Karsten Wedel Jacobsen

List of Publications by Citations

230 papers	28,003 citations	78 h-index	165 g-index
238 ext. papers	30,779 ext. citations	6.3 avg, IF	7.06 L-index

#	Paper	IF	Citations
230	Softening of nanocrystalline metals at very small grain sizes. *Nature*, **1998**, 391, 561-563	50.4	1370
229	Real-space grid implementation of the projector augmented wave method. *Physical Review B*, **2005**, 71,	3.3	1247
228	A maximum in the strength of nanocrystalline copper. *Science*, **2003**, 301, 1357-9	33.3	1111
227	The atomic simulation environment-a Python library for working with atoms. *Journal of Physics Condensed Matter*, **2017**, 29, 273002	1.8	1097
226	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	1092
225	. *Computing in Science and Engineering*, **2002**, 4, 56-66	1.5	974
224	Nudged elastic band method for finding minimum energy paths of transitions **1998**,		921
223	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. *Physical Review B*, **2012**, 85,	3.3	852
222	Phonon-limited mobility in n-type single-layer MoS2 from first principles. *Physical Review B*, **2012**, 85,	3.3	847
221	Interatomic interactions in the effective-medium theory. *Physical Review B*, **1987**, 35, 7423-7442	3.3	768
220	Atomic-scale simulations of the mechanical deformation of nanocrystalline metals. *Physical Review B*, **1999**, 60, 11971-11983	3.3	511
219	One-dimensional metallic edge states in MoS2. *Physical Review Letters*, **2001**, 87, 196803	7.4	506
218	Quantized conductance in an atom-sized point contact. *Physical Review Letters*, **1994**, 72, 2251-2254	7.4	402
217	The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals. *2D Materials*, **2018**, 5, 042002	5.9	399
216	Graphene on metals: A van der Waals density functional study. *Physical Review B*, **2010**, 81,	3.3	397
215	Phase diagrams for surface alloys. *Physical Review B*, **1997**, 56, 5822-5834	3.3	362
214	Mechanical Properties and Formation Mechanisms of a Wire of Single Gold Atoms. *Physical Review Letters*, **2001**, 87,	7.4	347

213	Atomic-scale insight into structure and morphology changes of MoS2 nanoclusters in hydrotreating catalysts. *Journal of Catalysis*, **2004**, 221, 510-522	7.3	324
212	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. *Journal of Chemical Physics*, **2010**, 132, 071101	3.9	319
211	Multidimensional potential energy surface for H2 dissociation over Cu(111). *Physical Review Letters*, **1994**, 73, 1400-1403	7.4	313
210	Atomic and electronic structure of MoS2 nanoparticles. *Physical Review B*, **2003**, 67,	3.3	312
209	Initial growth of Au on Ni(110): Surface alloying of immiscible metals. *Physical Review Letters*, **1993**, 71, 754-757	7.4	308
208	Computational screening of perovskite metal oxides for optimal solar light capture. *Energy and Environmental Science*, **2012**, 5, 5814-5819	35.4	301
207	Inelastic scattering in resonant tunneling. *Physical Review B*, **1989**, 40, 11834-11850	3.3	275
206	Quantized conductance in atom-sized wires between two metals. *Physical Review B*, **1995**, 52, 8499-8514	3.3	260
205	Effect of strain on surface diffusion and nucleation. *Physical Review B*, **1995**, 52, 14380-14383	3.3	257
204	Resonant tunneling with electron-phonon interaction: An exactly solvable model. *Physical Review Letters*, **1988**, 61, 1396-1399	7.4	253
203	Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates. *Science*, **2014**, 345, 197-200	33.3	244
202	Simulations of atomic-scale sliding friction. *Physical Review B*, **1996**, 53, 2101-2113	3.3	241
201	Localized atomic basis set in the projector augmented wave method. *Physical Review B*, **2009**, 80,	3.3	232
200	Chain formation of metal atoms. *Physical Review Letters*, **2001**, 87, 266101	7.4	227
199	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. *Physical Review B*, **1998**, 57, 3283-3294	3.3	225
198	Combined electronic structure and evolutionary search approach to materials design. *Physical Review Letters*, **2002**, 88, 255506	7.4	225
197	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. *Journal of Physical Chemistry Letters*, **2013**, 4, 222-6	6.4	221
196	Electrochemical CO2 and CO Reduction on Metal-Functionalized Porphyrin-like Graphene. *Journal of Physical Chemistry C*, **2013**, 117, 9187-9195	3.8	218

195	Fully self-consistent GW calculations for molecules. *Physical Review B*, **2010**, 81,	3.3	205
194	High-Entropy Alloys as a Discovery Platform for Electrocatalysis. *Joule*, **2019**, 3, 834-845	27.8	202
193	Enhancement of surface self-diffusion of platinum atoms by adsorbed hydrogen. *Nature*, **1999**, 398, 134-136	50.4	194
192	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. *Catalysis Letters*, **2011**, 141, 1067-1071	2.8	193
191	Conductance eigenchannels in nanocontacts. *Physical Review B*, **1997**, 56, 14956-14959	3.3	189
190	A semi-empirical effective medium theory for metals and alloys. *Surface Science*, **1996**, 366, 394-402	1.8	185
189	New cubic perovskites for one- and two-photon water splitting using the computational materials repository. *Energy and Environmental Science*, **2012**, 5, 9034	35.4	178
188	Density functional theory studies of screw dislocation core structures in bcc metals. *Philosophical Magazine*, **2003**, 83, 365-375	1.6	178
187	Bandgap calculations and trends of organometal halide perovskites. *APL Materials*, **2014**, 2, 081514	5.7	167
186	Island shape-induced transition from 2D to 3D growth for Pt/Pt(111). *Physical Review Letters*, **1995**, 74, 2295-2298	7.4	164
185	Chemistry of one-dimensional metallic edge states in MoS2nanoclusters. *Nanotechnology*, **2003**, 14, 385-389	3.4	163
184	Role of nonlocal exchange correlation in activated adsorption. *Physical Review Letters*, **1993**, 70, 3971-3974	7.4	155
183	Self-diffusion on copper surfaces. *Physical Review B*, **1991**, 44, 6523-6526	3.3	150
182	Atomic-scale determination of misfit dislocation loops at metal-metal interfaces. *Physical Review Letters*, **1995**, 75, 489-492	7.4	149
181	Bayesian error estimation in density-functional theory. *Physical Review Letters*, **2005**, 95, 216401	7.4	145
180	Apparent barrier height in scanning tunneling microscopy revisited. *Physical Review Letters*, **1996**, 76, 1485-1488	7.4	142
179	Theory of the oxygen-induced restructuring of Cu(110) and Cu(100) surfaces. *Physical Review Letters*, **1990**, 65, 1788-1791	7.4	139
178	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	2.3	137

177	Stretching dependence of the vibration modes of a single-molecule Pt–H2–Pt bridge. *Physical Review B*, **2005**, 71,	3.3	135
176	The Computational Materials Repository. *Computing in Science and Engineering*, **2012**, 14, 51-57	1.5	119
175	Oxygen chemisorption on Cu(110): A model for the c(6 x 2) structure. *Physical Review Letters*, **1990**, 65, 2027-2030	7.4	119
174	Theory of alkali-metal-induced reconstruction of fcc (110) surfaces. *Physical Review Letters*, **1988**, 60, 2496-2498	7.4	114
173	2-Photon tandem device for water splitting: comparing photocathode first versus photoanode first designs. *Energy and Environmental Science*, **2014**, 7, 2397-2413	35.4	112
172	Molecular transport calculations with Wannier functions. *Chemical Physics*, **2005**, 319, 111-125	2.3	111
171	Electronic structure, total energies, and STM images of clean and oxygen-covered Al(111). *Physical Review B*, **1995**, 52, 14954-14962	3.3	110
170	Linear density response function in the projector augmented wave method: Applications to solids, surfaces, and interfaces. *Physical Review B*, **2011**, 83,	3.3	107
169	Anisotropic corner diffusion as origin for dendritic growth on hexagonal substrates. *Surface Science* , **1996**, 349, L115-L122	1.8	106
168	New Light-Harvesting Materials Using Accurate and Efficient Bandgap Calculations. *Advanced Energy Materials*, **2015**, 5, 1400915	21.8	105
167	mBEEF: an accurate semi-local Bayesian error estimation density functional. *Journal of Chemical Physics*, **2014**, 140, 144107	3.9	101
166	Benchmark density functional theory calculations for nanoscale conductance. *Journal of Chemical Physics*, **2008**, 128, 114714	3.9	99
165	Stability and Electronic Properties of TiO2 Nanostructures With and Without B and N Doping. *Journal of Physical Chemistry C*, **2009**, 113, 12301-12308	3.8	94
164	Adsorption-induced restructuring of gold nanochains. *Physical Review B*, **2002**, 66,	3.3	93
163	Unraveling the acoustic electron-phonon interaction in graphene. *Physical Review B*, **2012**, 85,	3.3	91
162	Atomistic Determination of Cross-Slip Pathway and Energetics. *Physical Review Letters*, **1997**, 79, 3676-3679	7.4	91
161	Density Functional Simulation of a Breaking Nanowire. *Physical Review Letters*, **1999**, 82, 1538-1541	7.4	90
160	Cu cluster shell structure at elevated temperatures. *Physical Review Letters*, **1991**, 66, 2219-2222	7.4	90

159	Avalanche size scaling in sheared three-dimensional amorphous solid. *Physical Review Letters*, **2007**, 98, 095501	7.4	88
158	Scattering and conductance quantization in three-dimensional metal nanocontacts. *Physical Review B*, **1997**, 55, 2637-2650	3.3	87
157	Defect-Tolerant Monolayer Transition Metal Dichalcogenides. *Nano Letters*, **2016**, 16, 2234-9	11.5	86
156	Bayesian ensemble approach to error estimation of interatomic potentials. *Physical Review Letters*, **2004**, 93, 165501	7.4	84
155	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,	3.3	83
154	Simulations of the atomic structure, energetics, and cross slip of screw dislocations in copper. *Physical Review B*, **1997**, 56, 2977-2990	3.3	81
153	Thermal Diffusion Processes in Metal-Tip-Surface Interactions: Contact Formation and Adatom Mobility. *Physical Review Letters*, **1996**, 77, 5067-5070	7.4	79
152	Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organic-Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2016**, 7, 4346-4352	6.4	78
151	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, 14149-60	3.4	78
150	Fermi level alignment in molecular nanojunctions and its relation to charge transfer. *Physical Review B*, **2006**, 74,	3.3	76
149	Dissociation path for H2 on Al(110). *Physical Review Letters*, **1992**, 69, 1971-1974	7.4	76
148	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. *Journal of Chemical Physics*, **2009**, 131, 014101	3.9	74
147	Four-atom period in the conductance of monatomic Al wires. *Physical Review Letters*, **2003**, 91, 146801	7.4	73
146	Machine learning-based screening of complex molecules for polymer solar cells. *Journal of Chemical Physics*, **2018**, 148, 241735	3.9	71
145	Olesen et al. reply. *Physical Review Letters*, **1995**, 74, 2147	7.4	71
144	Nonlocal screening of plasmons in graphene by semiconducting and metallic substrates: first-principles calculations. *Physical Review Letters*, **2011**, 106, 146803	7.4	69
143	Atomistic simulation study of the shear-band deformation mechanism in Mg-Cu metallic glasses. *Physical Review B*, **2006**, 73,	3.3	69
142	Conductance calculations with a wavelet basis set. *Physical Review B*, **2003**, 67,	3.3	66

141	Surface stress, surface elasticity, and the size effect in surface segregation. *Physical Review B*, **1995**, 51, 10937-10946	3.3	66
140	Theory of adsorbate-induced surface relaxations: Hydrogen on Cu(110). *Physical Review Letters*, **1987**, 59, 2764-2767	7.4	66
139	Homoepitaxial Growth of Pt on Pt(100)-hex: Effects of Strongly Anisotropic Diffusion and Finite Island Sizes. *Physical Review Letters*, **1996**, 77, 87-90	7.4	65
138	Chemisorption of H, O, and S on Ni(110): general trends. *Surface Science*, **1992**, 272, 334-341	1.8	65
137	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. *Journal of Physical Chemistry Letters*, **2015**, 6, 1577-85	6.4	64
136	Sulfide perovskites for solar energy conversion applications: computational screening and synthesis of the selected compound LaYS3. *Energy and Environmental Science*, **2017**, 10, 2579-2593	35.4	61
135	Simulations of intergranular fracture in nanocrystalline molybdenum. *Acta Materialia*, **2004**, 52, 5019-5029	8.4	61
134	Conduction mechanism in a molecular hydrogen contact. *Physical Review Letters*, **2005**, 94, 036807	7.4	60
133	Heteroepitaxial subsurface growth mode resulting in interlayer mixing. *Physical Review B*, **1997**, 55, 1380-1383	3.3	59
132	Forces and conductances in a single-molecule bipyridine junction. *Physical Review B*, **2005**, 72,	3.3	59
131	Adsorption-induced step formation. *Physical Review Letters*, **2001**, 87, 126102	7.4	58
130	Self-consistent electronic structure and segregation profiles of the Cu-Ni (001) random-alloy surface. *Physical Review B*, **1994**, 49, 11383-11396	3.3	58
129	Partly occupied Wannier functions. *Physical Review Letters*, **2005**, 94, 026405	7.4	56
128	Determination of the of rate cross slip of screw dislocations. *Physical Review Letters*, **2000**, 85, 3866-9	7.4	55
127	Simulation of Cu-Mg metallic glass: Thermodynamics and structure. *Physical Review B*, **2004**, 69,	3.3	53
126	Island shapes in homoepitaxial growth of Pt(111). *Surface Science*, **1996**, 359, 37-44	1.8	53
125	Anharmonic stabilization and band gap renormalization in the perovskite CsSnI3. *Physical Review B*, **2015**, 92,	3.3	52
124	First-principles study of surface plasmons on Ag(111) and H/Ag(111). *Physical Review B*, **2011**, 84,	3.3	52

123	Rate Theory for Correlated Processes: Double Jumps in Adatom Diffusion. *Physical Review Letters*, **1997**, 79, 2843-2846	7.4	50
122	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. *New Journal of Physics*, **2013**, 15, 105026	2.9	49
121	Stacking fault energies in aluminium. *Journal of Physics Condensed Matter*, **1992**, 4, 10453-10460	1.8	48
120	Nature of dislocations in silicon. *Physical Review Letters*, **1995**, 75, 4444-4447	7.4	47
119	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 2244-2252	3.8	46
118	Many-atom interactions in metals. *Surface Science*, **1993**, 283, 277-282	1.8	46
117	Mechanisms of self-diffusion on Pt(110). *Physical Review B*, **1999**, 60, R5149-R5152	3.3	44
116	The energetics and dynamics of H2 dissociation on Al(110). *Surface Science*, **1994**, 304, 131-144	1.8	43
115	Melting a Copper Cluster: Critical-Droplet Theory. *Europhysics Letters*, **1994**, 26, 51-56	1.6	42
114	Interference and k-point sampling in the supercell approach to phase-coherent transport. *Physical Review B*, **2005**, 72,	3.3	41
113	Atomistic simulations of cross-slip of jogged screw dislocations in copper. *Philosophical Magazine Letters*, **2001**, 81, 137-144	1	41
112	H-H interactions in Pd. *Physical Review B*, **1989**, 40, 1993-1996	3.3	41
111	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. *Topics in Catalysis*, **2014**, 57, 265-272	2.3	40
110	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,	3.3	40
109	Electronic shell structure and chemisorption on gold nanoparticles. *Physical Review B*, **2011**, 84,	3.3	40
108	Ab initio potential for solids. *Physical Review B*, **1992**, 46, 3798-3809	3.3	40
107	Conventional and acoustic surface plasmons on noble metal surfaces: A time-dependent density functional theory study. *Physical Review B*, **2012**, 86,	3.3	39
106	Pareto-optimal alloys. *Applied Physics Letters*, **2003**, 83, 4527-4529	3.4	39

105	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		39
104	Chemisorption and vibration of hydrogen on Cu(111). *Surface Science*, **1993**, 285, 27-30	1.8	39
103	Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. *Nature Communications*, **2013**, 4, 2121	17.4	38
102	Oxidative trends of TiO2 hole trapping at anatase and rutile surfaces. *Energy and Environmental Science*, **2012**, 5, 9866	35.4	37
101	Oxygen adsorption on Pt(110)-(1 2): new high-coverage structures. *Surface Science*, **1999**, 430, L533-L539	1.8	37
100	Performance of genetic algorithms in search for water splitting perovskites. *Journal of Materials Science*, **2013**, 48, 6519-6534	4.3	35
99	Local Bayesian optimizer for atomic structures. *Physical Review B*, **2019**, 100,	3.3	34
98	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, 2414-8	6.4	33
97	Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes. *Physical Review B*, **2010**, 81,	3.3	33
96	Atomistic simulations of dislocation processes in copper. *Journal of Physics Condensed Matter*, **2002**, 14, 2929-2956	1.8	33
95	Comparative study of anchoring groups for molecular electronics: structure and conductance of Au-S-Au and Au-NH(2)-Au junctions. *Journal of Physics Condensed Matter*, **2008**, 20, 374101	1.8	32
94	Activation free energy and entropy for the normal and exchange selfdiffusion processes on Cu(100). *Surface Science*, **1993**, 289, 68-74	1.8	32
93	High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices. *ACS Energy Letters*, **2018**, 3, 436-446	20.1	31
92	Spatially resolved quantum plasmon modes in metallic nano-films from first-principles. *Physical Review B*, **2012**, 86,	3.3	31
91	Monte Carlo calculation of the thermal expansion coefficient of Al. *Physical Review B*, **1987**, 36, 5035-5036	3.3	31
90	Ab initio nonequilibrium quantum transport and forces with the real-space projector augmented wave method. *Physical Review B*, **2012**, 85,	3.3	30
89	Calculated optical absorption of different perovskite phases. *Journal of Materials Chemistry A*, **2015**, 3, 12343-12349	13	29
88	Exploration versus Exploitation in Global Atomistic Structure Optimization. *Journal of Physical Chemistry A*, **2018**, 122, 1504-1509	2.8	29

87	Determination of low-strain interfaces via geometric matching. *Physical Review B*, **2017**, 96,	3.3	29
86	Plasmons on the edge of MoS2 nanostructures. *Physical Review B*, **2014**, 90,	3.3	29
85	First-principles calculations of graphene nanoribbons in gaseous environments: Structural and electronic properties. *Physical Review B*, **2010**, 82,	3.3	29
84	Partly occupied Wannier functions: Construction and applications. *Physical Review B*, **2005**, 72,	3.3	29
83	Calculation of quantum tunneling for a spatially extended defect: the dislocation kink in copper has a low effective mass. *Physical Review Letters*, **2001**, 86, 1546-9	7.4	29
82	Heats of formation of solids with error estimation: The mBEEF functional with and without fitted reference energies. *Physical Review B*, **2015**, 91,	3.3	28
81	Electronic hole localization in rutile and anatase TiO2 □Self-interaction correction in □SCF DFT. *Chemical Physics Letters*, **2011**, 506, 42-45	2.5	28
80	mBEEF-vdW: Robust fitting of error estimation density functionals. *Physical Review B*, **2016**, 93,	3.3	27
79	Making the most of materials computations. *Science*, **2016**, 354, 180-181	33.3	27
78	Scanning Tunneling Microscopy Evidence for the Dissociation of Carbon Monoxide on Ruthenium Steps. *Journal of Physical Chemistry C*, **2012**, 116, 14350-14359	3.8	27
77	Nucleation of the Pt(111) reconstruction: a simulation study. *Surface Science*, **1994**, 317, 8-14	1.8	27
76	Electron transport in a Pt□OPt nanocontact: Density functional theory calculations. *Physical Review B*, **2006**, 73,	3.3	26
75	Atomic-scale structure of dislocations revealed by scanning tunneling microscopy and molecular dynamics. *Physical Review Letters*, **2002**, 88, 206106	7.4	26
74	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	6.4	24
73	Graphene Edges Dictate the Morphology of Nanoparticles during Catalytic Channeling. *Journal of Physical Chemistry C*, **2014**, 118, 4296-4302	3.8	24
72	Effective-medium tight-binding model for silicon. *Physical Review B*, **1994**, 50, 10727-10741	3.3	24
71	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	23
70	Effects of anisotropic diffusion and finite island sizes in homoepitaxial growth: Pt on Pt(100)-hex. *Surface Science*, **1998**, 400, 290-313	1.8	23

69	Mechanical deformation of nanocrystalline materials. *Philosophical Magazine Letters*, **1996**, 74, 339-344	1	23
68	Effective-medium calculations for hydrogen in Ni, Pd, and Pt. *Physical Review B*, **1990**, 41, 12413-12423	3.3	23
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66	Elastic effects behind cooperative bonding in beta-sheets. *Journal of the American Chemical Society*, **2004**, 126, 13140-3	16.4	22
65	Anab initiostudy of electron transport through nitrobenzene: the influence of leads and contacts. *Nanotechnology*, **2005**, 16, S155-S160	3.4	22
64	Inelastic scattering in metal-H2-metal junctions. *Physical Review B*, **2009**, 79,	3.3	21
63	Beta-sheet preferences from first principles. *Journal of the American Chemical Society*, **2003**, 125, 16383-6	16.4	21
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60	Kinematic generation of dislocations. *Philosophical Magazine Letters*, **1995**, 72, 245-250	1	20
59	Optimized and transferable densities from first-principles local density calculations. *Journal of Physics Condensed Matter*, **1991**, 3, 5437-5443	1.8	20
58	Theory of alkali-metal-induced reconstructions of fcc(100) surfaces. *Physical Review B*, **1992**, 45, 6893-6898	3.8	20
57	Critical current for the flow of superfluid3He in a confined geometry. *Journal of Low Temperature Physics*, **1987**, 67, 83-89	1.3	19
56	Dynamic breaking of a single gold bond. *Nature Communications*, **2017**, 8, 15931	17.4	18
55	IIDVI2 and IIIDIV2 Polytypes as Light Absorbers for Single Junction and Tandem Photovoltaic Devices. *Journal of Physical Chemistry C*, **2017**, 121, 17780-17786	3.8	18
54	A simple and realistic model system for studying hydrogen bonds in -sheets. *Journal of Chemical Physics*, **2003**, 118, 9783-9794	3.9	18
53	Construction of New Electronic Density Functionals with Error Estimation Through Fitting. *Topics in Catalysis*, **2012**, 55, 402-417	2.3	17
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50	Analytic approach to charge transfer during atom-surface scattering. *Physical Review B*, **1989**, 40, 3417-3420	3.8	17
49	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	3.8	16
48	Atomistic simulations of MgCu metallic glasses: mechanical properties. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2004**, 387-389, 996-1000	5.3	16
47	High-throughput computational screening for two-dimensional magnetic materials based on experimental databases of three-dimensional compounds. *Npj Computational Materials*, **2020**, 6,	10.9	15
46	Atomically Thin Ordered Alloys of Transition Metal Dichalcogenides: Stability and Band Structures. *Journal of Physical Chemistry C*, **2016**, 120, 23024-23029	3.8	14
45	Simple model of stacking-fault energies. *Physical Review B*, **1993**, 47, 4916-4921	3.3	14
44	Electronic hole transfer in rutile and anatase TiO2: Effect of a delocalization error in the density functional theory on the charge transfer barrier height. *Physical Review B*, **2011**, 84,	3.3	13
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42	Anomalous conductance oscillations and half-metallicity in atomic Ag-O chains. *Physical Review Letters*, **2008**, 101, 096804	7.4	13
41	Rich Ground-State Chemical Ordering in Nanoparticles: Exact Solution of a Model for Ag-Au Clusters. *Physical Review Letters*, **2018**, 120, 256101	7.4	12
40	Computer simulations of nanoindentation in MgCu and CuZr metallic glasses. *Modelling and Simulation in Materials Science and Engineering*, **2010**, 18, 055006	2	12
39	Atomistic simulations of jog migration on extended screw dislocations. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2001**, 319-321, 119-123	5.3	12
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