Karsten Wedel Jacobsen

List of Publications by Year
in descending order

235	33,852	5896 81	3915 177
papers	citations	h-index	g-index

238	238	238	26227
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
2	Real-space grid implementation of the projector augmented wave method. Physical Review B, 2005, 71, .	3.2	1,606
3	Softening of nanocrystalline metals at very small grain sizes. Nature, 1998, 391, 561-563.	27.8	1,558
4	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	1.8	1,451
5	A Maximum in the Strength of Nanocrystalline Copper. Science, 2003, 301, 1357-1359.	12.6	1,296
6	Nudged elastic band method for finding minimum energy paths of transitions. , 1998, , .		1,161
7	An object-oriented scripting interface to a legacy electronic structure code. Computing in Science and Engineering, 2002, 4, 56-66.	1.2	1,117
8	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. Physical Review B, 2012, 85, .	3.2	1,087
9	Phonon-limited mobility in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type single-layer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2012, 85, .	3.2	1,033
10	Interatomic interactions in the effective-medium theory. Physical Review B, 1987, 35, 7423-7442.	3.2	868
11	The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals. 2D Materials, 2018, 5, 042002.	4.4	711
12	Atomic-scale simulations of the mechanical deformation of nanocrystalline metals. Physical Review B, 1999, 60, 11971-11983.	3.2	569
13	One-Dimensional Metallic Edge States inMoS2. Physical Review Letters, 2001, 87, 196803.	7.8	563
14	High-Entropy Alloys as a Discovery Platform for Electrocatalysis. Joule, 2019, 3, 834-845.	24.0	464
15	Graphene on metals: A van der Waals density functional study. Physical Review B, 2010, 81, .	3.2	431
16	Quantized conductance in an atom-sized point contact. Physical Review Letters, 1994, 72, 2251-2254.	7.8	414
17	Phase diagrams for surface alloys. Physical Review B, 1997, 56, 5822-5834.	3.2	391
18	Mechanical Properties and Formation Mechanisms of a Wire of Single Gold Atoms. Physical Review Letters, 2001, 87, .	7.8	379

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19	Atomic-scale insight into structure and morphology changes of MoS2 nanoclusters in hydrotreating catalysts. Journal of Catalysis, 2004, 221, 510-522.	6.2	379
20	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. Journal of Chemical Physics, 2010, 132, 071101.	3.0	367
21	Computational screening of perovskite metal oxides for optimal solar light capture. Energy and Environmental Science, 2012, 5, 5814-5819.	30.8	354
22	Atomic and electronic structure ofMoS2nanoparticles. Physical Review B, 2003, 67, .	3.2	352
23	Multidimensional Potential Energy Surface forH2Dissociation over Cu(111). Physical Review Letters, 1994, 73, 1400-1403.	7.8	334
24	Initial growth of Au on Ni(110): Surface alloying of immiscible metals. Physical Review Letters, 1993, 71, 754-757.	7.8	325
25	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	12.6	319
26	Quantized conductance in atom-sized wires between two metals. Physical Review B, 1995, 52, 8499-8514.	3.2	307
27	Localized atomic basis set in the projector augmented wave method. Physical Review B, 2009, 80, .	3.2	297
28	Simulations of atomic-scale sliding friction. Physical Review B, 1996, 53, 2101-2113.	3.2	289
29	Inelastic scattering in resonant tunneling. Physical Review B, 1989, 40, 11834-11850.	3.2	285
30	Effect of strain on surface diffusion and nucleation. Physical Review B, 1995, 52, R14380-R14383.	3.2	274
31	Resonant Tunneling with Electron-Phonon Interaction: An Exactly Solvable Model. Physical Review Letters, 1988, 61, 1396-1399.	7.8	270
32	Electrochemical CO₂ and CO Reduction on Metal-Functionalized Porphyrin-like Graphene. Journal of Physical Chemistry C, 2013, 117, 9187-9195.	3.1	260
33	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	4.6	249
34	Combined Electronic Structure and Evolutionary Search Approach to Materials Design. Physical Review Letters, 2002, 88, 255506.	7.8	248
35	Chain Formation of Metal Atoms. Physical Review Letters, 2001, 87, 266101.	7.8	242
36	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. Physical Review B, 1998, 57, 3283-3294.	3.2	235

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37	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. Catalysis Letters, 2011, 141, 1067-1071.	2.6	234
38	Fully self-consistent GW calculations for molecules. Physical Review B, 2010, 81, .	3.2	225
39	Bandgap calculations and trends of organometal halide perovskites. APL Materials, 2014, 2, .	5.1	222
40	Enhancement of surface self-diffusion of platinum atoms by adsorbed hydrogen. Nature, 1999, 398, 134-136.	27.8	221
41	Chemistry of one-dimensional metallic edge states in MoS2nanoclusters. Nanotechnology, 2003, 14, 385-389.	2.6	212
42	New cubic perovskites for one- and two-photon water splitting using the computational materials repository. Energy and Environmental Science, 2012, 5, 9034.	30.8	211
43	A semi-empirical effective medium theory for metals and alloys. Surface Science, 1996, 366, 394-402.	1.9	205
44	Density functional theory studies of screw dislocation core structures in bcc metals. Philosophical Magazine, 2003, 83, 365-375.	1.6	197
45	Conductance eigenchannels in nanocontacts. Physical Review B, 1997, 56, 14956-14959.	3.2	196
46	Apparent Barrier Height in Scanning Tunneling Microscopy Revisited. Physical Review Letters, 1996, 76, 1485-1488.	7.8	180
47	Island Shape-Induced Transition from 2D to 3D Growth for Pt/Pt(111). Physical Review Letters, 1995, 74, 2295-2298.	7.8	171
48	Role of nonlocal exchange correlation in activated adsorption. Physical Review Letters, 1993, 70, 3971-3974.	7.8	170
49	Bayesian Error Estimation in Density-Functional Theory. Physical Review Letters, 2005, 95, 216401.	7.8	163
50	Atomic-Scale Determination of Misfit Dislocation Loops at Metal-Metal Interfaces. Physical Review Letters, 1995, 75, 489-492.	7.8	158
51	The Computational Materials Repository. Computing in Science and Engineering, 2012, 14, 51-57.	1.2	153
52	Wetting/ non-wetting phenomena during catalysis: Evidence from in situ on-line EXAFS studies of Cu-based catalysts. Topics in Catalysis, 1994, 1, 367-376.	2.8	152
53	Self-diffusion on copper surfaces. Physical Review B, 1991, 44, 6523-6526.	3.2	151
54	Theory of the oxygen-induced restructuring of Cu(110) and Cu(100) surfaces. Physical Review Letters, 1990, 65, 1788-1791.	7.8	150

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55	Stretching dependence of the vibration modes of a single-moleculePtâˆ'H2âˆ'Ptbridge. Physical Review B, 2005, 71, .	3.2	142
56	Linear density response function in the projector augmented wave method: Applications to solids, surfaces, and interfaces. Physical Review B, 2011, 83, .	3.2	142
57	2-Photon tandem device for water splitting: comparing photocathode first versus photoanode first designs. Energy and Environmental Science, 2014, 7, 2397-2413.	30.8	130
58	Oxygen chemisorption on Cu(110): A model for thec(6Ã—2) structure. Physical Review Letters, 1990, 65, 2027-2030.	7.8	129
59	New Lightâ€Harvesting Materials Using Accurate and Efficient Bandgap Calculations. Advanced Energy Materials, 2015, 5, 1400915.	19.5	124
60	Unraveling the acoustic electron-phonon interaction in graphene. Physical Review B, 2012, 85, .	3.2	122
61	Theory of Alkali-Metal-Induced Reconstruction of fcc (110) Surfaces. Physical Review Letters, 1988, 60, 2496-2498.	7.8	121
62	Molecular transport calculations with Wannier functions. Chemical Physics, 2005, 319, 111-125.	1.9	120
63	Electronic structure, total energies, and STM images of clean and oxygen-covered Al(111). Physical Review B, 1995, 52, 14954-14962.	3.2	118
64	mBEEF: An accurate semi-local Bayesian error estimation density functional. Journal of Chemical Physics, 2014, 140, 144107.	3.0	117
65	Anisotropic corner diffusion as origin for dendritic growth on hexagonal substrates. Surface Science, 1996, 349, L115-L122.	1.9	112
66	Defect-Tolerant Monolayer Transition Metal Dichalcogenides. Nano Letters, 2016, 16, 2234-2239.	9.1	111
67	Benchmark density functional theory calculations for nanoscale conductance. Journal of Chemical Physics, 2008, 128, 114714.	3.0	109
68	Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organicâ€"Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 4346-4352.	4.6	107
69	Adsorption-induced restructuring of gold nanochains. Physical Review B, 2002, 66, .	3.2	102
70	Stability and Electronic Properties of TiO₂ Nanostructures With and Without B and N Doping. Journal of Physical Chemistry C, 2009, 113, 12301-12308.	3.1	102
71	Atomistic Determination of Cross-Slip Pathway and Energetics. Physical Review Letters, 1997, 79, 3676-3679.	7.8	98
72	Density Functional Simulation of a Breaking Nanowire. Physical Review Letters, 1999, 82, 1538-1541.	7.8	97

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73	Avalanche Size Scaling in Sheared Three-Dimensional Amorphous Solid. Physical Review Letters, 2007, 98, 095501.	7.8	97
74	Cu cluster shell structure at elevated temperatures. Physical Review Letters, 1991, 66, 2219-2222.	7.8	95
75	Bayesian Ensemble Approach to Error Estimation of Interatomic Potentials. Physical Review Letters, 2004, 93, 165501.	7.8	95
76	Machine learning-based screening of complex molecules for polymer solar cells. Journal of Chemical Physics, 2018, 148, 241735.	3.0	94
77	Scattering and conductance quantization in three-dimensional metal nanocontacts. Physical Review B, 1997, 55, 2637-2650.	3.2	93
78	Matching conditions in the quasicontinuum method: Removal of the error introduced at the interface between the coarse-grained and fully atomistic region. Physical Review B, 2004, 69, .	3.2	93
79	Simulations of the atomic structure, energetics, and cross slip of screw dislocations in copper. Physical Review B, 1997, 56, 2977-2990.	3.2	92
80	Sulfide perovskites for solar energy conversion applications: computational screening and synthesis of the selected compound LaYS₃. Energy and Environmental Science, 2017, 10, 2579-2593.	30.8	91
81	Thermal Diffusion Processes in Metal-Tip-Surface Interactions: Contact Formation and Adatom Mobility. Physical Review Letters, 1996, 77, 5067-5070.	7.8	87
82	Fermi level alignment in molecular nanojunctions and its relation to charge transfer. Physical Review B, 2006, 74, .	3.2	84
83	Ab Initio van der Waals Interactions in Simulations of Water Alter Structure from Mainly Tetrahedral to High-Density-Like. Journal of Physical Chemistry B, 2011, 115, 14149-14160.	2.6	83
84	Four-Atom Period in the Conductance of Monatomic Al Wires. Physical Review Letters, 2003, 91, 146801.	7.8	82
85	Atomistic simulation study of the shear-band deformation mechanism in Mg-Cu metallic glasses. Physical Review B, 2006, 73, .	3.2	82
86	Dissociation path forH2on Al(110). Physical Review Letters, 1992, 69, 1971-1974.	7.8	80
87	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	3.0	77
88	Anharmonic stabilization and band gap renormalization in the perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CsSnI</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2015, 92, .	3.2	76
89	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. Journal of Physical Chemistry Letters, 2015, 6, 1577-1585.	4.6	75
90	Conductance calculations with a wavelet basis set. Physical Review B, 2003, 67, .	3.2	74

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91	Olesenet al.Reply:. Physical Review Letters, 1995, 74, 2147-2147.	7.8	73
92	Nonlocal Screening of Plasmons in Graphene by Semiconducting and Metallic Substrates: First-Principles Calculations. Physical Review Letters, 2011, 106, 146803.	7.8	73
93	Chemisorption of H, O, and S on Ni(110): general trends. Surface Science, 1992, 272, 334-341.	1.9	70
94	Surface stress, surface elasticity, and the size effect in surface segregation. Physical Review B, 1995, 51, 10937-10946.	3.2	69
95	Simulations of intergranular fracture in nanocrystalline molybdenum. Acta Materialia, 2004, 52, 5019-5029.	7.9	69
96	Theory of Adsorbate-Induced Surface Relaxations: Hydrogen on Cu(110). Physical Review Letters, 1987, 59, 2764-2767.	7.8	67
97	Homoepitaxial Growth of Pt on Pt(100)-hex: Effects of Strongly Anisotropic Diffusion and Finite Island Sizes. Physical Review Letters, 1996, 77, 87-90.	7.8	66
98	Adsorption-Induced Step Formation. Physical Review Letters, 2001, 87, 126102.	7.8	65
99	Forces and conductances in a single-molecule bipyridine junction. Physical Review B, 2005, 72, .	3.2	65
100	Partly Occupied Wannier Functions. Physical Review Letters, 2005, 94, 026405.	7.8	64
101	First-principles study of surface plasmons on Ag(111) and H/Ag(111). Physical Review B, 2011, 84, .	3.2	64
102	Conduction Mechanism in a Molecular Hydrogen Contact. Physical Review Letters, 2005, 94, 036807.	7.8	63
103	Critical current for the flow of superfluid3He in a confined geometry. Journal of Low Temperature Physics, 1987, 67, 83-89.	1.4	61
104	Self-consistent electronic structure and segregation profiles of the Cu-Ni (001) random-alloy surface. Physical Review B, 1994, 49, 11383-11396.	3.2	61
105	Heteroepitaxial subsurface growth mode resulting in interlayer mixing. Physical Review B, 1997, 55, 1380-1383.	3.2	61
106	Determination of the of Rate Cross Slip of Screw Dislocations. Physical Review Letters, 2000, 85, 3866-3869.	7.8	61
107	High-throughput computational screening for two-dimensional magnetic materials based on experimental databases of three-dimensional compounds. Npj Computational Materials, 2020, 6, .	8.7	60
108	Island shapes in homoepitaxial growth of Pt(111). Surface Science, 1996, 359, 37-44.	1.9	58

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109	Simulation of Cu-Mg metallic glass: Thermodynamics and structure. Physical Review B, 2004, 69, .	3.2	57
110	Local Bayesian optimizer for atomic structures. Physical Review B, 2019, 100, .	3.2	57
111	Exploration versus Exploitation in Global Atomistic Structure Optimization. Journal of Physical Chemistry A, 2018, 122, 1504-1509.	2.5	56
112	Stacking fault energies in aluminium. Journal of Physics Condensed Matter, 1992, 4, 10453-10460.	1.8	54
113	Nature of Dislocations in Silicon. Physical Review Letters, 1995, 75, 4444-4447.	7.8	52
114	Rate Theory for Correlated Processes: Double Jumps in Adatom Diffusion. Physical Review Letters, 1997, 79, 2843-2846.	7.8	52
115	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. Journal of Physical Chemistry C, 2011, 115, 2244-2252.	3.1	52
116	Conventional and acoustic surface plasmons on noble metal surfaces: A time-dependent density functional theory study. Physical Review B, 2012, 86, .	3.2	51
117	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. New Journal of Physics, 2013, 15, 105026.	2.9	51
118	High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices. ACS Energy Letters, 2018, 3, 436-446.	17.4	51
119	Many-atom interactions in metals. Surface Science, 1993, 283, 277-282.	1.9	50
120	The energetics and dynamics of H2 dissociation on Al(110). Surface Science, 1994, 304, 131-144.	1.9	48
121	Nanoscale plasticity. Nature Materials, 2002, 1, 15-16.	27.5	48
122	Interference andk-point sampling in the supercell approach to phase-coherent transport. Physical Review B, 2005, 72, .	3.2	47
123	Optical properties of bulk semiconductors and graphene/boron nitride: The Bethe-Salpeter equation with derivative discontinuity-corrected density functional energies. Physical Review B, 2012, 86, .	3.2	47
124	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. Topics in Catalysis, 2014, 57, 265-272.	2.8	47
125	Determination of low-strain interfaces via geometric matching. Physical Review B, 2017, 96, .	3.2	47
126	Atomistic simulations of cross-slip of jogged screw dislocations in copper. Philosophical Magazine Letters, 2001, 81, 137-144.	1.2	46

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127	Melting a Copper Cluster: Critical-Droplet Theory. Europhysics Letters, 1994, 26, 51-56.	2.0	45
128	Mechanisms of self-diffusion on Pt(110). Physical Review B, 1999, 60, R5149-R5152.	3.2	45
129	Simulation of structure and annihilation of screw dislocation dipoles. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2000, 80, 1273-1290.	0.6	44
130	Electronic shell structure and chemisorption on gold nanoparticles. Physical Review B, 2011, 84, .	3.2	44
131	H-H interactions in Pd. Physical Review B, 1989, 40, 1993-1996.	3.2	43
132	Ab initiopotential for solids. Physical Review B, 1992, 46, 3798-3809.	3.2	43
133	Chemisorption and vibration of hydrogen on Cu(111). Surface Science, 1993, 285, 27-30.	1.9	43
134	Pareto-optimal alloys. Applied Physics Letters, 2003, 83, 4527-4529.	3.3	43
135	Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. Nature Communications, 2013, 4, 2121.	12.8	43
136	Performance of genetic algorithms in search for water splitting perovskites. Journal of Materials Science, 2013, 48, 6519-6534.	3.7	42
137	Oxidative trends of TiO2â€”hole trapping at anatase and rutile surfaces. Energy and Environmental Science, 2012, 5, 9866.	30.8	41
138	Direct Dynamics Studies of a Binuclear Metal Complex in Solution: The Interplay Between Vibrational Relaxation, Coherence, and Solvent Effects. Journal of Physical Chemistry Letters, 2014, 5, 2414-2418.	4.6	39
139	Atomistic simulations of dislocation processes in copper. Journal of Physics Condensed Matter, 2002, 14, 2929-2956.	1.8	38
140	Partly occupied Wannier functions: Construction and applications. Physical Review B, 2005, 72, .	3.2	38
141	Oxygen adsorption on Pt(110)-(1Ã—2): new high-coverage structures. Surface Science, 1999, 430, L533-L539.	1.9	37
142	Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes. Physical Review B, 2010, 81, .	3.2	37
143	Spatially resolved quantum plasmon modes in metallic nano-films from first-principles. Physical Review B, 2012, 86, .	3.2	36
144	Plasmons on the edge of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">MoS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>nanostructures. Physical Review B, 2014, 90, .	3.2	36

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145	Calculated optical absorption of different perovskite phases. Journal of Materials Chemistry A, 2015, 3, 12343-12349.	10.3	35
146	mBEEF-vdW: Robust fitting of error estimation density functionals. Physical Review B, 2016, 93, .	3.2	35
147	Making the most of materials computations. Science, 2016, 354, 180-181.	12.6	35
148	Optimized and transferable densities from first-principles local density calculations. Journal of Physics Condensed Matter, 1991, 3, 5437-5443.	1.8	34
149	Atomic-Scale Structure of Dislocations Revealed by Scanning Tunneling Microscopy and Molecular Dynamics. Physical Review Letters, 2002, 88, 206106.	7.8	34
150	Comparative study of anchoring groups for molecular electronics: structure and conductance of Auâ€“Sâ€“Au and Auâ€“NH2â€“Au junctions. Journal of Physics Condensed Matter, 2008, 20, 374101.	1.8	34
151	Calculation of Quantum Tunneling for a Spatially Extended Defect: The Dislocation Kink in Copper Has a Low Effective Mass. Physical Review Letters, 2001, 86, 1546-1549.	7.8	33
152	First-principles calculations of graphene nanoribbons in gaseous environments: Structural and electronic properties. Physical Review B, 2010, 82, .	3.2	33
153	Ab initiononequilibrium quantum transport and forces with the real-space projector augmented wave method. Physical Review B, 2012, 85, .	3.2	33
154	Heats of formation of solids with error estimation: The mBEEF functional with and without fitted reference energies. Physical Review B, 2015, 91, .	3.2	33
155	Monte Carlo calculation of the thermal expansion coefficient of Al. Physical Review B, 1987, 36, 5035-5036.	3.2	32
156	Activation free energy and entropy for the normal and exchange selfdiffusion processes on Cu(100). Surface Science, 1993, 289, 68-74.	1.9	32
157	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. Journal of Chemical Theory and Computation, 2017, 13, 6010-6022.	5.3	32
158	Shining Light on Sulfide Perovskites: LaYS₃ Material Properties and Solar Cells. Chemistry of Materials, 2019, 31, 3359-3369.	6.7	32
159	Scanning Tunneling Microscopy Evidence for the Dissociation of Carbon Monoxide on Ruthenium Steps. Journal of Physical Chemistry C, 2012, 116, 14350-14359.	3.1	30
160	Definition of a scoring parameter to identify low-dimensional materials components. Physical Review Materials, 2019, 3, .	2.4	30
161	Nucleation of the Pt(111) reconstruction: a simulation study. Surface Science, 1994, 317, 8-14.	1.9	29
162	Electronic hole localization in rutile and anatase TiO2 â€“ Self-interaction correction in Î”-SCF DFT. Chemical Physics Letters, 2011, 506, 42-45.	2.6	29

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163	Graphene Edges Dictate the Morphology of Nanoparticles during Catalytic Channeling. Journal of Physical Chemistry C, 2014, 118, 4296-4302.	3.1	29
164	Mechanical deformation of nanocrystalline materials. Philosophical Magazine Letters, 1996, 74, 339-344.	1.2	28
165	Electron transport in aPtâ^'COâ^'Ptnanocontact: Density functional theory calculations. Physical Review B, 2006, 73, .	3.2	28
166	Dynamic breaking of a single gold bond. Nature Communications, 2017, 8, 15931.	12.8	28
167	Effective-medium tight-binding model for silicon. Physical Review B, 1994, 50, 10727-10741.	3.2	27
168	Effective-medium calculations for hydrogen in Ni, Pd, and Pt. Physical Review B, 1990, 41, 12413-12423.	3.2	25
169	Î²-Sheet Preferences from First Principles. Journal of the American Chemical Society, 2003, 125, 16383-16386.	13.7	24
170	Elastic Effects behind Cooperative Bonding in Î²-Sheets. Journal of the American Chemical Society, 2004, 126, 13140-13143.	13.7	24
171	Designing rules and probabilistic weighting for fast materials discovery in the Perovskite structure. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 055007.	2.0	24
172	Strain sensitivity of band gaps of Sn-containing semiconductors. Physical Review B, 2015, 91, .	3.2	24
173	A theoretical study of carbon chemisorption on nickel surfaces. Surface Science, 1986, 166, 539-553.	1.9	23
174	Kinematic generation of dislocations. Philosophical Magazine Letters, 1995, 72, 245-250.	1.2	23
175	Effects of anisotropic diffusion and finite island sizes in homoepitaxial growth. Surface Science, 1998, 400, 290-313.	1.9	23
176	Anab initiostudy of electron transport through nitrobenzene: the influence of leads and contacts. Nanotechnology, 2005, 16, S155-S160.	2.6	23
177	Importance of the Reorganization Energy Barrier in Computational Design of Porphyrin-Based Solar Cells with Cobalt-Based Redox Mediators. Journal of Physical Chemistry C, 2015, 119, 12792-12800.	3.1	23
178	Global optimization of atomic structures with gradient-enhanced Gaussian process regression. Physical Review B, 2021, 103, .	3.2	22
179	Inelastic scattering in metal-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:ma junctions. Physical Review B, 2009, 79, .	3.2	21
180	Effect of edge plasmons on the optical properties of <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 monolayer flakes. Physical Review B, 2017, 96, .	3.2	21

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181	Theory of alkali-metal-induced reconstructions of fcc(100) surfaces. Physical Review B, 1992, 45, 6893-6898.	3.2	20
182	Polarization and charge transfer during the dissociation of H2 on Al(110). Surface Science, 1993, 297, L68-L72.	1.9	20
183	Atomically Thin Ordered Alloys of Transition Metal Dichalcogenides: Stability and Band Structures. Journal of Physical Chemistry C, 2016, 120, 23024-23029.	3.1	20
184	A simple and realistic model system for studying hydrogen bonds in Î²-sheets. Journal of Chemical Physics, 2003, 118, 9783-9794.	3.0	19
185	Construction of New Electronic Density Functionals with Error Estimation Through Fitting. Topics in Catalysis, 2012, 55, 402-417.	2.8	19
186	An effective-medium theory approach to ordering in Cu-Au alloys. Journal of Physics Condensed Matter, 1992, 4, 7191-7202.	1.8	18
187	Construction of transferable spherically averaged electron potentials. Journal of Physics Condensed Matter, 1994, 6, 5415-5421.	1.8	18
188	IIâ€“IVâ€“V₂ and IIIâ€“IIIâ€“V₂ Polytypes as Light Absorbers for Single Junction and Tandem Photovoltaic Devices. Journal of Physical Chemistry C, 2017, 121, 17780-17786.	3.1	18
189	Analytic approach to charge transfer during atom-surface scattering. Physical Review B, 1989, 40, 3417-3420.	3.2	17
190	Atomistic simulations of Mgâ€“Cu metallic glasses: mechanical properties. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 387-389, 996-1000.	5.6	16
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