Matthias Scheffler

List of Publications by Year
in descending order

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386	56,980	643 123	1158 229
papers	citations	h-index	g-index

398	398	398	33956
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accurate Molecular Van Der Waals Interactions from Ground-State Electron Density and Free-Atom Reference Data. Physical Review Letters, 2009, 102, 073005.	7.8	4,824
2	Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). Physical Review B, 1992, 46, 16067-16080.	3.2	2,339
3	Ab initio molecular simulations with numeric atom-centered orbitals. Computer Physics Communications, 2009, 180, 2175-2196.	7.5	2,170
4	Composition, structure, and stability ofRuO2(110)as a function of oxygen pressure. Physical Review B, 2001, 65, .	3.2	1,771
5	Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory. Computer Physics Communications, 1999, 119, 67-98.	7.5	1,313
6	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	7.8	1,120
7	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
8	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	10.3	778
9	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.	7.5	660
10	Big Data of Materials Science: Critical Role of the Descriptor. Physical Review Letters, 2015, 114, 105503.	7.8	658
11	The CO/Pt(111) Puzzle. Journal of Physical Chemistry B, 2001, 105, 4018-4025.	2.6	642
12	CO Oxidation as a Prototypical Reaction for Heterogeneous Processes. Angewandte Chemie - International Edition, 2011, 50, 10064-10094.	13.8	639
13	Resolution-of-identity approach to Hartreeâ€“Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. New Journal of Physics, 2012, 14, 053020.	2.9	549
14	Trends of the surface relaxations, surface energies, and work functions of the 4dtransition metals. Physical Review B, 1992, 46, 4816-4829.	3.2	532
15	Analysis of separable potentials. Physical Review B, 1991, 44, 8503-8513.	3.2	508
16	Density-Functional Theory with Screened vanÂderÂWaals Interactions for the Modeling of Hybrid Inorganic-Organic Systems. Physical Review Letters, 2012, 108, 146103.	7.8	503
17	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. Journal of Chemical Theory and Computation, 2013, 9, 3404-3419.	5.3	499
18	The Hematite (Î±- Fe2O3) (0001) Surface: Evidence for Domains of Distinct Chemistry. Physical Review Letters, 1998, 81, 1038-1041.	7.8	490

#	Article	IF	Citations
19	Hallmark of Perfect Graphene. Physical Review Letters, 2004, 92, 225502.	7.8	487
20	Random-phase approximation and its applications in computational chemistry and materials science. Journal of Materials Science, 2012, 47, 7447-7471.	3.7	479
21	Effect of the Environment onÎ±â˜Al2O3(0001) Surface Structures. Physical Review Letters, 2000, 84, 3650-3653.	7.8	473
22	Efficient integration for all-electron electronic structure calculation using numeric basis functions. Journal of Computational Physics, 2009, 228, 8367-8379.	3.8	454
23	Phonon- Versus Electron-Mediated Desorption and Oxidation of CO on Ru(0001). Science, 1999, 285, 1042-1045.	12.6	443
24	Composition and structure of theRuO2(110)surface in anO2and CO environment: Implications for the catalytic formation ofCO2. Physical Review B, 2003, 68, .	3.2	442
25	Adatom diffusion at GaN (0001) and (000Ì„) surfaces. Applied Physics Letters, 1998, 73, 487-489.	3.3	436
26	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
27	GaAs equilibrium crystal shape from first principles. Physical Review B, 1996, 54, 8844-8855.	3.2	383
28	First-Principles Atomistic Thermodynamics for Oxidation Catalysis: Surface Phase Diagrams and Catalytically Interesting Regions. Physical Review Letters, 2003, 90, 046103.	7.8	382
29	Evidence for site-sensitive screening of core holes at the Si and Ge (001) surface. Physical Review Letters, 1993, 71, 2338-2341.	7.8	377
30	Six-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Pd(100): Steering and Steric Effects. Physical Review Letters, 1995, 75, 2718-2721.	7.8	358
31	On the Accuracy of DFT for Describing Hydrogen Bonds:â€‰ Dependence on the Bond Directionality. Journal of Physical Chemistry A, 2004, 108, 5692-5698.	2.5	354
32	Sources of Electrical Conductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 055502.	7.8	352
33	SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. Physical Review Materials, 2018, 2, .	2.4	349
34	Multidimensional Potential Energy Surface forH2Dissociation over Cu(111). Physical Review Letters, 1994, 73, 1400-1403.	7.8	334
35	Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. Chemical Physics Letters, 2004, 395, 210-215.	2.6	311
36	First-principles kinetic Monte Carlo simulations for heterogeneous catalysis: Application to the CO oxidation atRuO2(110). Physical Review B, 2006, 73, .	3.2	299

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37	Adatom Kinetics On and Below the Surface: The Existence of a New Diffusion Channel. Physical Review Letters, 2003, 90, 056101.	7.8	293
38	The Steady State of Heterogeneous Catalysis, Studied by First-Principles Statistical Mechanics. Physical Review Letters, 2004, 93, 116105.	7.8	289
39	NOMAD: The FAIR concept for big data-driven materials science. MRS Bulletin, 2018, 43, 676-682.	3.5	288
40	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	5.3	280
41	Structural, Electronic, and Chemical Properties of Nanoporous Carbon. Physical Review Letters, 2006, 96, 046806.	7.8	272
42	Theoretical Evidence for an Optically Inducible Structural Transition of the Isolated As Antisite in GaAs: Identification and Explanation ofEL2?. Physical Review Letters, 1988, 60, 2183-2186.	7.8	267
43	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3944-3951.	5.3	265
44	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
45	Reconstruction mechanism of fcc transition metal (001) surfaces. Physical Review Letters, 1993, 71, 1051-1054.	7.8	262
46	Dissociation ofO2at Al(111): The Role of Spin Selection Rules. Physical Review Letters, 2005, 94, 036104.	7.8	259
47	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. MRS Bulletin, 2010, 35, 435-442.	3.5	257
48	Oxygen adsorption on Ag(111): A density-functional theory investigation. Physical Review B, 2002, 65, .	3.2	256
49	Improving the efficiency of FP-LAPW calculations. Computer Physics Communications, 2000, 126, 294-309.	7.5	252
50	Converged properties of clean metal surfaces by all-electron first-principles calculations. Surface Science, 2006, 600, 703-715.	1.9	252
51	Self-consistent study of the electronic and structural properties of the clean Si(001)(2 Ã— 1) surface. Applied Surface Science, 1992, 56-58, 15-19.	6.1	250
52	Simultaneous calculation of the equilibrium atomic structure and its electronic ground state using density-functional theory. Computer Physics Communications, 1994, 79, 447-465.	7.5	249
53	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	3.2	243
54	Insightful classification of crystal structures using deep learning. Nature Communications, 2018, 9, 2775.	12.8	237

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55	Theory of self-diffusion at and growth of Al(111). Physical Review Letters, 1994, 72, 254-257.	7.8	231
56	Island Nucleation in Thin-Film Epitaxy: A First-Principles Investigation. Physical Review Letters, 2000, 84, 5371-5374.	7.8	226
57	The influence of lateral interactions on the vibrational spectrum of adsorbed CO. Surface Science, 1979, 81, 562-570.	1.9	225
58	Dispersion-corrected MÃ¸llerâ€“Plesset second-order perturbation theory. Journal of Chemical Physics, 2009, 131, 094106.	3.0	223
59	First-principles modeling of localized<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>states with the<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:mo>@</mml:mo><mml:mtext>LDA</mml:mtext><mml:mr Physical Review B, 2010, 82, .	3.2	222
60	Structure and Stability of a High-Coverage(1Ã—1)Oxygen Phase on Ru(0001). Physical Review Letters, 1996, 77, 3371-3374.	7.8	220
61	Calculated atomic structures and electronic properties of GaP, InP, GaAs, and InAs (110) surfaces. Physical Review B, 1991, 44, 6188-6198.	3.2	219
62	The adsorption of oxygen at GaN surfaces. Applied Physics Letters, 1999, 74, 1695-1697.	3.3	219
63	Defect Formation Energies without the Band-Gap Problem: Combining Density-Functional Theory and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Approach for the Silicon Self-Interstitial. Physical Review Letters, 2009, 102, 026402.	7.8	218
64	Modeling Adsorption and Reactions of Organic Molecules at Metal Surfaces. Accounts of Chemical Research, 2014, 47, 3369-3377.	15.6	218
65	Abinitiocalculations of energies and self-diffusion on flat and stepped surfaces of Al and their implications on crystal growth. Physical Review B, 1996, 53, 4958-4973.	3.2	212
66	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. Journal of Chemical Physics, 2008, 129, 194111.	3.0	211
67	Local Chemical Reactivity of a Metal Alloy Surface. Physical Review Letters, 1995, 74, 3487-3490.	7.8	210
68	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. Journal of Chemical Physics, 2007, 127, 184104.	3.0	208
69	A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. Catalysis Reviews - Science and Engineering, 2011, 53, 424-514.	12.9	205
70	Surface core-level shifts of some 4d-metal single-crystal surfaces: Experiments andabinitiocalculations. Physical Review B, 1994, 50, 17525-17533.	3.2	201
71	The Pd()â€“R27Â°-O surface oxide revisited. Surface Science, 2003, 541, 101-112.	1.9	201
72	Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange correlation. Physical Review B, 1998, 57, 2134-2145.	3.2	197

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73	Catalysis and corrosion: the theoretical surface-science context. Surface Science, 2002, 500, 368-394.	1.9	197
74	Thermodynamic stability of PdO surfaces. Physical Review B, 2004, 69, .	3.2	193
75	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	7.8	193
76	Beyond the Random-Phase Approximation for the Electron Correlation Energy: The Importance of Single Excitations. Physical Review Letters, 2011, 106, 153003.	7.8	193
77	Influence of surface stress on the equilibrium shape of strained quantum dots. Physical Review B, 1998, 58, 4566-4571.	3.2	192
78	Unusual chemisorption geometry of Na on Al(111). Physical Review Letters, 1991, 67, 2163-2166.	7.8	191
79	Electronic band structure of zirconia and hafnia polymorphs from the<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>perspective. Physical Review B, 2010, 81, .	3.2	191
80	GaAs(001) Surface under Conditions of Low As Pressure: Evidence for a Novel Surface Geometry. Physical Review Letters, 2000, 85, 3890-3893.	7.8	189
81	Electronic and structural properties of GaN by the full-potential linear muffin-tin orbitals method: The role of thedelectrons. Physical Review B, 1993, 47, 13353-13362.	3.2	188
82	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. New Journal of Physics, 2018, 20, 063020.	2.9	185
83	First-Principles Theory of Surface Thermodynamics and Kinetics. Physical Review Letters, 1999, 83, 2993-2996.	7.8	181
84	Jahn-Teller Stabilization of a â€œPolarâ€•Metal Oxide Surface:Fe3O4(001). Physical Review Letters, 2005, 94, 126101.	7.8	180
85	Why is a Noble Metal Catalytically Active? The Role of the O-Ag Interaction in the Function of Silver as an Oxidation Catalyst. Physical Review Letters, 2003, 90, 256102.	7.8	178
86	Insights into the function of silver as an oxidation catalyst byab initioatomistic thermodynamics. Physical Review B, 2003, 68, .	3.2	178
87	Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code WIEN. Computer Physics Communications, 1996, 94, 31-48.	7.5	177
88	Novel Diffusion Mechanism on the GaAs(001) Surface: The Role of Adatom-Dimer Interaction. Physical Review Letters, 1997, 79, 5278-5281.	7.8	175
89	Isolated arsenic-antisite defect in GaAs and the properties ofEL2. Physical Review B, 1989, 40, 10391-10401.	3.2	172
90	Strain dependence of surface diffusion: Ag on Ag(111) and Pt(111). Physical Review B, 1997, 55, 6750-6753.	3.2	171

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91	The NOMAD laboratory: from data sharing to artificial intelligence. JPhys Materials, 2019, 2, 036001.	4.2	171
92	Adsorption of Xe Atoms on Metal Surfaces: New Insights from First-Principles Calculations. Physical Review Letters, 2003, 90, 066104.	7.8	168
93	Preserving the Half-Metallicity at the Heusler AlloyCo2MnSi(001)Surface: A Density Functional Theory Study. Physical Review Letters, 2005, 94, 096402.	7.8	167
94	Quantum Theory of Dissociative Chemisorption on Metal Surfaces. Accounts of Chemical Research, 2002, 35, 193-200.	15.6	165
95	Structure Determination of Isolated Metal Clusters via Far-Infrared Spectroscopy. Physical Review Letters, 2004, 93, 023401.	7.8	161
96	Theoretical study of O adlayers on Ru(0001). Physical Review B, 1996, 54, 2868-2872.	3.2	160
97	Atomic Structure of theGaAs(001)â˜(2Ã—4)Surface Resolved Using Scanning Tunneling Microscopy and First-Principles Theory. Physical Review Letters, 1999, 83, 2989-2992.	7.8	159
98	Ab initioquantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). Physical Review B, 1998, 57, 2493-2506.	3.2	158
99	First-Principles Optical Spectra for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers in MgO. Physical Review Letters, 2012, 108, 126404.	7.8	157
100	Beyond Scaling Relations for the Description of Catalytic Materials. ACS Catalysis, 2019, 9, 2752-2759.	11.2	157
101	Localized and Itinerant States in Lanthanide Oxides United by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi><mml:mtext>â€‰</mml:mtext><mml:mo>@</mml:mo><mml:mtext> Physical Review Letters, 2009, 102, 126403.	7.8	156
102	Ghost states for separable, norm-conserving, Iab initioP pseudopotentials. Physical Review B, 1990, 41, 12264-12267.	3.2	155
103	Benchmark of<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>methods for azabenzenes. Physical Review B, 2012, 86, .	3.2	154
104	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. Applied Physics Letters, 2009, 95, .	3.3	151
105	Negative thermal expansion of diamond and zinc-blende semiconductors. Physical Review Letters, 1989, 63, 290-293.	7.8	147
106	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). Physical Review B, 2009, 80, .	3.2	147
107	High-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Cu(111). Physical Review Letters, 1994, 73, 3121-3124.	7.8	145
108	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	7.8	143

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109	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. New Journal of Physics, 2013, 15, 053046.	2.9	143
110	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	2.9	137
111	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. Applied Physics Letters, 2012, 100, .	3.3	136
112	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. Physical Review B, 2003, 67, .	3.2	135
113	Self-consistent<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>: All-electron implementation with localized basis functions. Physical Review B, 2013, 88, .	3.2	135
114	Theory of adsorption and surfactant effect of Sb on Ag(111). Physical Review Letters, 1993, 71, 2437-2440.	7.8	134
115	Anisotropy of Growth of the Close-Packed Surfaces of Silver. Physical Review Letters, 1996, 77, 1095-1098.	7.8	133
116	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. Computer Physics Communications, 2015, 192, 60-69.	7.5	133
117	Mechanisms of island formation of alkali-metal adsorbates on Al(111). Physical Review Letters, 1993, 71, 577-580.	7.8	129
118	Oxygen Overlayers on Pd(111) Studied by Density Functional Theoryâ€. Journal of Physical Chemistry B, 2004, 108, 14477-14483.	2.6	129
119	Alloy surface segregation in reactive environments: First-principles atomistic thermodynamics study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>Ag</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>Pd</mml:mi><mml:mn> oxygen atmospheres. Physical Review B, 2008, 77, .	3.2	129
120	Effect of a humid environment on the surface structure ofRuO2(110). Physical Review B, 2003, 67, .	3.2	127
121	First-Principles Statistical Mechanics Study of the Stability of a Subnanometer Thin Surface Oxide in Reactive Environments: CO Oxidation at Pd(100). Physical Review Letters, 2007, 98, 046101.	7.8	127
122	Origins of optical absorption and emission lines in AlN. Applied Physics Letters, 2014, 105, .	3.3	127
123	Total-energy gradients and lattice distortions at point defects in semiconductors. Physical Review B, 1985, 31, 6541-6551.	3.2	125
124	First-principles calculation of the thermal properties of silver. Physical Review B, 1999, 59, 965-969.	3.2	124
125	Two-Step Mechanism for Low-Temperature Oxidation of Vacancies in Graphene. Physical Review Letters, 2009, 102, 166104.	7.8	122
126	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. Chemical Physics Letters, 2002, 352, 311-317.	2.6	120

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127	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. Journal of Chemical Physics, 2007, 126, 204711.	3.0	120
128	Metastable precursors during the oxidation of the Ru(0001) surface. Physical Review B, 2002, 65, .	3.2	119
129	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. Journal of Chemical Physics, 2013, 139, 154702.	3.0	119
130	COoxidation atPd(100): A first-principles constrained thermodynamics study. Physical Review B, 2007, 75, .	3.2	116
131	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. Physical Review B, 2013, 88, .	3.2	115
132	Descriptions of surface chemical reactions using a neural network representation of the potential-energy surface. Physical Review B, 2006, 73, .	3.2	113
133	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. Physical Review B, 2013, 88, .	3.2	113
134	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Physical Review B, 2008, 77, .	3.2	112
135	Magnetism in C- or N-doped MgO and ZnO: A Density-Functional Study of Impurity Pairs. Physical Review Letters, 2010, 105, 267203.	7.8	111
136	Towards an Exact Treatment of Exchange and Correlation in Materials: Application to the â€œCO Adsorption Puzzleâ€•and Other Systems. Physical Review Letters, 2007, 98, 176103.	7.8	110
137	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metalâ^Phthalocyanine Dimers. Journal of Chemical Theory and Computation, 2010, 6, 81-90.	5.3	109
138	Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor. Physical Review B, 2013, 87, .	3.2	109
139	When seeing is not believing: Oxygen on Ag(111), a simple adsorption system?. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1487-1497.	2.1	108
140	Influence of the Core-Valence Interaction and of the Pseudopotential Approximation on the Electron Self-Energy in Semiconductors. Physical Review Letters, 2008, 101, 106404.	7.8	107
141	Physical origin of exchange diffusion on fcc(100) metal surfaces. Physical Review B, 1997, 56, R15569-R15572.	3.2	104
142	Concentration of Vacancies at Metal-Oxide Surfaces: Case Study of MgO(100). Physical Review Letters, 2013, 111, 045502.	7.8	104
143	Temperatureâ€Đependent Morphology, Magnetic and Optical Properties of Liâ€Đoped MgO. ChemCatChem, 2010, 2, 854-862.	3.7	102
144	Roadmap on organicâ€“inorganic hybrid perovskite semiconductors and devices. APL Materials, 2021, 9, .	5.1	102

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145	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.	2.6	100
146	Effects of strain on the band structure of group-III nitrides. Physical Review B, 2014, 90, .	3.2	100
147	Learning physical descriptors for materials science by compressed sensing. New Journal of Physics, 2017, 19, 023017.	2.9	100
148	Parameter-free calculations of total energies, interatomic forces and vibrational entropies of defects in semiconductors. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 107-121.	0.6	99
149	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. Physical Review Letters, 1998, 80, 3097-3100.	7.8	99
150	Examination of the concept of degree of rate control by first-principles kinetic Monte Carlo simulations. Surface Science, 2009, 603, 1724-1730.	1.9	99
151	Unraveling the Stability of Polypeptide Helices: Critical Role of van der Waals Interactions. Physical Review Letters, 2011, 106, 118102.	7.8	97
152	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. New Journal of Physics, 2015, 17, 093020.	2.9	97
153	Simultaneous learning of several materials properties from incomplete databases with multi-task SISSO. JPhys Materials, 2019, 2, 024002.	4.2	97
154	Electronic properties of lanthanide oxides from the<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>perspective. Physical Review B, 2012, 86, .	3.2	96
155	New Perspective on Formation Energies and Energy Levels of Point Defects in Nonmetals. Physical Review Letters, 2012, 108, 066404.	7.8	96
156	Xe adsorption on metal surfaces: First-principles investigations. Physical Review B, 2005, 72, .	3.2	94
157	Partial Dissociation of Water on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>001</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 252 Td (stretchy="false Review Letters, 2009, 103, 176102.	7.8	94
158	Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. Journal of Chemical Physics, 2009, 130, 184707.	3.0	94
159	Atomic and electronic structures of GaAs(110) and their alkali-adsorption-induced changes. Physical Review Letters, 1991, 67, 1031-1034.	7.8	92
160	Effect of strain on surface diffusion in semiconductor heteroepitaxy. Physical Review B, 2001, 64, .	3.2	92
161	All-electron formalism for total energy strain derivatives and stress tensor components for numeric atom-centered orbitals. Computer Physics Communications, 2015, 190, 33-50.	7.5	92
162	AB Initio Atomistic Thermodynamics and Statistical Mechanics of Surface Properties and Functions. , 2005, , 149-194.		91

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163	Island morphology and adatom self-diffusion on Pt(111). Physical Review B, 1998, 57, 1881-1889.	3.2	90
164	Experimental and theoretical study of oxygen adsorption structures on Ag(111). Physical Review B, 2009, 80, .	3.2	90
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