Georg Kresse

List of Publications by Year
in descending order

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378	316,300	863 117	75 371
papers	citations	h-index	g-index

385	385	385	81296
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Efficient iterative schemes forab initiototal-energy calculations using a plane-wave basis set. Physical Review B, 1996, 54, 11169-11186.	1.1	88,250
2	From ultrasoft pseudopotentials to the projector augmented-wave method. Physical Review B, 1999, 59, 1758-1775.	1.1	61,625
3	Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Computational Materials Science, 1996, 6, 15-50.	1.4	54,900
4	Ab initiomolecular dynamics for liquid metals. Physical Review B, 1993, 47, 558-561.	1.1	35,096
5	Ab initiomolecular-dynamics simulation of the liquid-metalâ€“amorphous-semiconductor transition in germanium. Physical Review B, 1994, 49, 14251-14269.	1.1	17,829
6	Ab initiomolecular dynamics for open-shell transition metals. Physical Review B, 1993, 48, 13115-13118.	1.1	6,534
7	Norm-conserving and ultrasoft pseudopotentials for first-row and transition elements. Journal of Physics Condensed Matter, 1994, 6, 8245-8257.	0.7	2,947
8	Linear optical properties in the projector-augmented wave methodology. Physical Review B, 2006, 73, .	1.1	2,450
9	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	16.4	1,967
10	Screened hybrid density functionals applied to solids. Journal of Chemical Physics, 2006, 124, 154709.	1.2	1,915
11	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
12	Self-consistentGWcalculations for semiconductors and insulators. Physical Review B, 2007, 75, .	1.1	800
13	Implementation and performance of the frequency-dependentGWmethod within the PAW framework. Physical Review B, 2006, 74, .	1.1	785
14	Ab initio molecular dynamics for liquid metals. Journal of Non-Crystalline Solids, 1995, 192-193, 222-229.	1.5	756
15	The Perdewâ€“Burkeâ€“Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set. Journal of Chemical Physics, 2005, 122, 234102.	1.2	754
16	Fully unconstrained noncollinear magnetism within the projector augmented-wave method. Physical Review B, 2000, 62, 11556-11570.	1.1	707
17	Ab initio Force Constant Approach to Phonon Dispersion Relations of Diamond and Graphite. Europhysics Letters, 1995, 32, 729-734.	0.7	663
18	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655

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19	First-principles investigation of phase stability inLixCoO2. Physical Review B, 1998, 58, 2975-2987.	1.1	632
20	Accurate Quasiparticle Spectra from Self-ConsistentGWCalculations with Vertex Corrections. Physical Review Letters, 2007, 99, 246403.	2.9	606
21	Hybrid functional studies of the oxygen vacancy in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2010, 81, .	1.1	554
22	Hybrid functionals applied to rare-earth oxides: The example of ceria. Physical Review B, 2007, 75, .	1.1	502
23	Hybrid functionals applied to extended systems. Journal of Physics Condensed Matter, 2008, 20, 064201.	0.7	500
24	Novel Stabilization Mechanism on Polar Surfaces: ZnO(0001)-Zn. Physical Review Letters, 2003, 90, 016102.	2.9	493
25	Quasiparticle band structure based on a generalized Kohn-Sham scheme. Physical Review B, 2007, 76, .	1.1	483
26	Why does the B3LYP hybrid functional fail for metals?. Journal of Chemical Physics, 2007, 127, 024103.	1.2	481
27	Accurate surface and adsorption energies from many-body perturbation theory. Nature Materials, 2010, 9, 741-744.	13.3	476
28	Towards an exact description of electronic wavefunctions in real solids. Nature, 2013, 493, 365-370.	13.7	440
29	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> a potential photovoltaic material: A hybrid Hartree-Fock density functional theory study. Physical Review B, 2009, 79, .	1.1	402
30	Assessing the quality of the random phase approximation for lattice constants and atomization energies of solids. Physical Review B, 2010, 81, .	1.1	398
31	Theory of the crystal structures of selenium and tellurium: The effect of generalized-gradient corrections to the local-density approximation. Physical Review B, 1994, 50, 13181-13185.	1.1	378
32	Direct View at Excess Electrons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and Anatase. Physical Review Letters, 2014, 113, 086402.	2.9	373
33	Ab initiocalculation of the structural and electronic properties of carbon and boron nitride using ultrasoft pseudopotentials. Physical Review B, 1994, 50, 15606-15622.	1.1	370
34	Ab initiocalculation of the lattice dynamics and phase diagram of boron nitride. Physical Review B, 1999, 59, 8551-8559.	1.1	359
35	Accurate Bulk Properties from Approximate Many-Body Techniques. Physical Review Letters, 2009, 103, 056401.	2.9	359
36	Ab initiostudy of the (0001) surfaces of hematite and chromia: Influence of strong electronic correlations. Physical Review B, 2004, 70, .	1.1	357

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37	Ab Initio Study of the H2â€“H2S/MoS2 Gasâ€“Solid Interface: The Nature of the Catalytically Active Sites. Journal of Catalysis, 2000, 189, 129-146.	3.1	350
38	Structure of the Ultrathin Aluminum Oxide Film on NiAl(110). Science, 2005, 308, 1440-1442.	6.0	342
39	Shape and Edge Sites Modifications of MoS2 Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study. Journal of Catalysis, 2002, 207, 76-87.	3.1	337
40	Density functional study of CO on Rh(111). Physical Review B, 2004, 70, .	1.1	337
41	Competing stabilization mechanism for the polar ZnO(0001)-Zn surface. Physical Review B, 2003, 68, .	1.1	335
42	Cohesive Properties and Asymptotics of the Dispersion Interaction in Graphite by the Random Phase Approximation. Physical Review Letters, 2010, 105, 196401.	2.9	330
43	Cohesive energy curves for noble gas solids calculated by adiabatic connection fluctuation-dissipation theory. Physical Review B, 2008, 77, .	1.1	327
44	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. Physical Review B, 1997, 56, 15629-15646.	1.1	324
45	Structure, Energetics, and Electronic Properties of the Surface of a Promoted MoS2 Catalyst: An ab Initio Local Density Functional Study. Journal of Catalysis, 2000, 190, 128-143.	3.1	321
46	Accurate density functional calculations for the phonon dispersion relations of graphite layer and carbon nanotubes. Physical Review B, 2003, 67, .	1.1	310
47	Dielectric properties and excitons for extended systems from hybrid functionals. Physical Review B, 2008, 78, .	1.1	303
48	First-principles calculations of the radial breathing mode of single-wall carbon nanotubes. Physical Review B, 1998, 58, R8869-R8872.	1.1	294
49	First-principles study of the adsorption of atomic H on Ni (111), (100) and (110). Surface Science, 2000, 459, 287-302.	0.8	294
50	Improved hybrid functional for solids: The HSEsol functional. Journal of Chemical Physics, 2011, 134, 024116.	1.2	292
51	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. Physical Review B, 2007, 75, .	1.1	288
52	Defect formation and phase stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu material. Physical Review B, 2010, 81, .	1.1	287
53	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. Physical Review B, 2010, 82, .	1.1	279
54	Calculation of the magnetic anisotropy with projected-augmented-wave methodology and the case study of disordered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review B, 2016, 93, .	1.1	279

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55	Performance of the Vienna ab initio simulation package (VASP) in chemical applications. Computational and Theoretical Chemistry, 2003, 624, 37-45.	1.5	275
56	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. Physical Review B, 2014, 90, .	1.1	271
57	Two-Dimensional Oxide on Pd(111). Physical Review Letters, 2002, 88, 246103.	2.9	267
58	The viscosity of liquid iron at the physical conditions of the Earth's core. Nature, 1998, 392, 805-807.	13.7	259
59	Theory of polaron bandwidth narrowing in organic molecular crystals. Physical Review B, 2004, 69, .	1.1	253
60	Phase Transitions of Hybrid Perovskites Simulated by Machine-Learning Force Fields Trained on the Fly with Bayesian Inference. Physical Review Letters, 2019, 122, 225701.	2.9	250
61	Tunable ferroelectric polarization and its interplay with spinâ€“orbit coupling in tin iodide perovskites. Nature Communications, 2014, 5, 5900.	5.8	247
62	Structure and dynamics of liquid iron under Earthâ€™s core conditions. Physical Review B, 2000, 61, 132-142.	1.1	245
63	Dimer reconstruction and electronic surface states on clean and hydrogenated diamond (100) surfaces. Physical Review B, 1996, 53, 7334-7351.	1.1	240
64	Graphene on Ni(111): Strong interaction and weak adsorption. Physical Review B, 2011, 84, .	1.1	239
65	Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites. Scientific Reports, 2016, 6, 28618.	1.6	234
66	On-the-fly machine learning force field generation: Application to melting points. Physical Review B, 2019, 100, .	1.1	233
67	Electronic correlation effects in transition-metal sulfides. Journal of Physics Condensed Matter, 2003, 15, 979-996.	0.7	231
68	Making the random phase approximation to electronic correlation accurate. Journal of Chemical Physics, 2009, 131, 154115.	1.2	227
69	Significance of single-electron energies for the description of CO on Pt(111). Physical Review B, 2003, 68, .	1.1	225
70	A systematic study of the surface energetics and structure of TiO2(110) by first-principles calculations. Surface Science, 1997, 385, 386-394.	0.8	224
71	The shortcomings of semi-local and hybrid functionals: what we can learn from surface science studies. New Journal of Physics, 2008, 10, 063020.	1.2	222
72	The AM05 density functional applied to solids. Journal of Chemical Physics, 2008, 128, 084714.	1.2	220

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73	<math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mtext>/</mml:mtext></mml:mrow><mml:msub><mml:mrow><mml:mtext>BaTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></math> using the projector augmented wave method: Performance of hybrid and semilocal functionals. Physical Review B, 2008, 78, .	1.1	219
74	Adsorption and diffusion of water on graphene from first principles. Physical Review B, 2011, 84, .	1.1	218
75	Molecular adsorption on the surface of strongly correlated transition-metal oxides: A case study for CO/NiO(100). Physical Review B, 2004, 69, .	1.1	216
76	Theory of Spin-Conserving Excitation of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi><mml:mo>â^'</mml:mo><mml:msup><mml:mi>V</mml:mi><mml:mo>â^'</mml:mo></mml:msup> in Diamond. Physical Review Letters, 2009, 103, 186404.	2.9	206
77	High Pressure Polymorphism in Silica. Physical Review Letters, 1998, 80, 2145-2148.	2.9	205
78	Self-Limited Growth of a Thin Oxide Layer on Rh(111). Physical Review Letters, 2004, 92, 126102.	2.9	198
79	Second-order MÃ¸llerâ€“Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. Journal of Chemical Physics, 2009, 130, 184103.	1.2	194
80	The adsorption and dissociation of ROH molecules on TiO2(110). Surface Science, 1998, 409, 336-349.	0.8	192
81	Dissociation and sticking ofH2on the Ni(111), (100), and (110) substrate. Physical Review B, 2000, 62, 8295-8305.	1.1	191
82	Ionization Potentials of Solids: The Importance of Vertex Corrections. Physical Review Letters, 2014, 112, 096401.	2.9	184
83	Structural and electronic properties of lead chalcogenides from first principles. Physical Review B, 2007, 75, .	1.1	182
84	Phonon Softening in Metallic Nanotubes by a Peierls-like Mechanism. Physical Review Letters, 2002, 88, 235506.	2.9	180
85	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	1.1	180
86	Accurate band structures and effective masses for InP, InAs, and InSb using hybrid functionals. Physical Review B, 2009, 80, .	1.1	177
87	BrÃ¸nsted Acid Sites in HSAPO-34 and Chabazite:â€‰ An Ab Initio Structural Study. Journal of Physical Chemistry B, 1998, 102, 5573-5580.	1.2	166
88	Heyd-Scuseria-Ernzerhof hybrid functional for calculating the lattice dynamics of semiconductors. Physical Review B, 2009, 80, .	1.1	164
89	First-principles calculations to describe zirconia pseudopolymorphs. Physical Review B, 1999, 59, 4044-4052.	1.1	162
90	Ab initiocalculation of the origin of the distortion of Î±-PbO. Physical Review B, 1999, 59, 8481-8486.	1.1	160

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91	Density functional theory study of MnO by a hybrid functional approach. Physical Review B, 2005, 72, .	1.1	160
92	Predictive<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m using plane waves and pseudopotentials. Physical Review B, 2014, 90, .	1.1	157
93	Site preference of CO chemisorbed on Pt(111) from density functional calculations. Surface Science, 2003, 530, 71-87.	0.8	155
94	Transition metals to sulfur binding energies relationship to catalytic activities in HDS: back to Sabatier with first principle calculations1This work has been undertaken within the â€œGdR Dynamique MolÃ©culaire Quantique AppliquÃ©e Ã la Catalyseâ€, a joint project of Centre National de la Recherche Scientifique, Technische UniversitÃt Wien, and Institut FranÃ§ais du PÃ©trole.1. Catalysis Today, 1999, 50, 629-636.	2.2	152
95	Second-order MÃ¸llerâ€“Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. Journal of Chemical Physics, 2010, 133, 074107.	1.2	147
96	Stabilization Principles for Polar Surfaces of ZnO. ACS Nano, 2011, 5, 5987-5994.	7.3	144
97	Structure ofAg(111)â^'p(4Ã—4)â^'O: No Silver Oxide. Physical Review Letters, 2006, 96, 146102.	2.9	141
98	Dual behavior of excess electrons in rutile TiO₂. Physica Status Solidi - Rapid Research Letters, 2013, 7, 199-203.	1.2	140
99	Cubic scaling algorithm for the random phase approximation: Self-interstitials and vacancies in Si. Physical Review B, 2014, 90, .	1.1	138
100	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	1.2	137
101	Chemisorption of H on Pd(111): Anabinitioapproach with ultrasoft pseudopotentials. Physical Review B, 1996, 54, 2157-2166.	1.1	135
102	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. Physical Review B, 2007, 76, .	1.1	133
103	Ab initio simulation of the metal/nonmetal transition in expanded fluid mercury. Physical Review B, 1997, 55, 7539-7548.	1.1	131
104	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	1.2	131
105	Adsorption Sites and Ligand Effect for CO on an Alloy Surface: A Direct View. Physical Review Letters, 2001, 87, 036103.	2.9	129
106	Adsorption of Thiophene on the Catalytically Active Surface ofMoS2: AnAb InitioLocal-Density-Functional Study. Physical Review Letters, 1998, 80, 1481-1484.	2.9	128
107	Adsorption of Methanol on TiO2(110):Â A First-Principles Investigation. Journal of Physical Chemistry B, 1998, 102, 2017-2026.	1.2	127
108	Atomic and electronic structure of icosahedral Al-Pd-Mn alloys and approximant phases. Physical Review B, 1995, 51, 17355-17378.	1.1	124

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109	First-order phase transitions by first-principles free-energy calculations: The melting of Al. Physical Review B, 1998, 57, 8223-8234.	1.1	124
110	Growth and structure of ultrathin vanadium oxide layers on Pd(111). Physical Review B, 2000, 61, 13945-13954.	1.1	124
111	Why clathrates are good thermoelectrics: A theoretical study of Sr8Ga16Ge30. Journal of Chemical Physics, 1999, 111, 3133-3144.	1.2	123
112	Oxygen-Deficient Line Defects in an Ultrathin Aluminum Oxide Film. Physical Review Letters, 2006, 97, 046101.	2.9	123
113	Nanotemplate with Holes: Ultrathin Alumina onNi3Al(111). Physical Review Letters, 2007, 99, 196104.	2.9	122
114	Unraveling the Jahn-Teller effect in Mn-doped GaN using the Heyd-Scuseria-Ernzerhof hybrid functional. Physical Review B, 2009, 79, .	1.1	122
115	Anomalous behavior of the semiconducting gap inWO3from first-principles calculations. Physical Review B, 1999, 59, 2684-2693.	1.1	121
116	Ab initiocalculations of the cohesive, elastic, and dynamical properties ofCoSi2by pseudopotential and all-electron techniques. Physical Review B, 1996, 54, 1729-1734.	1.1	120
117	Abâ€initio theory of semiconductor band structures: New developments and progress. Physica Status Solidi (B): Basic Research, 2009, 246, 1877-1892.	0.7	120
118	Structural and electronic properties of rhodium surfaces: an ab initio approach. Surface Science, 1996, 346, 300-321.	0.8	118
119	Ab initiodensity functional studies of transition-metal sulphides: I. Crystal structure and cohesive properties. Journal of Physics Condensed Matter, 1997, 9, 11085-11106.	0.7	118
120	Atomic and electronic structure of diamond (111) surfaces I. Reconstruction and hydrogen-induced de-reconstruction of the one dangling-bond surface. Surface Science, 1996, 366, 445-463.	0.8	117
121	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. Journal of Chemical Theory and Computation, 2011, 7, 2780-2785.	2.3	117
122	Low Scaling Algorithms for the Random Phase Approximation: Imaginary Time and Laplace Transformations. Journal of Chemical Theory and Computation, 2014, 10, 2498-2507.	2.3	117
123	Cubic scaling<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> Towards fast quasiparticle calculations. Physical Review B, 2016, 94, .	1.1	113
124	Novel Interface-Mediated Metastable Oxide Phases: Vanadium Oxides on Pd(111). Physical Review Letters, 2001, 87, 086102.	2.9	112
125	Relaxed core projector-augmented-wave method. Journal of Chemical Physics, 2006, 125, 104101.	1.2	112
126	Ab initiodensity functional studies of transition-metal sulphides: II. Electronic structure. Journal of Physics Condensed Matter, 1997, 9, 11107-11140.	0.7	109

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127	Structural and electronic properties of the MoS2(101Ì„0) edge-surface. Surface Science, 1998, 407, 237-250.	0.8	108
128	Surface oxides on close-packed surfaces of late transition metals. Journal of Physics Condensed Matter, 2006, 18, R481-R499.	0.7	107
129	Indirect-to-direct gap transition in strained and unstrained<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Sn</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math> Physical Review B, 2014, 89, .	1.1	107
130	Optimized norm-conserving pseudopotentials. Journal of Physics Condensed Matter, 1992, 4, 7451-7468.	0.7	106
131	First principles calculations on crystalline and liquid iron at Earth's core conditions. Faraday Discussions, 1997, 106, 205-218.	1.6	106
132	Maximally localized Wannier functions in LaMnO₃within PBE +U, hybrid functionals and partially self-consistent GW: an efficient route to constructab initiotight-binding parameters for e_gperovskites. Journal of Physics Condensed Matter, 2012, 24, 235602.	0.7	106
133	Behavior of Methylammonium Dipoles in MAPbX₃ (X = Br and I). Journal of Physical Chemistry Letters, 2017, 8, 4113-4121.	2.1	103
134	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row andd-electron elements. Physical Review B, 2000, 61, 4576-4587.	1.1	102
135	Charge Trapping at the Step Edges of TiO₂ Anatase (101). Angewandte Chemie - International Edition, 2014, 53, 4714-4716.	7.2	102
136	Structure of a thin oxide film on Rh(100). Physical Review B, 2005, 71, .	1.1	101
137	Calculations of ZnO properties using the Heyd-Scuseria-Ernzerhof screened hybrid density functional. Physical Review B, 2009, 80, .	1.1	101
138	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. Physical Review B, 2012, 86, .	1.1	101
139	Beyond the Tamm-Dancoff approximation for extended systems using exact diagonalization. Physical Review B, 2015, 92, .	1.1	101
140	Morphology of mesoscopic Rh and Pd nanoparticles under oxidizing conditions. Physical Review B, 2007, 76, .	1.1	100
141	The multiferroic phase of DyFeO₃: anab initiostudy. New Journal of Physics, 2010, 12, 093026.	1.2	100
142	Lattice constants and cohesive energies of alkali, alkaline-earth, and transition metals: Random phase approximation and density functional theory results. Physical Review B, 2013, 87, .	1.1	100
143	On-the-Fly Active Learning of Interatomic Potentials for Large-Scale Atomistic Simulations. Journal of Physical Chemistry Letters, 2020, 11, 6946-6955.	2.1	100
144	Ab Initiothermodynamic and elastic properties of alkaline-earth metals and their hydrides. Physical Review B, 2007, 76, .	1.1	99

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145	The surface oxide: A LEED, DFT and STM study. Surface Science, 2007, 601, 1574-1581.	0.8	96
146	Polaronic Hole Trapping in Doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaBiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 102, 256402.	2.9	93
147	Anionic Chemistry of Noble Gases: Formation of Mgâ€“NG (NG = Xe, Kr, Ar) Compounds under Pressure. Journal of the American Chemical Society, 2015, 137, 14122-14128.	6.6	91
148	Comment on â€œTaming multiple valency with density functionals: A case study of defective ceriaâ€• Physical Review B, 2005, 72, .	1.1	90
149	First-principles study of Cu₂ZnSnS₄and the related band offsets for photovoltaic applications. Journal of Physics Condensed Matter, 2011, 23, 404203.	0.7	90
150	Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks. Nature Communications, 2018, 9, 4899.	5.8	90
151	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. Journal of Physical Chemistry Letters, 2019, 10, 358-368.	2.1	90
152	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. Journal of Chemical Physics, 2007, 127, 054101.	1.2	89
153	Ab-initio calculations of the 6D potential energy surfaces for the dissociative adsorption of H2 on the (100) surfaces of Rh, Pd and Ag. Surface Science, 1998, 397, 116-136.	0.8	88
154	Atomic-level growth study of vanadium oxide nanostructures on Rh(111). Physical Review B, 2004, 69, .	1.1	87
155	Density functional theory calculations of adsorption of water at calcium oxide and calcium fluoride surfaces. Surface Science, 2000, 452, 9-19.	0.8	83
156	First principles calculation of oxygen adsorption and reconstruction of Cu(110) surface. Surface Science, 1998, 415, 194-211.	0.8	80
157	Comparison of the full-potential and frozen-core approximation approaches to density-functional calculations of surfaces. Physical Review B, 2006, 73, .	1.1	80
158	Correlation energy for the homogeneous electron gas: Exact Bethe-Salpeter solution and an approximate evaluation. Physical Review B, 2016, 93, .	1.1	80
159	Surface structures of ultrathin vanadium oxide films on Pd(). Surface Science, 2001, 495, 91-106.	0.8	79
160	Structural, vibrational, and quasiparticle properties of the Peierls semiconductorBaBiO3: A hybrid functional and self-consistentGW+vertex-correctionsstudy. Physical Review B, 2010, 81, .	1.1	79
161	Structure and dynamics of liquid selenium. Physical Review B, 1998, 57, 10482-10495.	1.1	78
162	Planar Vanadium Oxide Clusters: Two-Dimensional Evaporation and Diffusion on Rh(111). Physical Review Letters, 2004, 92, 206103.	2.9	77

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163	Stabilization mechanism for the polar ZnO(000<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 752 Td (xmlns:mml="http:/ Physical Review B, 2013, 87, .	1.1	77
164	Reduction of vanadium-oxide monolayer structures. Physical Review B, 2005, 71, .	1.1	76
165	GW100: A Plane Wave Perspective for Small Molecules. Journal of Chemical Theory and Computation, 2017, 13, 635-648.	2.3	74
166	First-principles calculations for the surface termination of pure and yttria-doped zirconia surfaces. Physical Review B, 2004, 69, .	1.1	73
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