

Christoph Freysoldt

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6174257/publications.pdf>

Version: 2024-02-01

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	First-principles calculations for point defects in solids. <i>Reviews of Modern Physics</i> , 2014, 86, 253-305.	45.6	1,967
2	Fully <i>Ab Initio</i> Finite-Size Corrections for Charged-Defect Supercell Calculations. <i>Physical Review Letters</i> , 2009, 102, 016402.	7.8	1,093
3	Electrostatic interactions between charged defects in supercells. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1067-1076.	1.5	395
4	Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. <i>New Journal of Physics</i> , 2005, 7, 126-126.	2.9	263
5	Atom probe tomography. <i>Nature Reviews Methods Primers</i> , 2021, 1, .	21.2	131
6	Advances in Density-Functional Calculations for Materials Modeling. <i>Annual Review of Materials Research</i> , 2019, 49, 1-30.	9.3	87
7	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	79
8	The object-oriented DFT program library S/PHI/nX. <i>Computer Physics Communications</i> , 2011, 182, 543-554.	7.5	77
9	Screening in two dimensions: $G \cdot W$ calculations for surfaces and thin films using the repeated-slab approach. <i>Physical Review B</i> , 2008, 77, .		71
10	First-principles calculations for charged defects at surfaces, interfaces, and two-dimensional materials in the presence of electric fields. <i>Physical Review B</i> , 2018, 97, .	3.2	71
11	Accurate electronic free energies of the d^3 transition metals at high temperatures. <i>Physical Review B</i> , 2019, 100, 045111.	3.2	70
12	Controlling Polarization at Insulating Surfaces: Quasiparticle Calculations for Molecules Adsorbed on Insulator Films. <i>Physical Review Letters</i> , 2009, 103, 056803.	7.8	65
13	Ultrathin Oxides: Bulk-Oxide-Like Model Surfaces or Unique Films?. <i>Physical Review Letters</i> , 2007, 99, 086101.	7.8	53
14	Electron and chemical reservoir corrections for point-defect formation energies. <i>Physical Review B</i> , 2016, 93, .	3.2	50
15	Titelbild: Discovery of Elusive K_4O_6 , a Compound Stabilized by Configurational Entropy of Polarons (<i>Angew. Chem.</i> 1/2019). <i>Angewandte Chemie</i> , 2019, 131, 1-1.	2.0	49
16	Direct minimization technique for metals in density functional theory. <i>Physical Review B</i> , 2009, 79, .	3.2	47
17	Dielectric anisotropy in the GW space-time method. <i>Computer Physics Communications</i> , 2007, 176, 1-13.	7.5	46
18	Dielectric Properties of Nanoconfined Water: A Canonical Thermopotentiostat Approach. <i>Physical Review Letters</i> , 2021, 126, 136803.	7.8	42

#	ARTICLE	IF	CITATIONS
19	Elastically frustrated rehybridization: Origin of chemical order and compositional limits in InGaN quantum wells. Physical Review Materials, 2018, 2.	2.4	36
20	Native defects in hexagonalI^2-Si3N4. Physical Review B, 2019, 100, 115402.	3.2	35
21	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. Journal of Physical Chemistry C, 2019, 123, 3180-3187.	3.1	34
22	Finite-size corrections for defect-involving vertical transitions in supercell calculations. Physical Review B, 2020, 101, .	3.2	32
23	Combined multifrequency EPR and DFT study of dangling bonds in generalized plane-wave formulation of Si:H. Physical Review B, 2011, 84, .	3.2	31
24	Plane-wave implementation of the real-space formalism and continuum elasticity approach to elastic and electronic properties of semiconductor nanostructures. Computational Materials Science Communications, 2010, 181, 765-771.	3.0	31
25	Plane-wave implementation of the real-space formalism and continuum elasticity theory. Computer Physics Communications, 2010, 181, 765-771.	7.5	28
26	An ab initio study of CO adsorption on ceria(110). Chemical Physics, 2005, 318, 180-190.	1.9	27
27	Imaging individual solute atoms at crystalline imperfections in metals. New Journal of Physics, 2019, 21, 123020.	2.9	26
28	Native and hydrogen-containing point defects in Mg3N4: A density functional theory study. Physical Review B, 2010, 81, .	3.2	24
29	A flexible, plane-wave based multiband $\mathbf{k} \cdot \mathbf{p}$ model. Optical and Quantum Electronics, 2012, 44, 183-188.	3.3	24
30	<i>Ab Initio</i> Description of Bond Breaking in Large Electric Fields. Physical Review Letters, 2020, 124, 176801.	7.8	24
31	Stability of charged sulfur vacancies in 2D and bulk MoS2 from plane-wave density functional theory with electrostatic corrections. Physical Review Materials, 2020, 4, .	2.4	24
32	Negatively Charged Ions on Mg(0001) Surfaces: Appearance and Origin of Attractive Adsorbate-Adsorbate Interactions. Physical Review Letters, 2014, 113, 136102.	7.8	21
33	Ordering phenomena and formation of nanostructures in GaNxN$1-x$ layers coherently grown on GaN(0001). Physical Review B, 2014, 90, .	3.2	20
34	Generalized dipole correction for charged surfaces in the repeated-slab approach. Physical Review B, 2020, 102, .	3.2	20
35	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
36	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

#	ARTICLE	IF	CITATIONS
37	Dangling-bond defect in a-Si:H: Characterization of network and strain effects by first-principles calculation of the EPR parameters. <i>Physical Review B</i> , 2013, 87, .	3.2	15
38	Atomic relaxation around defects in magnetically disordered materials computed by atomic spin constraints within an efficient Lagrange formalism. <i>Physical Review B</i> , 2020, 102, .	3.2	15
39	The dangling-bond defect in amorphous silicon: Statistical random versus kinetically driven defect geometries. <i>Journal of Non-Crystalline Solids</i> , 2012, 358, 2063-2066.	3.1	14
40	<i>Ab initio</i> EPR parameters for dangling-bond defect complexes in silicon: Effect of Jahn-Teller distortion. <i>Physical Review B</i> , 2012, 85, .	3.2	14
41	Quasiparticle band offsets of semiconductor heterojunctions from a generalized marker method. <i>Physical Review B</i> , 2011, 84, .	3.2	12
42	Effect of Cd diffusion on the electrical properties of the Cu(In,Ga)Se ₂ thin-film solar cell. <i>Solar Energy Materials and Solar Cells</i> , 2021, 224, 110989.	6.2	12
43	Influence of Coligands on the EPR Hyperfine Coupling Constants of the Cu(I)â ⁺ NO System â ⁺ A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1582-1588.	2.5	11
44	Discovery of Elusive K ₄ O ₆ , a Compound Stabilized by Configurational Entropy of Polarons. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 149-153.	13.8	9
45	First-principles investigation of charged dopants and dopant-vacancy defect complexes in monolayer MoS_2 . <i>Physical Review Materials</i> , 2020, 4, .		9
46	Electronic structure of metastable bcc Cuâ ⁺ Cr alloy thin films: Comparison of electron energy-loss spectroscopy and first-principles calculations. <i>Ultramicroscopy</i> , 2017, 178, 96-104.	1.9	8
47	Status and Direction of Atom Probe Analysis of Frozen Liquids. <i>Microscopy and Microanalysis</i> , 2022, 28, 1150-1167.	0.4	8
48	Specification of an extensible and portable file format for electronic structure and crystallographic data. <i>Computational Materials Science</i> , 2008, 43, 1056-1065.	3.0	7
49	<i>Ab initio</i> study of electron paramagnetic resonance hyperfine structure of the silicon dangling bond: Role of the local environment. <i>Physical Review B</i> , 2011, 83, .	3.2	7
50	On-the-fly parameterization of internal coordinate force constants for quasi-Newton geometry optimization in atomistic calculations. <i>Computational Materials Science</i> , 2017, 133, 71-81.	3.0	7
51	First-Principles Study of Intrinsic Defects in Ammonia Borane. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22680-22689.	3.1	7
52	Revealing atomic-scale vacancy-solute interaction in nickel. <i>Scripta Materialia</i> , 2021, 203, 114036.	5.2	7
53	Role of biaxial strain and microscopic ordering for structural and electronic properties of $\text{In}_x\text{Ga}_{1-x}\text{N}$. <i>Physical Review B</i> , 2015, 92, .	3.2	6
54	Limitations of empirical supercell extrapolation for calculations of point defects in bulk, at surfaces, and in two-dimensional materials. <i>Physical Review B</i> , 2022, 105, .	3.2	6

#	ARTICLE	IF	CITATIONS
55	Dangling bonds in amorphous silicon investigated by multifrequency EPR. Journal of Non-Crystalline Solids, 2012, 358, 2067-2070.	3.1	5
56	Interfacial Structure and Chemistry of GaN on Ge(111). Physical Review Letters, 2013, 111, 256101.	7.8	5
57	Charged vacancy defects in monolayer phosphorene. Physical Review Materials, 2021, 5, .	2.4	5
58	Difference in linear polarization of biaxially strained $I_n G_a$	3.2	3
59	Construction and performance of fully numerical optimum atomic basis sets. Physical Review B, 2011, 84, .	3.2	2
60	Discovery of Elusive K_4O_6 , a Compound Stabilized by Configurational Entropy of Polarons. Angewandte Chemie, 2019, 131, 155-159.	2.0	2
61	A flexible, plane-wave-based formulation of continuum elasticity and multiband k & p models. , 2011, , .		1
62	Cd and impurity redistribution at the p-n junction of CIGS based solar cells resolved by atom-probe tomography. , 2015, , .		1
63	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