants Research, 2009, 20, 1191-1199.	1.9	68
280	Using ab initio calculations in designing bcc Mgâ€“Li alloys for ultra-lightweight applications. Acta Materialia, 2009, 57, 69-76.	3.8	135
281	Atomistic calculations on interfaces: Bridging the length and time scales. European Physical Journal: Special Topics, 2009, 177, 41-57.	1.2	9
282	The influence of body mass index, age, implants, and dental restorations on image quality of cone beam computed tomography. Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics, 2009, 108, e108-e116.	1.6	30
283	Intraoral molluscum contagiosum imitating a squamous-cell carcinoma in an immunocompetent person â€“ case report and review of the literature. International Journal of Oral and Maxillofacial Surgery, 2009, 38, 802-805.	0.7	11
284	Understanding the Phase Transitions of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Ni</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>MnGa</mml:mi></mml:math>Magn Shape Memory System from First Principles. Physical Review Letters, 2009, 102, 035702.	2.9	138
285	FullyAb InitioFinite-Size Corrections for Charged-Defect Supercell Calculations. Physical Review Letters, 2009, 102, 016402.	2.9	1,093
286	Direct minimization technique for metals in density functional theory. Physical Review B, 2009, 79, .	1.1	47
287	Ab initioup to the melting point: Anharmonicity and vacancies in aluminum. Physical Review B, 2009, 79, .	1.1	232
288	Pressure dependence of the Curie temperature in bcc iron studied byab initiosimulations. Physical Review B, 2009, 79, .	1.1	49

#	Article	IF	Citations
289	Comparison of cone-beam imaging with orthopantomography and computerized tomography for assessment in presurgical implant dentistry. International Journal of Oral and Maxillofacial Implants, 2009, 24, 216-25.	0.6	54
290	Exciting prospects for solids: Exactâ€exchange based functionals meet quasiparticle energy calculations. Physica Status Solidi (B): Basic Research, 2008, 245, 929-945.	0.7	83
291	Modern Developments in Multiphysics Materials Simulations. Physica Status Solidi (B): Basic Research, 2008, 245, 2617-2617.	0.7	1
292	A comparison of polycrystalline elastic properties computed by analytic homogenization schemes and FEM. Physica Status Solidi (B): Basic Research, 2008, 245, 2630-2635.	0.7	23
293	Multiscale simulation of polycrystal mechanics of textured Î²â€Ti alloys using ab initio and crystalâ€based finite element methods. Physica Status Solidi (B): Basic Research, 2008, 245, 2642-2648.	0.7	26
294	Error propagation in multiscale approaches to the elasticity of polycrystals. Physica Status Solidi (B): Basic Research, 2008, 245, 2636-2641.	0.7	15
295	A map for phase-change materials. Nature Materials, 2008, 7, 972-977.	13.3	637
296	Solitary Hydatid Cyst in the Mandible: Case Report and Review of the Literature. Journal of Oral and Maxillofacial Surgery, 2008, 66, 1731-1736.	0.5	8
297	Comparison of atomistic and continuum theoretical approaches to determine electronic properties of GaN/AlN quantum dots. Physical Review B, 2008, 78, .	1.1	58
298	Comparison of cone-beam volumetric imaging and combined plain radiographs for localization of the mandibular canal before removal of impacted lower third molars. Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics, 2008, 105, 633-642.	1.6	54
299	Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. Physical Review B, 2008, 77, .	1.1	347
300	First-Principles Free-Energy Analysis of Helix Stability:â€‰ The Origin of the Low Entropy in Ï€ Helices. Journal of Physical Chemistry B, 2008, 112, 4109-4112.	1.2	16
301	Free energy of bcc iron: Integratedab initioderivation of vibrational, electronic, and magnetic contributions. Physical Review B, 2008, 78, .	1.1	188
302	Diagnostic quality of multiplanar reformations obtained with a newly developed cone beam device for maxillofacial imaging. Dentomaxillofacial Radiology, 2008, 37, 1-9.	1.3	26
303	Ab Initio Study of Elastic Properties in Fe3Al-based Alloys. Materials Research Society Symposia Proceedings, 2008, 1128, 20401.	0.1	4
304	Determination of symmetry reduced structures using a soft phonon analysis for magnetic shape memory alloys (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064219.	0.7	2
305	Theory-guided design of Ti-based binaries for human implants (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064221.	0.7	0
306	Compositional Correlation and Anticorrelation in Quaternary Alloys: Competition Between Bulk Thermodynamics and Surface Kinetics. Physical Review Letters, 2007, 99, 206103.	2.9	16

#	Article	IF	Citations
307	Geometric accuracy of a newly developed cone-beam device for maxillofacial imaging. Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics, 2007, 104, 551-559.	1.6	158
308	Intraoperative navigation in the maxillofacial area based on 3D imaging obtained by a cone-beam device. International Journal of Oral and Maxillofacial Surgery, 2007, 36, 687-694.	0.7	49
309	Ab initiostudy of the thermodynamic properties of nonmagnetic elementary fcc metals: Exchange-correlation-related error bars and chemical trends. Physical Review B, 2007, 76, .	1.1	218
310	Theory-guided bottom-up design of Î²-titanium alloys as biomaterials based on first principles calculations: Theory and experiments. Acta Materialia, 2007, 55, 4475-4487.	3.8	220
311	HYDROGEN IN SEMICONDUCTORS. Annual Review of Materials Research, 2006, 36, 179-198.	4.3	150
312	Understanding Si adsorption on GaN(0001) surfaces using first-principles calculations. Physical Review B, 2006, 73, .	1.1	43
313	Band gap and band parameters of InN and GaN from quasiparticle energy calculations based on exact-exchange density-functional theory. Applied Physics Letters, 2006, 89, 161919.	1.5	145
314	Peri-Implant Bone Organization Under Immediate Loading State. Circularly Polarized Light Analyses: A Minipig Study. Journal of Periodontology, 2006, 77, 152-160.	1.7	61
315	Lateral femoral cutaneous nerve and iliac crest bone graftsâ€"anatomical and clinical considerations. International Journal of Oral and Maxillofacial Surgery, 2006, 35, 366-372.	0.7	59
316	CVD Growth of Group-III Nitride Semiconductors: An ab Initio Based Multiscale Study. ECS Meeting Abstracts, 2006, , .	0.0	0
317	Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. Physical Review B, 2006, 74, .	1.1	89
318	Surface Structure and Adatom Kinetics of Group-III Nitrides. , 2006, , 295-318.		1
319	Generalized Wannier functions: An efficient way to constructab-initio tight-binding parameters for group-III nitrides. Physica Status Solidi (B): Basic Research, 2006, 243, 1583-1587.	0.7	7
320	Polarity inversion of GaN(0001) surfaces induced by Si adsorption. Surface Science, 2006, 600, 335-339.	0.8	11
321	First-principles calculations of the structural and electronic properties of cleanGaN(0001)surfaces. Physical Review B, 2006, 73, .	1.1	107
322	Energy-dependent contrast in atomic-scale spin-polarized scanning tunneling microscopy ofMn3N2(010): Experiment and first-principles theory. Physical Review B, 2006, 74, .	1.1	38
323	Bulk Electronic Structure of Metals Resolved with Scanning Tunneling Microscopy. Physical Review Letters, 2006, 96, 046801.	2.9	15
324	Comparison of static and dynamic computer-assisted guidance methods in implantology. International Journal of Computerized Dentistry, 2006, 9, 23-35.	0.2	48

#	Article	IF	Citations
325	Exact-exchange calculations of the electronic structure of AlN, GaN and InN. Computer Physics Communications, 2005, 169, 28-31.	3.0	19
326	A case of chronic calcium pyrophosphate dihydrate crystal disease (tophaceous pseudogout) in the temporomandibular joint. Oral Diseases, 2005, 11, 113-115.	1.5	21
327	Quantitative evaluation of the fibrin clot extension on different implant surfaces: Anin vitro study. Journal of Biomedical Materials Research - Part B Applied Biomaterials, 2005, 74B, 636-642.	1.6	50
328	Recent advances in atomic-scale spin-polarized scanning tunneling microscopy. Microscopy Research and Technique, 2005, 66, 72-84.	1.2	7
329	Metal-adlayer-stabilized ZnO(0001) surfaces: Toward a new growth mode for oxides. Applied Physics Letters, 2005, 87, 141914.	1.5	20
330	Role of semicore states in the electronic structure of group-III nitrides: An exact-exchange study. Physical Review B, 2005, 72, .	1.1	39
331	Chemically orderedAlxGa1â^'xNalloys:â€ƒSpontaneous formation of natural quantum wells. Physical Review B, 2005, 71, .	1.1	53
332	Phonon spectra and thermodynamic properties of the infinite polyalanineÎ±helix: A density-functional-theory-based harmonic vibrational analysis. Physical Review E, 2005, 71, 031911.	0.8	13
333	Structural Transitions in the Polyalanine Î±-Helix under Uniaxial Strain. Journal of the American Chemical Society, 2005, 127, 17241-17244.	6.6	23
334	CombiningGWcalculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. New Journal of Physics, 2005, 7, 126-126.	1.2	263
335	On the Accuracy of DFT for Describing Hydrogen Bonds:â€‰ Dependence on the Bond Directionality. Journal of Physical Chemistry A, 2004, 108, 5692-5698.	1.1	354
336	Aspects of spin-polarized scanning tunneling microscopy at the atomic scale: experiment, theory, and simulation. Surface Science, 2004, 561, 154-170.	0.8	19
337	First-principles calculations for defects and impurities: Applications to III-nitrides. Journal of Applied Physics, 2004, 95, 3851-3879.	1.1	2,695
338	Strong affinity of hydrogen for the GaN(000-1) surface: Implications for molecular beam epitaxy and metalorganic chemical vapor deposition. Applied Physics Letters, 2004, 85, 3429-3431.	1.5	81
339	Strain Induced Deep Electronic States around Threading Dislocations in GaN. Physical Review Letters, 2004, 93, 196401.	2.9	107
340	Growth and Proliferation of Human Osteoblasts on Different Bone Graft Substitutes An In Vitro Study. Implant Dentistry, 2004, 13, 171-179.	1.7	76
341	COMPARISON OF DIFFERENT REGISTRATION METHODS FOR NAVIGATION IN CRANIO-MAXILLOFACIAL SURGERY. , 2004, , .		0
342	Bone contact, growth, and density around immediately loaded implants in the mandible of mini pigs. Clinical Oral Implants Research, 2003, 14, 312-321.	1.9	114

#	Article	IF	Citations
343	Surfactants and antisurfactants on group-III-nitride surfaces. Physica Status Solidi C: Current Topics in Solid State Physics, 2003, 0, 1651-1667.	0.8	51
344	Universal alignment of hydrogen levels in semiconductors, insulators and solutions. Nature, 2003, 423, 626-628.	13.7	1,111
345	Structure and energetics of nitride surfaces under MOCVD growth conditions. Journal of Crystal Growth, 2003, 248, 8-13.	0.7	39
346	Gallium adsorption on (0001) GaN surfaces. Physical Review B, 2003, 67, .	1.1	131
347	Reconstructions of the AlN(0001) surface. Physical Review B, 2003, 68, .	1.1	70
348	Density Functional Theory Study of the Cooperativity of Hydrogen Bonds in Finite and Infinite Î±-Helices. Journal of Physical Chemistry B, 2003, 107, 1432-1437.	1.2	100
349	Adatom Kinetics On and Below the Surface: The Existence of a New Diffusion Channel. Physical Review Letters, 2003, 90, 056101.	2.9	293
350	Growth and Surface Reconstructions of AlN(0001) Films. Materials Research Society Symposia Proceedings, 2003, 798, 383.	0.1	0
351	Morphology and surface reconstructions of GaN(11Ì„00) surfaces. Applied Physics Letters, 2003, 82, 1793-1795.	1.5	35
352	Al(111)-(3Ã—3)R30:On-top versus substitutional adsorption for Rb and K. Physical Review B, 2003, 68, .	1.1	3
353	Adatom density kinetic Monte Carlo: A hybrid approach to perform epitaxial growth simulations. Physical Review B, 2003, 68, .	1.1	30
354	Cohesive properties of group-III nitrides: A comparative study of all-electron and pseudopotential calculations using the generalized gradient approximation. Physical Review B, 2002, 65, .	1.1	126
355	Role of hydrogen in surface reconstructions and growth of GaN. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2002, 20, 1640.	1.6	31
356	Phase Transitions on Gan Surfaces. Materials Research Society Symposia Proceedings, 2002, 743, L3.9.1.	0.1	1
357	Morphology and surface reconstructions of m-plane GaN. Materials Research Society Symposia Proceedings, 2002, 743, L4.1.1.	0.1	2
358	Review of Structure of Bare and Adsorbate-Covered GaN(0001) Surfaces. MRS Internet Journal of Nitride Semiconductor Research, 2002, 7, 1.	1.0	62
359	First-Principles Surface Phase Diagram for Hydrogen on GaN Surfaces. Physical Review Letters, 2002, 88, 066103.	2.9	229
360	Adsorption and incorporation of silicon at GaN(0001) surfaces. Applied Physics Letters, 2002, 80, 2008-2010.	1.5	57

#	Article	IF	Citations
361	Indium incorporation and surface segregation during InGaN growth by molecular beam epitaxy: experiment and theory. MRS Internet Journal of Nitride Semiconductor Research, 2001, 6, 1.	1.0	46
362	Ab initio Analysis of Surface Structure and Adatom Kinetics of Group-III Nitrides. Physica Status Solidi (B): Basic Research, 2001, 227, 93-114.	0.7	49
363	Silicon on GaN(0001) and (0001Ì„) surfaces. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2001, 19, 1619.	1.6	8
364	First-principles studies of beryllium doping of GaN. Physical Review B, 2001, 63, .	1.1	133
365	Identification of surface anion antisite defects in (110) surfaces of IIIâ€“V semiconductors. Applied Physics Letters, 2001, 79, 2877-2879.	1.5	20
366	Limits and accuracy of valence force field models forInxGa1â^'xNalloys. Physical Review B, 2001, 63, .	1.1	50
367	Controlling the conductivity of wide-band-gap semiconductors. Springer Proceedings in Physics, 2001, , 3-8.	0.1	0
368	Stability, diffusion, and complex formation of beryllium in wurtzite GaN. Materials Research Society Symposia Proceedings, 2000, 639, 431.	0.1	1
369	Theory of surfaces and interfaces of group III-nitrides. Applied Surface Science, 2000, 159-160, 355-359.	3.1	30
370	SURFACE MORPHOLOGY OF GaN SURFACES DURING MOLECULAR BEAM EPITAXY. Surface Review and Letters, 2000, 07, 601-606.	0.5	17
371	Surface structures and growth kinetics of InGaN(0001) grown by molecular beam epitaxy. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2000, 18, 2284.	1.6	72
372	Symmetric Versus Nonsymmetric Structure of the Phosphorus Vacancy on InP(110). Physical Review Letters, 2000, 84, 5816-5819.	2.9	44
373	Structure of GaN(0001):â€ƒThe laterally contracted Ga bilayer model. Physical Review B, 2000, 61, 9932-9935.	1.1	322
374	Spontaneous Formation of Indium-Rich Nanostructures on InGaN(0001) Surfaces. Physical Review Letters, 2000, 85, 1902-1905.	2.9	95
375	Arsenic impurities in GaN. Applied Physics Letters, 2000, 76, 1009-1011.	1.5	59
376	Indium incorporation and surface segregation during InGaN growth by molecular beam epitaxy. Materials Research Society Symposia Proceedings, 2000, 639, 261.	0.1	0
377	Guided bone regeneration with titanium membranes: a clinical study. British Journal of Oral and Maxillofacial Surgery, 2000, 38, 312-315.	0.4	96
378	Doping of AlGaN Alloys. MRS Internet Journal of Nitride Semiconductor Research, 1999, 4, 890-901.	1.0	29

#	Article	IF	Citations
379	Theory of Hydrogen in GaN. Semiconductors and Semimetals, 1999, , 479-502.	0.4	18
380	Indium-induced changes in GaN(0001) surface morphology. Physical Review B, 1999, 60, R8473-R8476.	1.1	148
381	Surface energetics, pit formation, and chemical ordering in InGaN alloys. Applied Physics Letters, 1999, 74, 2319-2321.	1.5	226
382	Doping of AlxGa1â^'xN alloys. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 59, 253-257.	1.7	37
383	The adsorption of oxygen at GaN surfaces. Applied Physics Letters, 1999, 74, 1695-1697.	1.5	219
384	GaN(0001) surface structures studied using scanning tunneling microscopy and first-principles total energy calculations. Surface Science, 1999, 423, 70-84.	0.8	118
385	Chemical trends for acceptor impurities in GaN. Journal of Applied Physics, 1999, 85, 3003-3005.	1.1	95
386	Modeling of Structural and Elastic Properties of InxGa1â€“xN Alloys. Materials Research Society Symposia Proceedings, 1999, 584, 215.	0.1	1
387	Defects and Defect Reactions in Semiconductor Nitrides. Acta Physica Polonica A, 1999, 96, 613-627.	0.2	25
388	Bone condensing in the placement of endosteal palatal implants: a case report. International Journal of Oral and Maxillofacial Implants, 1999, 14, 849-52.	0.6	13
389	Scanning tunneling microscopy of the GaN(000 $ar{1}$]]) surface. Applied Physics A: Materials Science and Processing, 1998, 66, S947-S951.	1.1	30
390	Theory of doping and defects in IIIâ€“V nitrides. Journal of Crystal Growth, 1998, 189-190, 505-510.	0.7	202
391	Adatom diffusion at GaN (0001) and (000Ì„) surfaces. Applied Physics Letters, 1998, 73, 487-489.	1.5	436
392	Reconstructions of GaN(0001) and (000Ì„) surfaces: Ga-rich metallic structures. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1998, 16, 2242.	1.6	228
393	Determination of wurtzite GaN lattice polarity based on surface reconstruction. Applied Physics Letters, 1998, 72, 2114-2116.	1.5	305
394	Electronic and structural properties of vacancies on and below the GaP(110) surface. Physical Review B, 1998, 58, 1392-1400.	1.1	43
395	Wurtzite GaN surface structures studied by scanning tunneling microscopy and reflection high energy electron diffraction. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1998, 16, 1641-1645.	0.9	91
396	Possibility of a Mott-Hubbard ground state for the SiC(0001) surface. Physical Review B, 1998, 57, R4230-R4232.	1.1	75

#	Article	IF	Citations
397	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. Physical Review Letters, 1998, 80, 3097-3100.	2.9	99
398	Doping of Aigan Alloys. Materials Research Society Symposia Proceedings, 1998, 537, 1.	0.1	5
399	Surface Structures, Surfactants and Diffusion at Cubic and Wurtzite GaN. MRS Internet Journal of Nitride Semiconductor Research, 1998, 3, 1.	1.0	38
400	Energetics of H andNH2on GaN(101Â¯0) and implications for the origin of nanopipe defects. Physical Review B, 1997, 56, R4325-R4328.	1.1	93
401	Defects and Doping in III-V Nitrides. Materials Science Forum, 1997, 258-263, 19-26.	0.3	8
402	Scanning tunneling microscopy observation of surface reconstruction of GaN on sapphire and 6H-SiC. Materials Research Society Symposia Proceedings, 1997, 482, 428.	0.1	1
403	Atomic structure and stability of AlN(0001) and (000Ì±1) surfaces. Physical Review B, 1997, 55, 13878-13883.	1.1	127
404	Small valence-band offsets at GaN/InGaN heterojunctions. Applied Physics Letters, 1997, 70, 2577-2579.	1.5	134
405	Reconstructions of theGaN(0001Â¯)Surface. Physical Review Letters, 1997, 79, 3934-3937.	2.9	331
406	Density-functional theory calculations for poly-atomic systems: electronic structure, static and elastic properties and ab initio molecular dynamics. Computer Physics Communications, 1997, 107, 187-222.	3.0	660
407	Role of hydrogen in doping of GaN. Applied Physics Letters, 1996, 68, 1829-1831.	1.5	304
408	Gallium vacancies and the yellow luminescence in GaN. Applied Physics Letters, 1996, 69, 503-505.	1.5	1,063
409	Role Of Hydrogen And Hydrogen Complexes In Doping Of Gan. Materials Research Society Symposia Proceedings, 1996, 423, 619.	0.1	11
410	Theory ofGaN(101Â¯0)and (112Â¯0) surfaces. Physical Review B, 1996, 53, R10477-R10480.	1.1	324
411	Theory of Point Defects and Interfaces. Materials Research Society Symposia Proceedings, 1996, 449, 861.	0.1	20
412	Energetics of AlN Epitaxial Wetting Layers on SiC (0001). Materials Research Society Symposia Proceedings, 1996, 449, 899.	0.1	1
413	Native defects and impurities in GaN. FestkÃ¶rperprobleme, 1996, , 25-44.	0.7	47
414	Inversion Domain and Stacking Mismatch Boundaries in GaN. Physical Review Letters, 1996, 77, 103-106.	2.9	244

#	Article	IF	Citations
415	Energetics of AlN thin films and the implications for epitaxial growth on SiC. Physical Review B, 1996, 54, R17351-R17354.	1.1	23
416	Phase Stability and Electronic Structure of GaAs_{1â€“x}N_x Alloys. Materials Research Society Symposia Proceedings, 1995, 379, 3.	0.1	3
417	Tight-Binding Initialization for Generating High-Quality Initial Wave Functions: Application to Defects and Impurities in GaN. Materials Research Society Symposia Proceedings, 1995, 408, 43.	0.1	5
418	Theory of Defects in Wide-Band-Gap Semiconductors. Materials Research Society Symposia Proceedings, 1995, 378, 467.	0.1	2
419	Theory of Point Defects and Complexes in GaN. Materials Research Society Symposia Proceedings, 1995, 395, 645.	0.1	64
420	Theory of the adatom-induced reconstruction of the SiC(0001)â^š3Ã—â^š3 surface. Physical Review B, 1995, 52, R17001-R17004.	1.1	159
421	Hydrogen interactions with self-interstitials in silicon. Physical Review B, 1995, 52, R14320-R14323.	1.1	39
422	Electronic structure and phase stability ofGaAs1â^'xNxalloys. Physical Review B, 1995, 51, 10568-10571.	1.1	273
423	Hydrogen in GaN: Novel Aspects of a Common Impurity. Physical Review Letters, 1995, 75, 4452-4455.	2.9	421
424	Chemical trends and bonding mechanisms for isloated adsorbates on Al(111). Physical Review B, 1994, 49, 17242-17252.	1.1	75
425	Atomic and electronic structure of the GaAs/ZnSe(001) interface. Physical Review B, 1994, 50, 8616-8628.	1.1	84
426	Alkali-metal adsorbates on Aluminum (111): The interplay and competition of adsorbates-substrate and adsorbate-adsorbate interactions. Progress in Surface Science, 1994, 46, 295-304.	3.8	5
427	Alkali-metal adsorption on Al(111) and Al(100). Surface Science, 1994, 307-309, 8-15.	0.8	62
428	Atomic geometry and electronic structure of native defects in GaN. Physical Review B, 1994, 50, 8067-8070.	1.1	736
429	Electronic structure of R30Â°-Na and -K on Al(111): Comparison of â€œnormalâ€•and substitutional adsorption sites. Surface Science, 1993, 287-288, 559-563.	0.8	17
430	Theory of adsorption and desorption in high electric fields. Surface Science, 1993, 287-288, 572-576.	0.8	44
431	A step from surface fiction towards surface science. Journal of Physics Condensed Matter, 1993, 5, A91-A94.	0.7	9
432	Mechanisms of island formation of alkali-metal adsorbates on Al(111). Physical Review Letters, 1993, 71, 577-580.	2.9	129

#	Article	IF	Citations
433	Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). Physical Review B, 1992, 46, 16067-16080.	1.1	2,339
434	Self-consistent tight-binding total energy calculations: Application to GaAs/Si and ZnSe/GaAs (100) interfaces. Superlattices and Microstructures, 1992, 11, 393-398.	1.4	3
435	Atomic structure of (100) ZnSe/GaAs interfaces. Superlattices and Microstructures, 1992, 12, 225-230.	1.4	1
436	Unusual chemisorption geometry of Na on Al(111). Physical Review Letters, 1991, 67, 2163-2166.	2.9	191
437	Tight-binding calculations of total energies of macroscopic polar electron-core systems: Application to IIâ€“VI compounds. Journal of Crystal Growth, 1990, 101, 332-336.	0.7	3
438	Diamagnetic Shift of Bielectrons in BiI3. Physica Status Solidi (B): Basic Research, 1988, 145, 579-584.	0.7	2
439	The Relation between Shear Banding, Microstructure and Mechanical Properties in Mg and Mg-Y Alloys. Materials Science Forum, 0, 690, 202-205.	0.3	17
440	Quantum-Mechanical Study of Single-Crystalline and Polycrystalline Elastic Properties of Mg-Substituted Calcite Crystals. Key Engineering Materials, 0, 592-593, 335-341.	0.4	2