Joerg Neugebauer

List of Publications by Year
in descending order

440 papers	37,340 citations	3515 90 h-index	3638 180 g-index
468 all docs	468 docs citations	468 times ranked	25428 citing authors

#	Article	IF	Citations
1	First-principles calculations for defects and impurities: Applications to III-nitrides. Journal of Applied Physics, 2004, 95, 3851-3879.	1.1	2,695
2	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
3	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	16.4	1,967
4	Universal alignment of hydrogen levels in semiconductors, insulators and solutions. Nature, 2003, 423, 626-628.	13.7	1,111
5	FullyAb InitioFinite-Size Corrections for Charged-Defect Supercell Calculations. Physical Review Letters, 2009, 102, 016402.	2.9	1,093
6	Gallium vacancies and the yellow luminescence in GaN. Applied Physics Letters, 1996, 69, 503-505.	1.5	1,063
7	Atomic geometry and electronic structure of native defects in GaN. Physical Review B, 1994, 50, 8067-8070.	1.1	736
8	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
9	A map for phase-change materials. Nature Materials, 2008, 7, 972-977.	13.3	637
10	The relation between ductility and stacking fault energies in Mg and Mgâ€“Y alloys. Acta Materialia, 2012, 60, 3011-3021.	3.8	481
11	Adatom diffusion at GaN (0001) and (000Ì„1Ì„) surfaces. Applied Physics Letters, 1998, 73, 487-489.	1.5	436
12	Hydrogen in GaN: Novel Aspects of a Common Impurity. Physical Review Letters, 1995, 75, 4452-4455.	2.9	421
13	Electrostatic interactions between charged defects in supercells. Physica Status Solidi (B): Basic Research, 2011, 248, 1067-1076.	0.7	395
14	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
15	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
16	Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. Physical Review B, 2008, 77, .	1.1	347
17	Reconstructions of theGaN(0001Â¯)Surface. Physical Review Letters, 1997, 79, 3934-3937.	2.9	331
18	Theory ofGaN(101Â¯0)and (112Â¯0) surfaces. Physical Review B, 1996, 53, R10477-R10480.	1.1	324

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19	Structure of GaN(0001):â€ƒThe laterally contracted Ga bilayer model. Physical Review B, 2000, 61, 9932-9935.	1.1	322
20	Determination of wurtzite GaN lattice polarity based on surface reconstruction. Applied Physics Letters, 1998, 72, 2114-2116.	1.5	305
21	Role of hydrogen in doping of GaN. Applied Physics Letters, 1996, 68, 1829-1831.	1.5	304
22	Ultrastrong Mediumâ€Entropy Singleâ€Phase Alloys Designed via Severe Lattice Distortion. Advanced Materials, 2019, 31, e1807142.	11.1	301
23	Adatom Kinetics On and Below the Surface: The Existence of a New Diffusion Channel. Physical Review Letters, 2003, 90, 056101.	2.9	293
24	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
25	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. Acta Materialia, 2017, 136, 262-270.	3.8	275
26	Electronic structure and phase stability ofGaAs1â^'xNxalloys. Physical Review B, 1995, 51, 10568-10571.	1.1	273
27	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
28	Ductility improvement of Mg alloys by solid solution: Ab initio modeling, synthesis and mechanical properties. Acta Materialia, 2014, 70, 92-104.	3.8	250
29	Inversion Domain and Stacking Mismatch Boundaries in GaN. Physical Review Letters, 1996, 77, 103-106.	2.9	244
30	Ab initioup to the melting point: Anharmonicity and vacancies in aluminum. Physical Review B, 2009, 79, .	1.1	232
31	First-Principles Surface Phase Diagram for Hydrogen on GaN Surfaces. Physical Review Letters, 2002, 88, 066103.	2.9	229
32	Reconstructions of GaN(0001) and (0001Ì„) 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
33	Surface energetics, pit formation, and chemical ordering in InGaN alloys. Applied Physics Letters, 1999, 74, 2319-2321.	1.5	226
34	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
35	The adsorption of oxygen at GaN surfaces. Applied Physics Letters, 1999, 74, 1695-1697.	1.5	219
36	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

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37	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
38	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
39	Theory of doping and defects in IIIâ€“V nitrides. Journal of Crystal Growth, 1998, 189-190, 505-510.	0.7	202
40	Unusual chemisorption geometry of Na on Al(111). Physical Review Letters, 1991, 67, 2163-2166.	2.9	191
41	Free energy of bcc iron: Integratedab initioderivation of vibrational, electronic, and magnetic contributions. Physical Review B, 2008, 78, .	1.1	188
42	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
43	Large anisotropic adatom kinetics on nonpolar GaN surfaces: Consequences for surface morphologies and nanowire growth. Physical Review B, 2009, 79, .	1.1	172
44	Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. Acta Materialia, 2017, 123, 90-101.	3.8	161
45	Theory of the adatom-induced reconstruction of the SiC(0001)âˆš3Ã—âˆš3 surface. Physical Review B, 1995, 52, R17001-R17004.	1.1	159
46	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
47	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. Physical Review B, 2012, 85, .	1.1	157
48	HYDROGEN IN SEMICONDUCTORS. Annual Review of Materials Research, 2006, 36, 179-198.	4.3	150
49	Indium-induced changes in GaN(0001) surface morphology. Physical Review B, 1999, 60, R8473-R8476.	1.1	148
50	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
51	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
52	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
53	Trends in the elastic response of binary early transition metal nitrides. Physical Review B, 2012, 85, .	1.1	136
54	Using ab initio calculations in designing bcc Mgâ€“Li alloys for ultra-lightweight applications. Acta Materialia, 2009, 57, 69-76.	3.8	135

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55	Small valence-band offsets at GaN/InGaN heterojunctions. Applied Physics Letters, 1997, 70, 2577-2579.	1.5	134
56	First-principles studies of beryllium doping of GaN. Physical Review B, 2001, 63, .	1.1	133
57	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
58	Gallium adsorption on (0001) GaN surfaces. Physical Review B, 2003, 67, .	1.1	131
59	Mechanisms of island formation of alkali-metal adsorbates on Al(111). Physical Review Letters, 1993, 71, 577-580.	2.9	129
60	A rare-earth free magnesium alloy with improved intrinsic ductility. Scientific Reports, 2017, 7, 10458.	1.6	129
61	Atomic structure and stability of AlN(0001) and (000Ì±1) surfaces. Physical Review B, 1997, 55, 13878-13883.	1.1	127
62	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
63	Magnetic properties of the CrMnFeCoNi high-entropy alloy. Physical Review B, 2017, 96, .	1.1	124
64	GaN(0001) surface structures studied using scanning tunneling microscopy and first-principles total energy calculations. Surface Science, 1999, 423, 70-84.	0.8	118
65	Temperature Stabilized Surface Reconstructions at Polar ZnO(0001). Physical Review Letters, 2009, 103, 065502.	2.9	118
66	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
67	Understanding Anharmonicity in fcc Materials: From its Origin toabÂinitioStrategies beyond the Quasiharmonic Approximation. Physical Review Letters, 2015, 114, 195901.	2.9	115
68	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
69	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
70	Strain Induced Deep Electronic States around Threading Dislocations in GaN. Physical Review Letters, 2004, 93, 196401.	2.9	107
71	First-principles calculations of the structural and electronic properties of cleanGaN(0001)surfaces. Physical Review B, 2006, 73, .	1.1	107
72	First-principles study of the thermodynamics of hydrogen-vacancy interaction in fcc iron. Physical Review B, 2010, 82, .	1.1	106

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73	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
74	Ab initiostudy of H-vacancy interactions in fcc metals: Implications for the formation of superabundant vacancies. Physical Review B, 2014, 89, .	1.1	104
75	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
76	Density functional theory in materials science. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 438-448.	6.2	102
77	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
78	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
79	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
80	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
81	Guided bone regeneration with titanium membranes: a clinical study. British Journal of Oral and Maxillofacial Surgery, 2000, 38, 312-315.	0.4	96
82	Chemical trends for acceptor impurities in GaN. Journal of Applied Physics, 1999, 85, 3003-3005.	1.1	95
83	Spontaneous Formation of Indium-Rich Nanostructures on InGaN(0001) Surfaces. Physical Review Letters, 2000, 85, 1902-1905.	2.9	95
84	Structural stability and thermodynamics of CrN magnetic phases fromab initiocalculations and experiment. Physical Review B, 2014, 90, .	1.1	95
85	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
86	Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment. Physical Review Letters, 2014, 113, 165503.	2.9	93
87	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
88	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
89	Designing shape-memory Heusler alloys from first-principles. Applied Physics Letters, 2011, 99, .	1.5	91
90	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

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91	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
92	A machine learning approach to model solute grain boundary segregation. Npj Computational Materials, 2018, 4, .	3.5	89
93	Improved method of calculatingab initiohigh-temperature thermodynamic properties with application to ZrC. Physical Review B, 2015, 91, .	1.1	86
94	Vacancy formation energies in fcc metals: Influence of exchange-correlation functionals and correction schemes. Physical Review B, 2012, 85, .	1.1	85
95	Atomic and electronic structure of the GaAs/ZnSe(001) interface. Physical Review B, 1994, 50, 8616-8628.	1.1	84
96	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
97	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
98	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	3.5	79
99	The object-oriented DFT program library S/PHI/nX. Computer Physics Communications, 2011, 182, 543-554.	3.0	77
100	Growth and Proliferation of Human Osteoblasts on Different Bone Graft Substitutes An In Vitro Study. Implant Dentistry, 2004, 13, 171-179.	1.7	76
101	Chemical trends and bonding mechanisms for isloated adsorbates on Al(111). Physical Review B, 1994, 49, 17242-17252.	1.1	75
102	Possibility of a Mott-Hubbard ground state for the SiC(0001) surface. Physical Review B, 1998, 57, R4230-R4232.	1.1	75
103	Advancing density functional theory to finite temperatures: methods and applications in steel design. Journal of Physics Condensed Matter, 2012, 24, 053202.	0.7	75
104	A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron. Acta Materialia, 2015, 90, 69-76.	3.8	73
105	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
106	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
107	Thermodynamic properties of cementite (). Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 129-133.	0.7	72
108	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

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109	First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion. Physical Review Letters, 2018, 120, 246801.	2.9	71
110	Reconstructions of the AlN(0001) surface. Physical Review B, 2003, 68, .	1.1	70
111	Theory-Guided Materials Design of Multi-Phase Ti-Nb Alloys with Bone-Matching Elastic Properties. Materials, 2012, 5, 1853-1872.	1.3	70
112	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
113	Impact of nanodiffusion on the stacking fault energy in high-strength steels. Acta Materialia, 2014, 75, 147-155.	3.8	69
114	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
115	Accuracy of a newly developed integrated system for dental implant planning. Clinical Oral Implants Research, 2009, 20, 1191-1199.	1.9	68
116	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
117	Designing Heusler nanoprecipitates by elastic misfit stabilization in Feâ€“Mn maraging steels. Acta Materialia, 2014, 76, 94-105.	3.8	65
118	Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries. Physical Review Letters, 2018, 121, 015702.	2.9	65
119	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
120	Theory of Point Defects and Complexes in GaN. Materials Research Society Symposia Proceedings, 1995, 395, 645.	0.1	64
121	Ab Initio Based Understanding of the Segregation and Diffusion Mechanisms of Hydrogen in Steels. Jom, 2014, 66, 1399-1405.	0.9	64
122	pyiron: An integrated development environment for computational materials science. Computational Materials Science, 2019, 163, 24-36.	1.4	64
123	Alkali-metal adsorption on Al(111) and Al(100). Surface Science, 1994, 307-309, 8-15.	0.8	62
124	Review of Structure of Bare and Adsorbate-Covered GaN(0001) Surfaces. MRS Internet Journal of Nitride Semiconductor Research, 2002, 7, 1.	1.0	62
125	Extending the Concept of Defect Chemistry from Semiconductor Physics to Electrochemistry. Physical Review Applied, 2014, 1, .	1.5	62
126	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

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127	Deformationâ€Induced Martensite: A New Paradigm for Exceptional Steels. Advanced Materials, 2016, 28, 7753-7757.	11.1	61
128	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	1.1	61
129	Arsenic impurities in GaN. Applied Physics Letters, 2000, 76, 1009-1011.	1.5	59
130	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
131	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
132	Comparison of atomistic and continuum theoretical approaches to determine electronic properties of GaN/AlN quantum dots. Physical Review B, 2008, 78, .	1.1	58
133	Hydrogen adsorption on polar ZnO(0001)-Zn: Extending equilibrium surface phase diagrams to kinetically stabilized structures. Physical Review B, 2010, 82, .	1.1	58
134	Perspectives on point defect thermodynamics. Physica Status Solidi (B): Basic Research, 2014, 251, 97-129.	0.7	58
135	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
136	Adsorption and incorporation of silicon at GaN(0001) surfaces. Applied Physics Letters, 2002, 80, 2008-2010.	1.5	57
137	Rescaled Monte Carlo approach for magnetic systems:Ab initiothermodynamics of bcc iron. Physical Review B, 2010, 81, .	1.1	57
138	Ab initiobased determination of thermodynamic properties of cementite including vibronic, magnetic, and electronic excitations. Physical Review B, 2011, 84, .	1.1	57
139	AbÂinitioPrediction of Martensitic and Intermartensitic Phase Boundaries in Ni-Mn-Ga. Physical Review Letters, 2016, 116, 025503.	2.9	57
140	The Basics of Electronic Structure Theory for Periodic Systems. Frontiers in Chemistry, 2019, 7, 106.	1.8	57
141	Formation energies of point defects at finite temperatures. Physica Status Solidi (B): Basic Research, 2011, 248, 1295-1308.	0.7	56
142	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
143	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
144	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

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145	Chemically orderedAlxGa1â^'xNalloys:â€ƒSpontaneous formation of natural quantum wells. Physical Review B, 2005, 71, .	1.1	53
146	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
147	Efficient approach to compute melting properties fully from ab initio with application to Cu. Physical Review B, 2017, 96, .	1.1	53
148	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
149	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
150	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
151	Limits and accuracy of valence force field models forInxGa1â^'xNalloys. Physical Review B, 2001, 63, .	1.1	50
152	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
153	Electron and chemical reservoir corrections for point-defect formation energies. Physical Review B, 2016, 93, .	1.1	50
154	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
155	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
156	Pressure dependence of the Curie temperature in bcc iron studied byab initiosimulations. Physical Review B, 2009, 79, .	1.1	49
157	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
158	Comparison of static and dynamic computer-assisted guidance methods in implantology. International Journal of Computerized Dentistry, 2006, 9, 23-35.	0.2	48
159	Native defects and impurities in GaN. FestkÃ¶rperprobleme, 1996, , 25-44.	0.7	47
160	Direct minimization technique for metals in density functional theory. Physical Review B, 2009, 79, .	1.1	47
161	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
162	Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation. Acta Materialia, 2015, 85, 53-66.	3.8	47

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163	Calculating free energies of point defects from ab initio. Computational Materials Science, 2018, 148, 249-259.	1.4	47
164	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
165	Interplay between long-range elastic and short-range chemical interactions in Fe-C martensite formation. Physical Review B, 2009, 79, .	1.1	45
166	Role of spin quantization in determining the thermodynamic properties of magnetic transition metals. Physical Review B, 2011, 83, .	1.1	45
167	Hidden surface states at non-polar GaN (101Â¯) facets: Intrinsic pinning of nanowires. Applied Physics Letters, 2013, 103, .	1.5	45
168	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. Physical Review B, 2018, 97, .	1.1	45
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