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	Structure and energetics of liquid waterâ€“hydroxyl layers on Pt(111). Physical Chemistry Chemical Physics, 2022, 24, 9885-9890.	2.8	8
2	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	8.7	6
3	Computational exfoliation of atomically thin one-dimensional materials with application to Majorana bound states. Physical Review Materials, 2022, 6, .	2.4	4
4	Schottky barrier lowering due to interface states in 2D heterophase devices. Nanoscale Advances, 2021, 3, 567-574.	4.6	8
5	Global optimization of atomic structures with gradient-enhanced Gaussian process regression. Physical Review B, 2021, 103, .	3.2	22
6	Assessing the role of quantum effects in two-dimensional heterophase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoTe</mml:mi><mml:mn>2</mml:mn></mml:msub></m field effect transistors. Physical Review B, 2021, 104, .	3.2	2
7	Atomic Structure Optimization with Machine-Learning Enabled Interpolation between Chemical Elements. Physical Review Letters, 2021, 127, 166001.	7.8	11
8	Is the water/Pt(111) interface ordered at room temperature?. Journal of Chemical Physics, 2021, 155, 224701.	3.0	9
9	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
10	Bayesian error estimation in density functional theory. , 2020, , 77-91.		0
11	Machine learning with bond information for local structure optimizations in surface science. Journal of Chemical Physics, 2020, 153, 234116.	3.0	12
12	Minimum-strain symmetrization of Bravais lattices. Physical Review Research, 2020, 2, .	3.6	3
13	Reply to comment on â€˜The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystalsâ€™. 2D Materials, 2019, 6, 048002.	4.4	12
14	Local Bayesian optimizer for atomic structures. Physical Review B, 2019, 100, .	3.2	57
15	Materials property prediction using symmetry-labeled graphs as atomic position independent descriptors. Physical Review B, 2019, 100, .	3.2	9
16	Spontaneous breaking of time-reversal symmetry at the edges of 1Tâ€² monolayer transition metal dichalcogenides. Physical Review B, 2019, 99, .	3.2	8
17	Shining Light on Sulfide Perovskites: LaYS₃ Material Properties and Solar Cells. Chemistry of Materials, 2019, 31, 3359-3369.	6.7	32
18	High-Entropy Alloys as a Discovery Platform for Electrocatalysis. Joule, 2019, 3, 834-845.	24.0	464

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19	Definition of a scoring parameter to identify low-dimensional materials components. Physical Review Materials, 2019, 3, .	2.4	30
20	High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices. ACS Energy Letters, 2018, 3, 436-446.	17.4	51
21	Exploration versus Exploitation in Global Atomistic Structure Optimization. Journal of Physical Chemistry A, 2018, 122, 1504-1509.	2.5	56
22	The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals. 2D Materials, 2018, 5, 042002.	4.4	711
23	Machine learning-based screening of complex molecules for polymer solar cells. Journal of Chemical Physics, 2018, 148, 241735.	3.0	94
24	Rich Ground-State Chemical Ordering in Nanoparticles: Exact Solution of a Model for Ag-Au Clusters. Physical Review Letters, 2018, 120, 256101.	7.8	15
25	Chapter 3. Computational Screening of Light-absorbing Materials for Photoelectrochemical Water Splitting. RSC Energy and Environment Series, 2018, , 62-99.	0.5	2
26	Promising quaternary chalcogenides as high-band-gap semiconductors for tandem photoelectrochemical water splitting devices: A computational screening approach. Physical Review Materials, 2018, 2, .	2.4	16
27	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
28	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
29	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
30	Roughness in flatland. Nature Materials, 2017, 16, 1059-1060.	27.5	9
31	Determination of low-strain interfaces via geometric matching. Physical Review B, 2017, 96, .	3.2	47
32	Dynamic breaking of a single gold bond. Nature Communications, 2017, 8, 15931.	12.8	28
33	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
34	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
35	Defect Chemistry and Electrical Conductivity of Sm-Doped La_{1â€“x}Sr_xCoO_{3â^'Î´} for Solid Oxide Fuel Cells. Journal of Physical Chemistry C, 2017, 121, 15017-15027.	3.1	13
36	Defect-Tolerant Monolayer Transition Metal Dichalcogenides. Nano Letters, 2016, 16, 2234-2239.	9.1	111

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37	Atomically Thin Ordered Alloys of Transition Metal Dichalcogenides: Stability and Band Structures. Journal of Physical Chemistry C, 2016, 120, 23024-23029.	3.1	20
38	mBEEF-vdW: Robust fitting of error estimation density functionals. Physical Review B, 2016, 93, .	3.2	35
39	Making the most of materials computations. Science, 2016, 354, 180-181.	12.6	35
40	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
41	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
42	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
43	Band-gap engineering of functional perovskites through quantum confinement and tunneling. Physical Review B, 2015, 91, .	3.2	13
44	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
45	Strain sensitivity of band gaps of Sn-containing semiconductors. Physical Review B, 2015, 91, .	3.2	24
46	Calculated optical absorption of different perovskite phases. Journal of Materials Chemistry A, 2015, 3, 12343-12349.	10.3	35
47	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
48	New Lightâ€Harvesting Materials Using Accurate and Efficient Bandgap Calculations. Advanced Energy Materials, 2015, 5, 1400915.	19.5	124
49	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
50	mBEEF: An accurate semi-local Bayesian error estimation density functional. Journal of Chemical Physics, 2014, 140, 144107.	3.0	117
51	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
52	Graphene Edges Dictate the Morphology of Nanoparticles during Catalytic Channeling. Journal of Physical Chemistry C, 2014, 118, 4296-4302.	3.1	29
53	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	12.6	319
54	Bandgap calculations and trends of organometal halide perovskites. APL Materials, 2014, 2, .	5.1	222

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55	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
56	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. Topics in Catalysis, 2014, 57, 265-272.	2.8	47
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	Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. Nature Communications, 2013, 4, 2121.	12.8	43
59	Performance of genetic algorithms in search for water splitting perovskites. Journal of Materials Science, 2013, 48, 6519-6534.	3.7	42
60	Electrochemical CO₂ and CO Reduction on Metal-Functionalized Porphyrin-like Graphene. Journal of Physical Chemistry C, 2013, 117, 9187-9195.	3.1	260
61	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	4.6	249
62	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. New Journal of Physics, 2013, 15, 105026.	2.9	51
63	Bandgap Engineering of Double Perovskites for One- and Two-photon Water Splitting. Materials Research Society Symposia Proceedings, 2013, 1523, 601.	0.1	13
64	Unraveling the acoustic electron-phonon interaction in graphene. Physical Review B, 2012, 85, .	3.2	122
65	Conventional and acoustic surface plasmons on noble metal surfaces: A time-dependent density functional theory study. Physical Review B, 2012, 86, .	3.2	51
66	The Computational Materials Repository. Computing in Science and Engineering, 2012, 14, 51-57.	1.2	153
67	Spatially resolved quantum plasmon modes in metallic nano-films from first-principles. Physical Review B, 2012, 86, .	3.2	36
68	Computational screening of perovskite metal oxides for optimal solar light capture. Energy and Environmental Science, 2012, 5, 5814-5819.	30.8	354
69	Oxidative trends of TiO2â€"hole trapping at anatase and rutile surfaces. Energy and Environmental Science, 2012, 5, 9866.	30.8	41
70	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
71	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. Physical Review B, 2012, 85, .	3.2	1,087
72	Ab initiononequilibrium quantum transport and forces with the real-space projector augmented wave method. Physical Review B, 2012, 85, .	3.2	33

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73	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
74	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
75	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
76	Construction of New Electronic Density Functionals with Error Estimation Through Fitting. Topics in Catalysis, 2012, 55, 402-417.	2.8	19
77	Ab Initio Calculations of the Electronic Properties of Polypyridine Transition Metal Complexes and Their Adsorption on Metal Surfaces in the Presence of Solvent and Counterions. Journal of Physical Chemistry B, 2011, 115, 9410-9416.	2.6	14
78	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, .	3.2	14
79	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
80	Nonlocal Screening of Plasmons in Graphene by Semiconducting and Metallic Substrates: First-Principles Calculations. Physical Review Letters, 2011, 106, 146803.	7.8	73
81	First-principles study of surface plasmons on Ag(111) and H/Ag(111). Physical Review B, 2011, 84, .	3.2	64
82	Electronic shell structure and chemisorption on gold nanoparticles. Physical Review B, 2011, 84, .	3.2	44
83	Linear density response function in the projector augmented wave method: Applications to solids, surfaces, and interfaces. Physical Review B, 2011, 83, .	3.2	142
84	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. Journal of Physical Chemistry C, 2011, 115, 2244-2252.	3.1	52
85	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. Catalysis Letters, 2011, 141, 1067-1071.	2.6	234
86	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
87	First-principles modelling of scanning tunneling microscopy using non-equilibrium Greenâ€™s functions. Frontiers of Physics in China, 2010, 5, 369-379.	1.0	13
88	Designing multifunctional chemical sensors using Ni and Cu doped carbon nanotubes. Physica Status Solidi (B): Basic Research, 2010, 247, 2678-2682.	1.5	8
89	Fully self-consistent GW calculations for molecules. Physical Review B, 2010, 81, .	3.2	225
90	First-principles calculations of graphene nanoribbons in gaseous environments: Structural and electronic properties. Physical Review B, 2010, 82, .	3.2	33

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91	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. Journal of Chemical Physics, 2010, 132, 071101.	3.0	367
92	Computer simulations of nanoindentation in Mgâ€“Cu and Cuâ€“Zr metallic glasses. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 055006.	2.0	14
93	Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes. Physical Review B, 2010, 81, .	3.2	37
94	Graphene on metals: A van der Waals density functional study. Physical Review B, 2010, 81, .	3.2	431
95	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
96	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:math junctions. Physical Review B, 2009, 79, .	3.2	41
97	Localized atomic basis set in the projector augmented wave method. Physical Review B, 2009, 80, .	3.2	297
98	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
99	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
100	Anomalous Conductance Oscillations and Half-Metallicity in Atomic Ag-O Chains. Physical Review Letters, 2008, 101, 096804.	7.8	14
101	Benchmark density functional theory calculations for nanoscale conductance. Journal of Chemical Physics, 2008, 128, 114714.	3.0	109
102	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
103	Avalanche Size Scaling in Sheared Three-Dimensional Amorphous Solid. Physical Review Letters, 2007, 98, 095501.	7.8	97
104	Electronic-Structure-Based Design of Ordered Alloys. MRS Bulletin, 2006, 31, 986-990.	3.5	12
105	Atomistic simulation study of the shear-band deformation mechanism in Mg-Cu metallic glasses. Physical Review B, 2006, 73, .	3.2	82
106	Fermi level alignment in molecular nanojunctions and its relation to charge transfer. Physical Review B, 2006, 74, .	3.2	84
107	Electron transport in aPtâ^'COâ^'Ptnanocontact: Density functional theory calculations. Physical Review B, 2006, 73, .	3.2	28
108	Molecular transport calculations with Wannier functions. Chemical Physics, 2005, 319, 111-125.	1.9	120

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109	Anab initiostudy of electron transport through nitrobenzene: the influence of leads and contacts. Nanotechnology, 2005, 16, S155-S160.	2.6	23
110	Interference andk-point sampling in the supercell approach to phase-coherent transport. Physical Review B, 2005, 72, .	3.2	47
111	Partly occupied Wannier functions: Construction and applications. Physical Review B, 2005, 72, .	3.2	38
112	Partly Occupied Wannier Functions. Physical Review Letters, 2005, 94, 026405.	7.8	64
113	Stretching dependence of the vibration modes of a single-moleculePtâ^'H2â^'Ptbridge. Physical Review B, 2005, 71, .	3.2	142
114	Conduction Mechanism in a Molecular Hydrogen Contact. Physical Review Letters, 2005, 94, 036807.	7.8	63
115	Bayesian Error Estimation in Density-Functional Theory. Physical Review Letters, 2005, 95, 216401.	7.8	163
116	Real-space grid implementation of the projector augmented wave method. Physical Review B, 2005, 71, .	3.2	1,606
117	Forces and conductances in a single-molecule bipyridine junction. Physical Review B, 2005, 72, .	3.2	65
118	Simulation of Cu-Mg metallic glass: Thermodynamics and structure. Physical Review B, 2004, 69, .	3.2	57
119	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
120	Bayesian Ensemble Approach to Error Estimation of Interatomic Potentials. Physical Review Letters, 2004, 93, 165501.	7.8	95
121	Atomic-scale insight into structure and morphology changes of MoS2 nanoclusters in hydrotreating catalysts. Journal of Catalysis, 2004, 221, 510-522.	6.2	379
122	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
123	Simulations of intergranular fracture in nanocrystalline molybdenum. Acta Materialia, 2004, 52, 5019-5029.	7.9	69
124	Elastic Effects behind Cooperative Bonding in Î²-Sheets. Journal of the American Chemical Society, 2004, 126, 13140-13143.	13.7	24
125	A Maximum in the Strength of Nanocrystalline Copper. Science, 2003, 301, 1357-1359.	12.6	1,296
126	Chemistry of one-dimensional metallic edge states in MoS2nanoclusters. Nanotechnology, 2003, 14, 385-389.	2.6	212

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127	Atomic and electronic structure ofMoS2nanoparticles. Physical Review B, 2003, 67, .	3.2	352
128	Î²-Sheet Preferences from First Principles. Journal of the American Chemical Society, 2003, 125, 16383-16386.	13.7	24
129	Density functional theory studies of screw dislocation core structures in bcc metals. Philosophical Magazine, 2003, 83, 365-375.	1.6	197
130	Conductance calculations with a wavelet basis set. Physical Review B, 2003, 67, .	3.2	74
131	A simple and realistic model system for studying hydrogen bonds in Î²-sheets. Journal of Chemical Physics, 2003, 118, 9783-9794.	3.0	19
132	Pareto-optimal alloys. Applied Physics Letters, 2003, 83, 4527-4529.	3.3	43
133	Four-Atom Period in the Conductance of Monatomic Al Wires. Physical Review Letters, 2003, 91, 146801.	7.8	82
134	Atomic-Scale Structure of Dislocations Revealed by Scanning Tunneling Microscopy and Molecular Dynamics. Physical Review Letters, 2002, 88, 206106.	7.8	34
135	Combined Electronic Structure and Evolutionary Search Approach to Materials Design. Physical Review Letters, 2002, 88, 255506.	7.8	248
136	An object-oriented scripting interface to a legacy electronic structure code. Computing in Science and Engineering, 2002, 4, 56-66.	1.2	1,117
137	Atomistic simulations of dislocation processes in copper. Journal of Physics Condensed Matter, 2002, 14, 2929-2956.	1.8	38
138	Adsorption-induced restructuring of gold nanochains. Physical Review B, 2002, 66, .	3.2	102
139	Nanoscale plasticity. Nature Materials, 2002, 1, 15-16.	27.5	48
140	Atomistic simulations of cross-slip of jogged screw dislocations in copper. Philosophical Magazine Letters, 2001, 81, 137-144.	1.2	46
141	Atomistic simulations of jog migration on extended screw dislocations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2001, 319-321, 119-123.	5.6	12
142	Mechanical Properties and Formation Mechanisms of a Wire of Single Gold Atoms. Physical Review Letters, 2001, 87, .	7.8	379
143	Adsorption-Induced Step Formation. Physical Review Letters, 2001, 87, 126102.	7.8	65
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146	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
147	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
148	Surface chemistry in three dimensions: CO dissociation between two surfaces. Chemical Physics Letters, 2000, 322, 307-311.	2.6	2
149	Determination of the of Rate Cross Slip of Screw Dislocations. Physical Review Letters, 2000, 85, 3866-3869.	7.8	61
150	Nakamuraet al.Reply:. Physical Review Letters, 2000, 84, 2549-2549.	7.8	1
151	Density Functional Simulation of a Breaking Nanowire. Physical Review Letters, 1999, 82, 1538-1541.	7.8	97
152	Mechanisms of self-diffusion on Pt(110). Physical Review B, 1999, 60, R5149-R5152.	3.2	45
153	Enhancement of surface self-diffusion of platinum atoms by adsorbed hydrogen. Nature, 1999, 398, 134-136.	27.8	221
154	Oxygen adsorption on Pt(110)-(1Ã—2): new high-coverage structures. Surface Science, 1999, 430, L533-L539.	1.9	37
155	Atomic-scale simulations of the mechanical deformation of nanocrystalline metals. Physical Review B, 1999, 60, 11971-11983.	3.2	569
156	Atomic-Scale Modeling of the Annihilation of Jogged Screw Dislocation Dipoles. Materials Research Society Symposia Proceedings, 1999, 578, 217.	0.1	8
157	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. Physical Review B, 1998, 57, 3283-3294.	3.2	235
158	Softening of nanocrystalline metals at very small grain sizes. Nature, 1998, 391, 561-563.	27.8	1,558
159	Effects of anisotropic diffusion and finite island sizes in homoepitaxial growth. Surface Science, 1998, 400, 290-313.	1.9	23
160	Nudged elastic band method for finding minimum energy paths of transitions. , 1998, , .		1,161
161	Atomic-Scale Modeling of the Deformation of Nanocrystalline Metals. Materials Research Society Symposia Proceedings, 1998, 538, 299.	0.1	2
162	Heteroepitaxial subsurface growth mode resulting in interlayer mixing. Physical Review B, 1997, 55, 1380-1383.	3.2	61

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163	Scattering and conductance quantization in three-dimensional metal nanocontacts. Physical Review B, 1997, 55, 2637-2650.	3.2	93
164	Rate Theory for Correlated Processes: Double Jumps in Adatom Diffusion. Physical Review Letters, 1997, 79, 2843-2846.	7.8	52
165	Atomistic Determination of Cross-Slip Pathway and Energetics. Physical Review Letters, 1997, 79, 3676-3679.	7.8	98
166	Simulations of the atomic structure, energetics, and cross slip of screw dislocations in copper. Physical Review B, 1997, 56, 2977-2990.	3.2	92
167	Phase diagrams for surface alloys. Physical Review B, 1997, 56, 5822-5834.	3.2	391
168	Conductance eigenchannels in nanocontacts. Physical Review B, 1997, 56, 14956-14959.	3.2	196
169	Atomic structure and energetics of constricted screw dislocations in copper. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1997, 234-236, 544-547.	5.6	3
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172	Mechanical deformation of nanocrystalline materials. Philosophical Magazine Letters, 1996, 74, 339-344.	1.2	28
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174	Island shapes in homoepitaxial growth of Pt(111). Surface Science, 1996, 359, 37-44.	1.9	58
175	Incomplete melting of the Si(100) surface from molecular-dynamics simulations using the effective-medium tight-binding model. Surface Science, 1996, 360, 221-228.	1.9	10
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177	Thermal Diffusion Processes in Metal-Tip-Surface Interactions: Contact Formation and Adatom Mobility. Physical Review Letters, 1996, 77, 5067-5070.	7.8	87
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