Christoph Freysoldt

List of Publications by Year
in descending order

63 papers	5,706 citations	201674 27 h-index	118850 62 g-index
67 all docs	67 docs citations	67 times ranked	6699 citing authors

#	Article	IF	Citations
1	Reflections on the Spatial Performance of Atom Probe Tomography in the Analysis of Atomic Neighborhoods. Microscopy and Microanalysis, 2022, 28, 1116-1126.	0.4	16
2	Status and Direction of Atom Probe Analysis of Frozen Liquids. Microscopy and Microanalysis, 2022, 28, 1150-1167.	0.4	8
3	Limitations of empirical supercell extrapolation for calculations of point defects in bulk, at surfaces, and in two-dimensional materials. Physical Review B, 2022, 105, .	3.2	6
4	Dielectric Properties of Nanoconfined Water: A Canonical Thermopotentiostat Approach. Physical Review Letters, 2021, 126, 136803.	7.8	42
5	Effect of Cd diffusion on the electrical properties of the Cu(In,Ga)Se2 thin-film solar cell. Solar Energy Materials and Solar Cells, 2021, 224, 110989.	6.2	12
6	Atom probe tomography. Nature Reviews Methods Primers, 2021, 1, .	21.2	131
7	Segmentation of Static and Dynamic Atomic-Resolution Microscopy Data Sets with Unsupervised Machine Learning Using Local Symmetry Descriptors. Microscopy and Microanalysis, 2021, , 1-11.	0.4	1
8	Revealing atomic-scale vacancy-solute interaction in nickel. Scripta Materialia, 2021, 203, 114036.	5.2	7
9	Charged vacancy defects in monolayer phosphorene. Physical Review Materials, 2021, 5, .	2.4	5
10	Atomic relaxation around defects in magnetically disordered materials computed by atomic spin constraints within an efficient Lagrange formalism. Physical Review B, 2020, 102, .	3.2	15
11	Generalized dipole correction for charged surfaces in the repeated-slab approach. Physical Review B, 2020, 102, .	3.2	20
12	Finite-size corrections for defect-involving vertical transitions in supercell calculations. Physical Review B, 2020, 101, .	3.2	32
13	AbÂinitio Description of Bond Breaking in Large Electric Fields. Physical Review Letters, 2020, 124, 176801.	7.8	24
14	Stability of charged sulfur vacancies in 2D and bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm from plane-wave density functional theory with electrostatic corrections. Physical Review Materials, 2020, 4, .	2.4	24
15	First-principles investigation of charged dopants and dopant-vacancy defect complexes in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2020, 4, .	2.4	9
16	Titelbild: Discovery of Elusive K₄O₆, a Compound Stabilized by Configurational Entropy of Polarons (Angew. Chem. 1/2019). Angewandte Chemie, 2019, 131, 1-1.	2.0	49
17	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	8.7	79
18	Advances in Density-Functional Calculations for Materials Modeling. Annual Review of Materials Research, 2019, 49, 1-30.	9.3	87

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19	Imaging individual solute atoms at crystalline imperfections in metals. New Journal of Physics, 2019, 21, 123020.	2.9	26
20	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. Journal of Physical Chemistry C, 2019, 123, 3180-3187.	3.1	34
21	Discovery of Elusive K₄O₆, a Compound Stabilized by Configurational Entropy of Polarons. Angewandte Chemie, 2019, 131, 155-159.	2.0	2
22	Discovery of Elusive K₄O₆, a Compound Stabilized by Configurational Entropy of Polarons. Angewandte Chemie - International Edition, 2019, 58, 149-153.	13.8	9
23	First-principles calculations for charged defects at surfaces, interfaces, and two-dimensional materials in the presence of electric fields. Physical Review B, 2018, 97, .	3.2	71
24	Elastically frustrated rehybridization: Origin of chemical order and compositional limits in InGaN quantum wells. Physical Review Materials, 2018, 2, .	2.4	36
25	On-the-fly parameterization of internal coordinate force constants for quasi-Newton geometry optimization in atomistic calculations. Computational Materials Science, 2017, 133, 71-81.	3.0	7
26	Cd and Impurity Redistribution at the CdS/CIGS Interface After Annealing of CIGS-Based Solar Cells Resolved by Atom Probe Tomography. IEEE Journal of Photovoltaics, 2017, 7, 313-321.	2.5	19
27	First-Principles Study of Intrinsic Defects in Ammonia Borane. Journal of Physical Chemistry C, 2017, 121, 22680-22689.	3.1	7
28	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	3.2	70
29	Electronic structure of metastable bcc Cuâ€“Cr alloy thin films: Comparison of electron energy-loss spectroscopy and first-principles calculations. Ultramicroscopy, 2017, 178, 96-104.	1.9	8
30	Electron and chemical reservoir corrections for point-defect formation energies. Physical Review B, 2016, 93, .	3.2	50
31	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:mn>	3.2	6
32	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 mathvariant="normal">a</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></r	3.2	3
33	Cd and impurity redistribution at the p-n junction of CIGS based solar cells resolved by atom-probe tomography. , 2015, , .		1
34	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><mml:mi mathvariant="normal">N</mml:mi></mml:math>layers coherently grown on GaN(0001). Physical Review B, 2014, 90, .	3.2	20
35	Negatively Charged Ions on Mg(0001) Surfaces: Appearance and Origin of Attractive Adsorbate-Adsorbate Interactions. Physical Review Letters, 2014, 113, 136102.	7.8	21
36	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	45.6	1,967

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37	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...	3.0	31
38	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, .	3.2	15
39	Interfacial Structure and Chemistry of GaN on Ge(111). Physical Review Letters, 2013, 111, 256101.	7.8	5
40	The dangling-bond defect in amorphous silicon: Statistical random versus kinetically driven defect geometries. Journal of Non-Crystalline Solids, 2012, 358, 2063-2066.	3.1	14
41	Dangling bonds in amorphous silicon investigated by multifrequency EPR. Journal of Non-Crystalline Solids, 2012, 358, 2067-2070.	3.1	5
42	Ab initioEPR parameters for dangling-bond defect complexes in silicon: Effect of Jahn-Teller distortion. Physical Review B, 2012, 85, .	3.2	14
43	A flexible, plane-wave based multiband $${mathbf{k}cdotmathbf{p}}$$ model. Optical and Quantum Electronics, 2012, 44, 183-188.	3.3	24
44	A flexible, plane-wave-based formulation of continuum elasticity and multiband k·p models. , 2011, , .		1
45	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, .	3.2	31
46	Ab initiostudy of electron paramagnetic resonance hyperfine structure of the silicon dangling bond: Role of the local environment. Physical Review B, 2011, 83, .	3.2	7
47	Native defects in hexagonal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>I²</mml:mi></mml:mrow></mml:math>-Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: Physic...	3.2	35
48	Electrostatic interactions between charged defects in supercells. Physica Status Solidi (B): Basic Research, 2011, 248, 1067-1076.	1.5	395
49	The object-oriented DFT program library S/PHI/nX. Computer Physics Communications, 2011, 182, 543-554.	7.5	77
50	Construction and performance of fully numerical optimum atomic basis sets. Physical Review B, 2011, 84, .	3.2	2
51	Quasiparticle band offsets of semiconductor heterojunctions from a generalized marker method. Physical Review B, 2011, 84, .	3.2	12
52	Plane-wave implementation of the real-space formalism and continuum elasticity theory. Computer Physics Communications, 2010, 181, 765-771.	7.5	28
53	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:m... A density functional theory study. Physical Review B, 2010, 81, .	3.2	24
54	Controlling Polarization at Insulating Surfaces: Quasiparticle Calculations for Molecules Adsorbed on Insulator Films. Physical Review Letters, 2009, 103, 056803.	7.8	65

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55	FullyAb InitioFinite-Size Corrections for Charged-Defect Supercell Calculations. Physical Review Letters, 2009, 102, 016402.	7.8	1,093
56	Direct minimization technique for metals in density functional theory. Physical Review B, 2009, 79, .	3.2	47
57	Screening in two dimensions:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations for surfaces and thin films using the repeated-slab approach. Physical Review B, 2008, 77, .	3.2	71
58	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
59	Ultrathin Oxides: Bulk-Oxide-Like Model Surfaces or Unique Films?. Physical Review Letters, 2007, 99, 086101.	7.8	53
60	Dielectric anisotropy in the GW spaceâ€“time method. Computer Physics Communications, 2007, 176, 1-13.	7.5	46
61	An ab initio study of CO adsorption on ceria(110). Chemical Physics, 2005, 318, 180-190.	1.9	27
62	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	263
63	Influence of Coligands on the EPR Hyperfine Coupling Constants of the Cu(I)â^'NO System â^' A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 1582-1588.	2.5	11