Joerg Neugebauer

List of Publications by Year in Descending Order

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	Origins of the hydrogen signal in atom probe tomography: case studies of alkali and noble metals. *New Journal of Physics*, **2022**, 24, 013008	2.9	2
440	Ab initio investigations of point and complex defect structures in B2-FeAl. *Physical Review Materials* , **2022**, 6,	3.2	1
439	Controlled doping of electrocatalysts through engineering impurities.. *Advanced Materials*, **2022**, e2203030	24	2
438	Finite-size correction for slab supercell calculations of materials with spontaneous polarization. *Npj Computational Materials*, **2021**, 7,	10.9	2
437	A Combined Experimental and First-Principles Based Assessment of Finite-Temperature Thermodynamic Properties of Intermetallic AlSc. *Materials*, **2021**, 14,	3.5	1
436	Dielectric Properties of Nanoconfined Water: A Canonical Thermopotentiostat Approach. *Physical Review Letters*, **2021**, 126, 136803	7.4	15
435	Impact of Water Coadsorption on the Electrode Potential of H-Pt(1 1 1)-Liquid Water Interfaces. *Physical Review Letters*, **2021**, 126, 166802	7.4	11
434	B2 ordering in body-centered-cubic AlNbTiV refractory high-entropy alloys. *Physical Review Materials*, **2021**, 5,	3.2	5
433	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. *Npj Computational Materials*, **2021**, 7,	10.9	6
432	A fully automated approach to calculate the melting temperature of elemental crystals. *Computational Materials Science*, **2021**, 187, 110065	3.2	4
431	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,	3.2	2
430	Segmentation of Static and Dynamic Atomic-Resolution Microscopy Data Sets with Unsupervised Machine Learning Using Local Symmetry Descriptors. *Microscopy and Microanalysis*, **2021**, 1-11	0.5	0
429	Revealing atomic-scale vacancy-solute interaction in nickel. *Scripta Materialia*, **2021**, 203, 114036	5.6	1
428	Mechanism of collective interstitial ordering in Fe-C alloys. *Nature Materials*, **2020**, 19, 849-854	27	11
427	Interplay of Chemistry and Faceting at Grain Boundaries in a Model Al Alloy. *Physical Review Letters*, **2020**, 124, 106102	7.4	15
426	Phonons in magnetically disordered materials: Magnetic versus phononic time scales. *Physical Review B*, **2020**, 101,	3.3	5
425	Generalized dipole correction for charged surfaces in the repeated-slab approach. *Physical Review B* , **2020**, 102,	3.3	6

424	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	1.9	2
423	Ab initio Description of Bond Breaking in Large Electric Fields. *Physical Review Letters*, **2020**, 124, 176801	7.4	16
422	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,	3.3	7
421	Correlation analysis of strongly fluctuating atomic volumes, charges, and stresses in body-centered cubic refractory high-entropy alloys. *Physical Review Materials*, **2020**, 4,	3.2	14
420	Role of magnetic ordering for the design of quinary TWIP-TRIP high entropy alloys. *Physical Review Materials*, **2020**, 4,	3.2	11
419	Short-range order in face-centered cubic VCoNi alloys. *Physical Review Materials*, **2020**, 4,	3.2	8
418	Atomic scale configuration of planar defects in the Nb-rich C14 Laves phase NbFe2. *Acta Materialia*, **2020**, 183, 362-376	8.4	16
417	Atomic relaxation around defects in magnetically disordered materials computed by atomic spin constraints within an efficient Lagrange formalism. *Physical Review B*, **2020**, 102,	3.3	3
416	Anharmonic free energy of lattice vibrations in fcc crystals from a mean-field bond. *Physical Review B*, **2020**, 102,	3.3	1
415	Segregation-assisted spinodal and transient spinodal phase separation at grain boundaries. *Npj Computational Materials*, **2020**, 6,	10.9	11
414	Ab initio based method to study structural phase transitions in dynamically unstable crystals, with new insights on the to transformation in titanium. *Physical Review B*, **2019**, 100,	3.3	9
413	Deciphering Charge Transfer and Electronic Polarization Effects at Gold Nanocatalysts on Reduced Titania Support. *Journal of Physical Chemistry C*, **2019**, 123, 5495-5506	3.8	5
412	Invar effects in FeNiCo medium entropy alloys: From an Invar treasure map to alloy design. *Intermetallics*, **2019**, 111, 106520	3.5	17
411	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
410	Role of hole confinement in the recombination properties of InGaN quantum structures. *Scientific Reports*, **2019**, 9, 9047	4.9	6
409	Elasticity of Phases in Fe-Al-Ti Superalloys: Impact of Atomic Order and Anti-Phase Boundaries. *Crystals*, **2019**, 9, 299	2.3	8
408	pyiron: An integrated development environment for computational materials science. *Computational Materials Science*, **2019**, 163, 24-36	3.2	24
407	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

406	The Basics of Electronic Structure Theory for Periodic Systems. *Frontiers in Chemistry*, **2019**, 7, 106	5	29
405	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. *Npj Computational Materials*, **2019**, 5,	10.9	44
404	Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams. *Physical Review Materials*, **2019**, 3,	3.2	9
403	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. *Physical Review Materials*, **2019**, 3,	3.2	21
402	Imaging individual solute atoms at crystalline imperfections in metals. *New Journal of Physics*, **2019**, 21, 123020	2.9	18
401	Phonon Lifetimes throughout the Brillouin Zone at Elevated Temperatures from Experiment and Ab□nitio. *Physical Review Letters*, **2019**, 123, 235501	7.4	10
400	Ultrastrong Medium-Entropy Single-Phase Alloys Designed via Severe Lattice Distortion. *Advanced Materials*, **2019**, 31, e1807142	24	132
399	Transferability of interatomic potentials for molybdenum and silicon. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 025007	2	11
398	Discovery of Elusive K4O6, a Compound Stabilized by Configurational Entropy of Polarons. *Angewandte Chemie*, **2019**, 131, 155-159	3.6	0
397	Discovery of Elusive K O , a Compound Stabilized by Configurational Entropy of Polarons. *Angewandte Chemie - International Edition*, **2019**, 58, 149-153	16.4	4
396	Impact of local electrostatic field rearrangement on field ionization. *Journal Physics D: Applied Physics*, **2018**, 51, 105601	3	15
395	Selective Solvent-Induced Stabilization of Polar Oxide Surfaces in an Electrochemical Environment. *Physical Review Letters*, **2018**, 120, 066101	7.4	17
394	Calculating free energies of point defects from ab initio. *Computational Materials Science*, **2018**, 148, 249-259	3.2	31
393	Temperature-dependent phonon spectra of magnetic random solid solutions. *Npj Computational Materials*, **2018**, 4,	10.9	13
392	Ab initio simulation of hydrogen-induced decohesion in cementite-containing microstructures. *Acta Materialia*, **2018**, 150, 53-58	8.4	27
391	Advanced data mining in field ion microscopy. *Materials Characterization*, **2018**, 146, 307-318	3.9	7
390	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. *Physical Review B*, **2018**, 97,	3.3	23
389	Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries. *Physical Review Letters* , **2018**, 121, 015702	7.4	50

388	Modeling of Phase Equilibria in Ni-H: Bridging the Atomistic with the Continuum Scale. *Metals*, **2018**, 8, 280	2.3	2
387	First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion. *Physical Review Letters*, **2018**, 120, 246801	7.4	45
386	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	3.6	4
385	Elastically frustrated rehybridization: Origin of chemical order and compositional limits in InGaN quantum wells. *Physical Review Materials*, **2018**, 2,	3.2	26
384	Tetragonal fcc-Fe induced by ε-carbide precipitates: Atomic scale insights from correlative electron microscopy, atom probe tomography, and density functional theory. *Physical Review Materials*, **2018**, 2,	3.2	13
383	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,	3.2	9
382	Migration mechanisms of a faceted grain boundary. *Physical Review Materials*, **2018**, 2,	3.2	12
381	Precipitate-induced nonlinearities of diffusion along grain boundaries in Al-based alloys. *Physical Review Materials*, **2018**, 2,	3.2	7
380	{110} planar faults in strained bcc metals: Origins and implications of a commonly observed artifact of classical potentials. *Physical Review Materials*, **2018**, 2,	3.2	10
379	GB□tode: A grain boundary generation code. *Journal of Open Source Software*, **2018**, 3, 900	5.2	5
378	Impact of Co and Fe Doping on the Martensitic Transformation and the Magnetic Properties in Ni-Mn-Based Heusler Alloys. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1700455	1.3	12
377	Titelbild: Discovery of Elusive K4O6, a Compound Stabilized by Configurational Entropy of Polarons (Angew. Chem. 1/2019). *Angewandte Chemie*, **2018**, 131, 1	3.6	
376	Atomistic modelling of light-element co-segregation at structural defects in iron. *Procedia Structural Integrity*, **2018**, 13, 1099-1104	1	2
375	A machine learning approach to model solute grain boundary segregation. *Npj Computational Materials*, **2018**, 4,	10.9	58
374	Origin of the Low Magnetic Moment in Fe□AlTi: An Ab Initio Study. *Materials*, **2018**, 11,	3.5	14
373	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. *Physical Review B*, **2018**, 98,	3.3	33
372	Anomalous Phonon Lifetime Shortening in Paramagnetic CrN Caused by Spin-Lattice Coupling: A Combined Spin and Ab□nitio Molecular Dynamics Study. *Physical Review Letters*, **2018**, 121, 125902	7.4	25
371	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. *Entropy*, **2018**, 20,	2.8	42

370	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
369	Modelling of grain boundary dynamics using amplitude equations. *Continuum Mechanics and Thermodynamics*, **2017**, 29, 895-911	3.5	6
368	Fermi-level pinning and intrinsic surface states of Al1−xInxN(101̄0) surfaces. *Applied Physics Letters* , **2017**, 110, 022104	3.4	4
367	Atomistic Modeling-Based Design of Novel Materials . *Advanced Engineering Materials*, **2017**, 19, 1600688	3.5	10
366	Atomic structures of twin boundaries in hexagonal close-packed metallic crystals with particular focus on Mg. *Npj Computational Materials*, **2017**, 3,	10.9	26
365	Ab initio modelling of solute segregation energies to a general grain boundary. *Acta Materialia*, **2017**, 132, 138-148	8.4	21
364	Hydrogen behaviour at twist {110} grain boundaries in -Fe. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	11
363	Narrow Implants **2017**, 208-218		
362	100 years public−private partnership in metallurgical and materials science research. *Materials Today*, **2017**, 20, 335-337	21.8	
361	Ab initio explanation of disorder and off-stoichiometry in Fe-Mn-Al-C κ-carbides. *Physical Review B*, **2017**, 95,	3.3	24
360	Low-temperature features in the heat capacity of unary metals and intermetallics for the example of bulk aluminum and Al3Sc. *Physical Review B*, **2017**, 95,	3.3	7
359	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
358	High Fidelity Reconstruction of Experimental Field Ion Microscopy Data by Atomic Relaxation Simulations. *Microscopy and Microanalysis*, **2017**, 23, 642-643	0.5	5
357	A rare-earth free magnesium alloy with improved intrinsic ductility. *Scientific Reports*, **2017**, 7, 10458	4.9	95
356	Accurate electronic free energies of the 3d,4d, and 5d transition metals at high temperatures. *Physical Review B*, **2017**, 95,	3.3	46
355	Magnetic properties of the CrMnFeCoNi high-entropy alloy. *Physical Review B*, **2017**, 96,	3.3	74
354	Efficient approach to compute melting properties fully from ab initio with application to Cu. *Physical Review B*, **2017**, 96,	3.3	37
353	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. *Acta Materialia*, **2017**, 136, 262-270	8.4	179

352	Adsorption and desorption of hydrogen at nonpolar GaN(11□00) surfaces: Kinetics and impact on surface vibrational and electronic properties. *Physical Review B*, **2017**, 95,	3.3	12
351	Origin of Structural Modulations in Ultrathin Fe Films on Cu(001). *Physical Review Letters*, **2017**, 118, 236101	7.4	4
350	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
349	Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. *Acta Materialia*, **2017**, 123, 90-101	8.4	104
348	The Role of □Carbides as Hydrogen Traps in High-Mn Steels. *Metals*, **2017**, 7, 264	2.3	16
347	Thermomechanical response of NiTi shape-memory nanoprecipitates in TiV alloys. *Physical Review Materials*, **2017**, 1,	3.2	18
346	Influence of magnetic excitations on the phase stability of metals and steels. *Current Opinion in Solid State and Materials Science*, **2016**, 20, 77-84	12	21
345	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. *Acta Materialia*, **2016**, 102, 241-250	8.4	15
344	Interplay between interstitial displacement and displacive lattice transformations. *Physical Review B*, **2016**, 94,	3.3	10
343	The impact of carbon and oxygen in alpha-titanium: ab initio study of solution enthalpies and grain boundary segregation. *Journal of Physics Condensed Matter*, **2016**, 28, 385001	1.8	9
342	Nonlinear elastic effects in phase field crystal and amplitude equations: Comparison to ab initio simulations of bcc metals and graphene. *Physical Review B*, **2016**, 93,	3.3	14
341	Ab□initio Prediction of Martensitic and Intermartensitic Phase Boundaries in Ni-Mn-Ga. *Physical Review Letters*, **2016**, 116, 025503	7.4	44
340	Deformation-Induced Martensite: A New Paradigm for Exceptional Steels. *Advanced Materials*, **2016** , 28, 7753-7	24	48
339	Electron and chemical reservoir corrections for point-defect formation energies. *Physical Review B*, **2016**, 93,	3.3	42
338	First-principles investigation of hydrogen interaction with TiC precipitates in □Fe. *Physical Review B* , **2016**, 93,	3.3	75
337	Impact of local magnetism on stacking fault energies: A first-principles investigation for fcc iron. *Physical Review B*, **2016**, 93,	3.3	27
336	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
335	Scale bridging description of coherent phase equilibria in the presence of surfaces and interfaces. *Physical Review B*, **2016**, 94,	3.3	7

334	Atomistic migration mechanisms of atomically flat, stepped, and kinked grain boundaries. *Physical Review B*, **2016**, 94,	3.3	23
333	Combined atom probe tomography and density functional theory investigation of the Al off-stoichiometry of κ-carbides in an austenitic Fe-Mn-Al-C low density steel. *Acta Materialia*, **2016**, 106, 229-238	8.4	73
332	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	1	9
331	The structure and dynamics of chitin nanofibrils in an aqueous environment revealed by molecular dynamics simulations. *RSC Advances*, **2016**, 6, 30710-30721	3.7	16
330	Multiscale modeling of hydrogen enhanced homogeneous dislocation nucleation. *Acta Materialia*, **2016**, 107, 144-151	8.4	18
329	Impact of magnetic fluctuations on lattice excitations in fcc nickel. *Journal of Physics Condensed Matter*, **2016**, 28, 076002	1.8	13
328	Ab Initio Determined Phase Diagram of Clean and Solvated Muscovite Mica Surfaces. *Langmuir*, **2016**, 32, 1027-33	4	4
327	First-principles calculation of the elastic dipole tensor of a point defect: Application to hydrogen in α-zirconium. *Physical Review B*, **2016**, 94,	3.3	19
326	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
325	A QM/MM approach for low-symmetry defects in metals. *Computational Materials Science*, **2016**, 118, 259-268	3.2	6
324	Changes in volume during the four months' remodelling period of iliac crest grafts in reconstruction of the alveolar ridge. *British Journal of Oral and Maxillofacial Surgery*, **2016**, 54, 751-6	1.4	13
323	Ab initio-guided design of twinning-induced plasticity steels. *MRS Bulletin*, **2016**, 41, 320-325	3.2	21
322	Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires. *Acta Materialia*, **2016**, 111, 321-334	8.4	25
321	Functional adaptation of crustacean exoskeletal elements through structural and compositional diversity: a combined experimental and theoretical study. *Bioinspiration and Biomimetics*, **2016**, 11, 055006	2.6	30
320	Identification of bulk oxide defects in an electrochemical environment. *Faraday Discussions*, **2015**, 180, 97-112	3.6	22
319	A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron. *Acta Materialia*, **2015**, 90, 69-76	8.4	45
318	From wetting to melting along grain boundaries using phase field and sharp interface methods. *Computational Materials Science*, **2015**, 108, 293-300	3.2	3
317	Ab initio study of compositional trends in solid solution strengthening in metals with low Peierls stresses. *Acta Materialia*, **2015**, 98, 367-376	8.4	18

316	From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium. *Physical Review B*, **2015**, 92,	3.3	22
315	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
314	Structural transformations among austenite, ferrite and cementite in Fe□ alloys: A unified theory based on ab initio simulations. *Acta Materialia*, **2015**, 99, 281-289	8.4	46
313	Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation. *Acta Materialia*, **2015**, 85, 53-66	8.4	37
312	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	1.8	9
311	Importance of coordination number and bond length in titanium revealed by electronic structure investigations. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 1907-1924	1.3	22
310	Improved method of calculating ab initio high-temperature thermodynamic properties with application to ZrC. *Physical Review B*, **2015**, 91,	3.3	60
309	Role of biaxial strain and microscopic ordering for structural and electronic properties of InxGa1□N. *Physical Review B*, **2015**, 92,	3.3	4
308	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
307	Mechanisms and kinetics of the migration of grain boundaries containing extended defects. *Physical Review B*, **2015**, 92,	3.3	15
306	Difference in linear polarization of biaxially strained InxGa1□N alloys on nonpolar a-plane and m-plane GaN. *Physical Review B*, **2015**, 92,	3.3	3
305	Comparison of design and torque measurements of various manual wrenches. *International Journal of Oral and Maxillofacial Implants*, **2015**, 30, 526-33	2.8	5
304	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	2.5	23
303	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	2.9	13
302	Ab initio-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	1.3	14
301	Interplay of strain and interdiffusion in Heusler alloy bilayers. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 321-325	2.5	5
300	Rapid theory-guided prototyping of ductile Mg alloys: from binary to multi-component materials. *New Journal of Physics*, **2015**, 17, 093009	2.9	29
299	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

298	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,	3.3	17
297	Multiscale description of dislocation induced nano-hydrides. *Acta Materialia*, **2015**, 89, 50-59	8.4	21
296	Influence of the dislocation core on the glide of the <1 1 1>{1 1 0} edge dislocation in bcc-iron: An embedded atom method study. *Computational Materials Science*, **2014**, 87, 274-282	3.2	11
295	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
294	Ab initio based study of finite-temperature structural, elastic and thermodynamic properties of FeTi. *Intermetallics*, **2014**, 45, 11-17	3.5	13
293	Extending the Concept of Defect Chemistry from Semiconductor Physics to Electrochemistry. *Physical Review Applied*, **2014**, 1,	4.3	54
292	Understanding and controlling indium incorporation and surface segregation on InxGa1N surfaces: An ab initio approach. *Physical Review B*, **2014**, 89,	3.3	41
291	Scale bridging between atomistic and mesoscale modelling: applications of amplitude equation descriptions. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 034001	2	5
290	Ab initio study of point defects in NiTi-based alloys. *Physical Review B*, **2014**, 89,	3.3	23
289	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	2.5	9
288	Phase-field modeling of grain-boundary premelting using obstacle potentials. *Physical Review E*, **2014**, 90, 012401	2.4	18
287	Reliability evaluation of thermophysical properties from first-principles calculations. *Journal of Physics Condensed Matter*, **2014**, 26, 335401	1.8	8
286	A generalized plane-wave formulation of . *Computational Materials Science*, **2014**, 95, 280-287	3.2	24
285	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	1	11
284	Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment. *Physical Review Letters*, **2014**, 113, 165503	7.4	68
283	Ab Initio Based Understanding of the Segregation and Diffusion Mechanisms of Hydrogen in Steels. *Jom*, **2014**, 66, 1399-1405	2.1	31
282	Ductility improvement of Mg alloys by solid solution: Ab initio modeling, synthesis and mechanical properties. *Acta Materialia*, **2014**, 70, 92-104	8.4	189
281	Perspectives on point defect thermodynamics. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 97-129	1.3	45

280	Impact of nanodiffusion on the stacking fault energy in high-strength steels. *Acta Materialia*, **2014**, 75, 147-155	8.4	57
279	Designing Heusler nanoprecipitates by elastic misfit stabilization in Fe Mn maraging steels. *Acta Materialia*, **2014**, 76, 94-105	8.4	53
278	Role of the mesoscale in migration kinetics of flat grain boundaries. *Physical Review B*, **2014**, 89,	3.3	30
277	Impact of Mn on the solution enthalpy of hydrogen in austenitic Fe-Mn alloys: a first-principles study. *Journal of Computational Chemistry*, **2014**, 35, 2239-44	3.5	6
276	Ordering phenomena and formation of nanostructures in InxGa1 N layers coherently grown on GaN(0001). *Physical Review B*, **2014**, 90,	3.3	17
275	Structural stability and thermodynamics of CrN magnetic phases from ab initio calculations and experiment. *Physical Review B*, **2014**, 90,	3.3	78
274	Macroscopic elastic properties of textured ZrN-AlN polycrystalline aggregates: From ab initio calculations to grain-scale interactions. *Physical Review B*, **2014**, 90,	3.3	28
273	Origin of the unusually strong luminescence of a-type screw dislocations in GaN. *Physical Review B*, **2014**, 90,	3.3	18
272	Influence of short-range forces on melting along grain boundaries. *Physical Review B*, **2014**, 89,	3.3	6
271	Negatively charged ions on Mg(0001) surfaces: appearance and origin of attractive adsorbate-adsorbate interactions. *Physical Review Letters*, **2014**, 113, 136102	7.4	17
270	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
269	First-principles calculations for point defects in solids. *Reviews of Modern Physics*, **2014**, 86, 253-305	40.5	1431
268	Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite. *Acta Materialia*, **2013**, 61, 1773-1784	8.4	32
267	Polarization effects due to thickness fluctuations in nonpolar InGaN/GaN quantum wells. *Applied Physics Letters*, **2013**, 103, 073115	3.4	7
266	Hidden surface states at non-polar GaN (101 0) facets: Intrinsic pinning of nanowires. *Applied Physics Letters*, **2013**, 103, 152101	3.4	39
265	Ab Initio Guided Design of Materials **2013**, 481-495		
264	Ab initio study of thermodynamic, electronic, magnetic, structural, and elastic properties of Ni4N allotropes. *Physical Review B*, **2013**, 88,	3.3	18
263	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	1.2	15

262	Density functional theory in materials science. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 438-448	7.9	80
261	Ab initio based conformational study of the crystalline α-chitin. *Biopolymers*, **2013**, 99, 22-34	2.2	24
260	Basal and non-basal dislocation slip in MgγY. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2013**, 576, 61-68	5.3	153
259	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	4.1	25
258	CHAPTER 9:Multi-scale Modelling of a Biological Material: The Arthropod Exoskeleton. *RSC Smart Materials*, **2013**, 197-218	0.6	2
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