Joerg Neugebauer

List of Publications by Citations

441 papers	31,009 citations	80 h-index	165 g-index
465 ext. papers	34,197 ext. citations	4.7 avg, IF	7.48 L-index

#	Paper	IF	Citations
441	First-principles calculations for defects and impurities: Applications to III-nitrides. *Journal of Applied Physics*, **2004**, 95, 3851-3879	2.5	2330
440	Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). *Physical Review B*, **1992**, 46, 16067-16080	3.3	1987
439	First-principles calculations for point defects in solids. *Reviews of Modern Physics*, **2014**, 86, 253-305	40.5	1431
438	Universal alignment of hydrogen levels in semiconductors, insulators and solutions. *Nature*, **2003**, 423, 626-8	50.4	1003
437	Gallium vacancies and the yellow luminescence in GaN. *Applied Physics Letters*, **1996**, 69, 503-505	3.4	963
436	Fully ab initio finite-size corrections for charged-defect supercell calculations. *Physical Review Letters*, **2009**, 102, 016402	7.4	845
435	Atomic geometry and electronic structure of native defects in GaN. *Physical Review B*, **1994**, 50, 8067-8070	3.3	692
434	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	4.2	628
433	A map for phase-change materials. *Nature Materials*, **2008**, 7, 972-7	27	559
432	Adatom diffusion at GaN (0001) and (0001) surfaces. *Applied Physics Letters*, **1998**, 73, 487-489	3.4	400
431	Hydrogen in GaN: Novel aspects of a common impurity. *Physical Review Letters*, **1995**, 75, 4452-4455	7.4	390
430	The relation between ductility and stacking fault energies in Mg and Mg alloys. *Acta Materialia*, **2012**, 60, 3011-3021	8.4	359
429	On the Accuracy of DFT for Describing Hydrogen Bonds: Dependence on the Bond Directionality. *Journal of Physical Chemistry A*, **2004**, 108, 5692-5698	2.8	324
428	Electrostatic interactions between charged defects in supercells. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1067-1076	1.3	309
427	Reconstructions of the GaN(0001) Surface. *Physical Review Letters*, **1997**, 79, 3934-3937	7.4	309
426	Theory of GaN(101-bar0) and (112-bar0) surfaces. *Physical Review B*, **1996**, 53, R10477-R10480	3.3	309
425	Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. *Physical Review B*, **2008**, 77,	3.3	306

424	Structure of GaN(0001): The laterally contracted Ga bilayer model. *Physical Review B*, **2000**, 61, 9932-9935	3.3	296
423	Determination of wurtzite GaN lattice polarity based on surface reconstruction. *Applied Physics Letters*, **1998**, 72, 2114-2116	3.4	286
422	Role of hydrogen in doping of GaN. *Applied Physics Letters*, **1996**, 68, 1829-1831	3.4	278
421	Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one. *Acta Materialia*, **2015**, 100, 90-97	8.4	277
420	Adatom kinetics on and below the surface: the existence of a new diffusion channel. *Physical Review Letters*, **2003**, 90, 056101	7.4	267
419	Electronic structure and phase stability of GaAs1-xNx alloys. *Physical Review B*, **1995**, 51, 10568-10571	3.3	251
418	CombiningGWcalculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. *New Journal of Physics*, **2005**, 7, 126-126	2.9	250
417	Revealing the design principles of high-performance biological composites using ab initio and multiscale simulations: the example of lobster cuticle. *Advanced Materials*, **2010**, 22, 519-26	24	239
416	Inversion Domain and Stacking Mismatch Boundaries in GaN. *Physical Review Letters*, **1996**, 77, 103-106	7.4	217
415	First-principles surface phase diagram for hydrogen on GaN surfaces. *Physical Review Letters*, **2002**, 88, 066103	7.4	216
414	Surface energetics, pit formation, and chemical ordering in InGaN alloys. *Applied Physics Letters*, **1999**, 74, 2319-2321	3.4	213
413	Reconstructions of GaN(0001) and (0001) 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		211
412	The adsorption of oxygen at GaN surfaces. *Applied Physics Letters*, **1999**, 74, 1695-1697	3.4	197
411	Ductility improvement of Mg alloys by solid solution: Ab initio modeling, synthesis and mechanical properties. *Acta Materialia*, **2014**, 70, 92-104	8.4	189
410	Theory-guided bottom-up design of β-titanium alloys as biomaterials based on first principles calculations: Theory and experiments. *Acta Materialia*, **2007**, 55, 4475-4487	8.4	188
409	Ab initio up to the melting point: Anharmonicity and vacancies in aluminum. *Physical Review B*, **2009** , 79,	3.3	184
408	Ab initio study of the thermodynamic properties of nonmagnetic elementary fcc metals: Exchange-correlation-related error bars and chemical trends. *Physical Review B*, **2007**, 76,	3.3	184
407	Unusual chemisorption geometry of Na on Al(111). *Physical Review Letters*, **1991**, 67, 2163-2166	7.4	180

406	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. *Acta Materialia*, **2017**, 136, 262-270	8.4	179
405	Theory of doping and defects in III□V nitrides. *Journal of Crystal Growth*, **1998**, 189-190, 505-510	1.6	175
404	Large anisotropic adatom kinetics on nonpolar GaN surfaces: Consequences for surface morphologies and nanowire growth. *Physical Review B*, **2009**, 79,	3.3	160
403	Basal and non-basal dislocation slip in Mg□. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2013**, 576, 61-68	5.3	153
402	Free energy of bcc iron: Integrated ab initio derivation of vibrational, electronic, and magnetic contributions. *Physical Review B*, **2008**, 78,	3.3	152
401	Theory of the adatom-induced reconstruction of the SiC(0001) sqrt 3 x sqrt 3 surface. *Physical Review B*, **1995**, 52, 17001-17004	3.3	152
400	First-principles study on the interaction of H interstitials with grain boundaries in □and □Fe. *Physical Review B*, **2011**, 84,	3.3	150
399	Geometric accuracy of a newly developed cone-beam device for maxillofacial imaging. *Oral Surgery Oral Medicine Oral Pathology Oral Radiology and Endodontics*, **2007**, 104, 551-9		140
398	Indium-induced changes in GaN(0001) surface morphology. *Physical Review B*, **1999**, 60, R8473-R8476	3.3	140
397	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	3.4	134
396	Ultrastrong Medium-Entropy Single-Phase Alloys Designed via Severe Lattice Distortion. *Advanced Materials*, **2019**, 31, e1807142	24	132
395	Generation and performance of special quasirandom structures for studying the elastic properties of random alloys: Application to Al-Ti. *Physical Review B*, **2010**, 81,	3.3	129
394	HYDROGEN IN SEMICONDUCTORS. *Annual Review of Materials Research*, **2006**, 36, 179-198	12.8	127
393	Mechanisms of island formation of alkali-metal adsorbates on Al(111). *Physical Review Letters*, **1993** , 71, 577-580	7.4	126
392	Development and application of a Ni-Ti interatomic potential with high predictive accuracy of the martensitic phase transition. *Physical Review B*, **2015**, 92,	3.3	125
391	First-principles studies of beryllium doping of GaN. *Physical Review B*, **2001**, 63,	3.3	124
390	Understanding the phase transitions of the Ni2MnGa magnetic shape memory system from first principles. *Physical Review Letters*, **2009**, 102, 035702	7.4	123
389	Small valence-band offsets at GaN/InGaN heterojunctions. *Applied Physics Letters*, **1997**, 70, 2577-2579	3.4	122

388	Trends in the elastic response of binary early transition metal nitrides. *Physical Review B*, **2012**, 85,	3.3	121
387	Atomic structure and stability of AlN(0001) and (000 1) surfaces. *Physical Review B*, **1997**, 55, 13878-13883	3.3	120
386	Gallium adsorption on (0001) GaN surfaces. *Physical Review B*, **2003**, 67,	3.3	118
385	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,	3.3	118
384	Using ab initio calculations in designing bcc Mg□i alloys for ultra-lightweight applications. *Acta Materialia*, **2009**, 57, 69-76	8.4	115
383	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. *Physical Review B*, **2012**, 85,	3.3	114
382	GaN(0001) surface structures studied using scanning tunneling microscopy and first-principles total energy calculations. *Surface Science*, **1999**, 423, 70-84	1.8	113
381	Temperature stabilized surface reconstructions at polar ZnO(0001). *Physical Review Letters*, **2009**, 103, 065502	7.4	110
380	Hydrogen-enhanced local plasticity at dilute bulk H concentrations: The role of H□H interactions and the formation of local hydrides. *Acta Materialia*, **2011**, 59, 2969-2980	8.4	105
379	Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. *Acta Materialia*, **2017**, 123, 90-101	8.4	104
378	First-principles calculations of the structural and electronic properties of clean GaN(0001) surfaces. *Physical Review B*, **2006**, 73,	3.3	100
377	Density Functional Theory Study of the Cooperativity of Hydrogen Bonds in Finite and Infinite □-Helices. *Journal of Physical Chemistry B*, **2003**, 107, 1432-1437	3.4	99
376	Strain induced deep electronic states around threading dislocations in GaN. *Physical Review Letters*, **2004**, 93, 196401	7.4	98
375	Bone contact, growth, and density around immediately loaded implants in the mandible of mini pigs. *Clinical Oral Implants Research*, **2003**, 14, 312-21	4.8	96
374	A rare-earth free magnesium alloy with improved intrinsic ductility. *Scientific Reports*, **2017**, 7, 10458	4.9	95
373	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. *Physical Review Letters*, **1998**, 80, 3097-3100	7.4	92
372	Spontaneous formation of indium-rich nanostructures on InGaN(0001) surfaces. *Physical Review Letters*, **2000**, 85, 1902-5	7.4	91
371	Understanding Anharmonicity in fcc Materials: From its Origin to ab initio Strategies beyond the Quasiharmonic Approximation. *Physical Review Letters*, **2015**, 114, 195901	7.4	89

370	First-principles investigation of the effect of carbon on the stacking fault energy of Fe□ alloys. *Acta Materialia*, **2011**, 59, 3041-3048	8.4	89
369	Energetics of H and NH2 on GaN(101□0) and implications for the origin of nanopipe defects. *Physical Review B*, **1997**, 56, R4325-R4328	3.3	88
368	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, 129-45	4.1	87
367	First-principles study of the thermodynamics of hydrogen-vacancy interaction in fcc iron. *Physical Review B*, **2010**, 82,	3.3	85
366	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, 634-40		84
365	Chemical trends for acceptor impurities in GaN. *Journal of Applied Physics*, **1999**, 85, 3003-3005	2.5	84
364	Exciting prospects for solids: Exact-exchange based functionals meet quasiparticle energy calculations. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 929-945	1.3	82
363	Density functional theory in materials science. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 438-448	7.9	80
362	Ab initioand atomistic study of generalized stacking fault energies in Mg and Mg□ alloys. *New Journal of Physics*, **2013**, 15, 043020	2.9	80
361	Designing shape-memory Heusler alloys from first-principles. *Applied Physics Letters*, **2011**, 99, 191904	3.4	80
360	Guided bone regeneration with titanium membranes: a clinical study. *British Journal of Oral and Maxillofacial Surgery*, **2000**, 38, 312-5	1.4	80
359	Atomic and electronic structure of the GaAs/ZnSe(001) interface. *Physical Review B*, **1994**, 50, 8616-8628	3.3	79
358	Structural stability and thermodynamics of CrN magnetic phases from ab initio calculations and experiment. *Physical Review B*, **2014**, 90,	3.3	78
357	Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. *Physical Review B*, **2006**, 74,	3.3	78
356	First-principles investigation of hydrogen interaction with TiC precipitates in □Fe. *Physical Review B*, **2016**, 93,	3.3	75
355	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	3.4	75
354	Magnetic properties of the CrMnFeCoNi high-entropy alloy. *Physical Review B*, **2017**, 96,	3.3	74
353	Possibility of a Mott-Hubbard ground state for the SiC(0001) surface. *Physical Review B*, **1998**, 57, R4230-R4232	3.3	74

352	Combined atom probe tomography and density functional theory investigation of the Al off-stoichiometry of κ-carbides in an austenitic FeMnAlC low density steel. *Acta Materialia*, **2016**, 106, 229-238	8.4	73
351	Chemical trends and bonding mechanisms for isloated adsorbates on Al(111). *Physical Review B*, **1994**, 49, 17242-17252	3.3	73
350	Breakdown of the Arrhenius Law in Describing Vacancy Formation Energies: The Importance of Local Anharmonicity Revealed by Ab initio Thermodynamics. *Physical Review X*, **2014**, 4,	9.1	70
349	Growth and proliferation of human osteoblasts on different bone graft substitutes: an in vitro study. *Implant Dentistry*, **2004**, 13, 171-9	2.4	70
348	Vacancy formation energies in fcc metals: Influence of exchange-correlation functionals and correction schemes. *Physical Review B*, **2012**, 85,	3.3	69
347	Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment. *Physical Review Letters*, **2014**, 113, 165503	7.4	68
346	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		67
345	Advancing density functional theory to finite temperatures: methods and applications in steel design. *Journal of Physics Condensed Matter*, **2012**, 24, 053202	1.8	66
344	Reconstructions of the AlN(0001) surface. *Physical Review B*, **2003**, 68,	3.3	66
343	Thermodynamic properties of cementite (Fe3C). *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2010**, 34, 129-133	1.9	64
342	Theory-Guided Materials Design of Multi-Phase Ti-Nb Alloys with Bone-Matching Elastic Properties. *Materials*, **2012**, 5, 1853-1872	3.5	62
341	Ab initio study of H-vacancy interactions in fcc metals: Implications for the formation of superabundant vacancies. *Physical Review B*, **2014**, 89,	3.3	61
340	The object-oriented DFT program library S/PHI/nX. *Computer Physics Communications*, **2011**, 182, 543-554	4.2	61
339	Alkali-metal adsorption on Al(111) and Al(100). *Surface Science*, **1994**, 307-309, 8-15	1.8	61
338	Impact of lattice relaxations on phase transitions in a high-entropy alloy studied by machine-learning potentials. *Npj Computational Materials*, **2019**, 5,	10.9	60
337	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	8.4	60
336	Improved method of calculating ab initio high-temperature thermodynamic properties with application to ZrC. *Physical Review B*, **2015**, 91,	3.3	60
335	Accuracy of a newly developed integrated system for dental implant planning. *Clinical Oral Implants Research*, **2009**, 20, 1191-9	4.8	60

334	Theory of Point Defects and Complexes in GaN. *Materials Research Society Symposia Proceedings*, **1995**, 395, 645		60
333	Review of Structure of Bare and Adsorbate-Covered GaN(0001) Surfaces. *MRS Internet Journal of Nitride Semiconductor Research*, **2002**, 7, 1		59
332	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	2.9	58
331	A machine learning approach to model solute grain boundary segregation. *Npj Computational Materials*, **2018**, 4,	10.9	58
330	Impact of nanodiffusion on the stacking fault energy in high-strength steels. *Acta Materialia*, **2014**, 75, 147-155	8.4	57
329	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	2.8	57
328	Hydrogen adsorption on polar ZnO(0001)-Zn: Extending equilibrium surface phase diagrams to kinetically stabilized structures. *Physical Review B*, **2010**, 82,	3.3	56
327	Extending the Concept of Defect Chemistry from Semiconductor Physics to Electrochemistry. *Physical Review Applied*, **2014**, 1,	4.3	54
326	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	7.4	54
325	Designing Heusler nanoprecipitates by elastic misfit stabilization in Fe-Mn maraging steels. *Acta Materialia*, **2014**, 76, 94-105	8.4	53
324	Comparison of atomistic and continuum theoretical approaches to determine electronic properties of GaN/AlN quantum dots. *Physical Review B*, **2008**, 78,	3.3	53
323	Adsorption and incorporation of silicon at GaN(0001) surfaces. *Applied Physics Letters*, **2002**, 80, 2008-2010	3.4	52
322	Arsenic impurities in GaN. *Applied Physics Letters*, **2000**, 76, 1009-1011	3.4	52
321	Rescaled Monte Carlo approach for magnetic systems: Ab initio thermodynamics of bcc iron. *Physical Review B*, **2010**, 81,	3.3	51
320	Peri-implant bone organization under immediate loading state. Circularly polarized light analyses: a minipig study. *Journal of Periodontology*, **2006**, 77, 152-60	4.6	51
319	From electronic structure to phase diagrams: A bottom-up approach to understand the stability of titanium-transition metal alloys. *Acta Materialia*, **2016**, 113, 311-319	8.4	51
318	Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries. *Physical Review Letters* , **2018**, 121, 015702	7.4	50
317	Ab initio based determination of thermodynamic properties of cementite including vibronic, magnetic, and electronic excitations. *Physical Review B*, **2011**, 84,	3.3	50

316	Lateral femoral cutaneous nerve and iliac crest bone grafts--anatomical and clinical considerations. *International Journal of Oral and Maxillofacial Surgery*, **2006**, 35, 366-72	2.9	49
315	Deformation-Induced Martensite: A New Paradigm for Exceptional Steels. *Advanced Materials*, **2016**, 28, 7753-7	24	48
314	Limits and accuracy of valence force field models for InxGa1−xN alloys. *Physical Review B*, **2001**, 63,	3.3	48
313	Chemically ordered AlxGa1−xN alloys: Spontaneous formation of natural quantum wells. *Physical Review B*, **2005**, 71,	3.3	47
312	Ab initio Analysis of Surface Structure and Adatom Kinetics of Group-III Nitrides. *Physica Status Solidi (B): Basic Research*, **2001**, 227, 93-114	1.3	47
311	Structural transformations among austenite, ferrite and cementite in Fe–C alloys: A unified theory based on ab initio simulations. *Acta Materialia*, **2015**, 99, 281-289	8.4	46
310	Accurate electronic free energies of the 3d,4d, and 5d transition metals at high temperatures. *Physical Review B*, **2017**, 95,	3.3	46
309	A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron. *Acta Materialia*, **2015**, 90, 69-76	8.4	45
308	First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion. *Physical Review Letters*, **2018**, 120, 246801	7.4	45
307	Perspectives on point defect thermodynamics. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 97-129	1.3	45
306	Formation energies of point defects at finite temperatures. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1295-1308	1.3	45
305	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, 687-94	2.9	45
304	Surfactants and antisurfactants on group-III-nitride surfaces. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2003**, 1651-1667		45
303	Ab‐initio Prediction of Martensitic and Intermartensitic Phase Boundaries in Ni-Mn-Ga. *Physical Review Letters*, **2016**, 116, 025503	7.4	44
302	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. *Npj Computational Materials*, **2019**, 5,	10.9	44
301	Pressure dependence of the Curie temperature in bcc iron studied by ab initio simulations. *Physical Review B*, **2009**, 79,	3.3	44
300	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, 633-42; discussion 643		44
299	Comparison of static and dynamic computer-assisted guidance methods in implantology. *International Journal of Computerized Dentistry*, **2006**, 9, 23-35	4.5	44

298	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	2.8	44
297	Temperature-driven phase transitions from first principles including all relevant excitations: The fcc-to-bcc transition in Ca. *Physical Review B*, **2011**, 84,	3.3	43
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295	Native defects and impurities in GaN. *Festk□perprobleme*, **1996**, 25-44		43
294	First-principles calculations for charged defects at surfaces, interfaces, and two-dimensional materials in the presence of electric fields. *Physical Review B*, **2018**, 97,	3.3	43
293	Electron and chemical reservoir corrections for point-defect formation energies. *Physical Review B*, **2016**, 93,	3.3	42
292	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	16.4	42
291	Electronic and structural properties of vacancies on and below the GaP(110) surface. *Physical Review B*, **1998**, 58, 1392-1400	3.3	42
290	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. *Entropy*, **2018**, 20,	2.8	42
289	Understanding and controlling indium incorporation and surface segregation on InxGa1□N surfaces: An ab initio approach. *Physical Review B*, **2014**, 89,	3.3	41
288	Interplay between long-range elastic and short-range chemical interactions in Fe-C martensite formation. *Physical Review B*, **2009**, 79,	3.3	41
287	Theory of adsorption and desorption in high electric fields. *Surface Science*, **1993**, 287-288, 572-576	1.8	41
286	Direct minimization technique for metals in density functional theory. *Physical Review B*, **2009**, 79,	3.3	40
285	Understanding Si adsorption on GaN(0001) surfaces using first-principles calculations. *Physical Review B*, **2006**, 73,	3.3	40
284	Hidden surface states at non-polar GaN (101□0) facets: Intrinsic pinning of nanowires. *Applied Physics Letters*, **2013**, 103, 152101	3.4	39
283	Ab initio study of thermodynamic, structural, and elastic properties of Mg-substituted crystalline calcite. *Acta Biomaterialia*, **2010**, 6, 4506-12	10.8	39
282	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		39
281	Thermodynamics of grain boundary segregation, interfacial spinodal and their relevance for nucleation during solid-solid phase transitions. *Acta Materialia*, **2019**, 168, 109-120	8.4	38

280	Surface Structures, Surfactants and Diffusion at Cubic and Wurtzite GaN. *MRS Internet Journal of Nitride Semiconductor Research*, **1998**, 3, 1		38
279	Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation. *Acta Materialia*, **2015**, 85, 53-66	8.4	37
278	Efficient approach to compute melting properties fully from ab initio with application to Cu. *Physical Review B*, **2017**, 96,	3.3	37
277	Role of semicore states in the electronic structure of group-III nitrides: An exact-exchange study. *Physical Review B*, **2005**, 72,	3.3	37
276	Role of spin quantization in determining the thermodynamic properties of magnetic transition metals. *Physical Review B*, **2011**, 83,	3.3	36
275	Structure and energetics of nitride surfaces under MOCVD growth conditions. *Journal of Crystal Growth*, **2003**, 248, 8-13	1.6	36
274	Hydrogen interactions with self-interstitials in silicon. *Physical Review B*, **1995**, 52, 14320-14323	3.3	36
273	Computer-aided manufacturing technologies for guided implant placement. *Expert Review of Medical Devices*, **2010**, 7, 113-29	3.5	35
272	Symmetric versus nonsymmetric structure of the phosphorus vacancy on InP(110). *Physical Review Letters*, **2000**, 84, 5816-9	7.4	35
271	First-principles study of the thermodynamic and elastic properties of eutectic Fe□Ti alloys. *Acta Materialia*, **2012**, 60, 1594-1602	8.4	33
270	GaN(0001) surface states: Experimental and theoretical fingerprints to identify surface reconstructions. *Physical Review B*, **2013**, 88,	3.3	33
269	Orientational ordering of interstitial atoms and martensite formation in dilute Fe-based solid solutions. *Physical Review B*, **2011**, 83,	3.3	33
268	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. *Physical Review B*, **2018**, 98,	3.3	33
267	Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite. *Acta Materialia*, **2013**, 61, 1773-1784	8.4	32
266	Ab Initio-Based Prediction of Phase Diagrams: Application to Magnetic Shape Memory Alloys. *Advanced Engineering Materials*, **2012**, 14, 547-561	3.5	32
265	Morphology and surface reconstructions of GaN(11 00) surfaces. *Applied Physics Letters*, **2003**, 82, 1793-1795	3.4	32
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263	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,	3.3	31

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259	Ab initio study of the anomalous volume-composition dependence in Fe3Al alloys. *Intermetallics*, **2010**, 18, 1316-1321	3.5	30
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