Jakob SchiÃ¸tz

List of Publications by Year
in descending order

81 papers	11,475 citations	136885 32 h-index	79644 73 g-index
83 all docs	83 docs citations	83 times ranked	12061 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.	0.7	1,933
2	Softening of nanocrystalline metals at very small grain sizes. Nature, 1998, 391, 561-563.	13.7	1,558
3	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	0.7	1,451
4	A Maximum in the Strength of Nanocrystalline Copper. Science, 2003, 301, 1357-1359.	6.0	1,296
5	Tuning the activity of Pt alloy electrocatalysts by means of the lanthanide contraction. Science, 2016, 352, 73-76.	6.0	783
6	Robust structural identification via polyhedral template matching. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 055007.	0.8	580
7	Atomic-scale simulations of the mechanical deformation of nanocrystalline metals. Physical Review B, 1999, 60, 11971-11983.	1.1	569
8	Quantized conductance in an atom-sized point contact. Physical Review Letters, 1994, 72, 2251-2254.	2.9	414
9	Quantized conductance in atom-sized wires between two metals. Physical Review B, 1995, 52, 8499-8514.	1.1	307
10	Kinetic Implications of Dynamical Changes in Catalyst Morphology during Methanol Synthesis over Cu/ZnO Catalysts. Journal of Catalysis, 1997, 168, 133-142.	3.1	254
11	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï”</mml:mi></mml:math>self-consistent field method to obtain potential energy surfaces of excited molecules on surfaces. Physical Review B, 2008, 78, .	1.1	182
12	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.	1.3	152
13	Atomic-scale modeling of plastic deformation of nanocrystalline copper. Scripta Materialia, 2004, 51, 837-841.	2.6	142
14	A Deep Learning Approach to Identify Local Structures in Atomicâ€Resolution Transmission Electron Microscopy Images. Advanced Theory and Simulations, 2018, 1, 1800037.	1.3	139
15	Nano-scale effects in electrochemistry. Chemical Physics Letters, 2004, 390, 440-444.	1.2	126
16	Electrochemical control of quantum interference in anthraquinone-based molecular switches. Journal of Chemical Physics, 2010, 132, 224104.	1.2	98
17	Avalanche Size Scaling in Sheared Three-Dimensional Amorphous Solid. Physical Review Letters, 2007, 98, 095501.	2.9	97
18	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, .	1.1	93

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19	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.	1.2	83
20	Atomistic simulation study of the shear-band deformation mechanism in Mg-Cu metallic glasses. Physical Review B, 2006, 73, .	1.1	82
21	Strain-induced coarsening in nanocrystalline metals under cyclic deformation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 375-377, 975-979.	2.6	76
22	Olesenet al.Reply:. Physical Review Letters, 1995, 74, 2147-2147.	2.9	73
23	Simulations of intergranular fracture in nanocrystalline molybdenum. Acta Materialia, 2004, 52, 5019-5029.	3.8	69
24	Understanding the catalytic activity of gold nanoparticles through multi-scale simulations. Journal of Catalysis, 2011, 284, 34-41.	3.1	68
25	Hot-electron-mediated desorption rates calculated from excited-state potential energy surfaces. Physical Review B, 2009, 79, .	1.1	59
26	Simulation of Cu-Mg metallic glass: Thermodynamics and structure. Physical Review B, 2004, 69, .	1.1	57
27	Simulations of boundary migration during recrystallization using molecular dynamics. Acta Materialia, 2007, 55, 6383-6391.	3.8	49
28	Structure and reactivity of ruthenium nanoparticles. Physical Review B, 2008, 77, .	1.1	49
29	Nanoscale plasticity. Nature Materials, 2002, 1, 15-16.	13.3	48
30	Origin of Power Laws for Reactions at Metal Surfaces Mediated by Hot Electrons. Physical Review Letters, 2009, 103, 238301.	2.9	41
31	Sizeâ€Dependence of the Melting Temperature of Individual Au Nanoparticles. Particle and Particle Systems Characterization, 2019, 36, 1800480.	1.2	35
32	Atomic-Scale Structure of Dislocations Revealed by Scanning Tunneling Microscopy and Molecular Dynamics. Physical Review Letters, 2002, 88, 206106.	2.9	34
33	Correlation between diffusion barriers and alloying energy in binary alloys. Physical Chemistry Chemical Physics, 2016, 18, 3302-3307.	1.3	33
34	Dislocation nucleation and vacancy formation during high-speed deformation of fcc metals. Philosophical Magazine Letters, 2001, 81, 301-309.	0.5	30
35	Mechanical deformation of nanocrystalline materials. Philosophical Magazine Letters, 1996, 74, 339-344.	0.5	28
36	Effects of crack tip geometry on dislocation emission and cleavage: A possible path to enhanced ductility. Physical Review B, 1997, 55, 6211-6221.	1.1	28

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37	An Interatomic Potential for Studying CuZr Bulk Metallic Glasses. Advanced Engineering Materials, 2007, 9, 505-508.	1.6	26
38	Kinematic generation of dislocations. Philosophical Magazine Letters, 1995, 72, 245-250.	0.5	23
39	New Platinum Alloy Catalysts for Oxygen Electroreduction Based on Alkaline Earth Metals. Electrocatalysis, 2017, 8, 594-604.	1.5	23
40	Long time scale simulation of a grain boundary in copper. New Journal of Physics, 2009, 11, 073034.	1.2	20
41	MATERIALS SCIENCE: Nanocrystals Get Twins. Science, 2003, 300, 1244-1245.	6.0	19
42	Transformations of supported gold nanoparticles observed by in situ electron microscopy. Nanoscale, 2019, 11, 11885-11891.	2.8	19
43	Atomic structure of screw dislocations intersecting theAu(111)surface: A combined scanning tunneling microscopy and molecular dynamics study. Physical Review B, 2006, 74, .	1.1	18
44	Hot-electron-assisted femtochemistry at surfaces: A time-dependent density functional theory approach. Physical Review B, 2009, 79, .	1.1	18
45	Atomistic simulations of Mgâ€“Cu metallic glasses: mechanical properties. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 387-389, 996-1000.	2.6	16
46	Pt Gd alloy formation on Pt(111): Preparation and structural characterization. Surface Science, 2016, 652, 114-122.	0.8	16
47	Accuracy of surface strain measurements from transmission electron microscopy images of nanoparticles. Advanced Structural and Chemical Imaging, 2017, 3, 14.	4.0	16
48	Rich Ground-State Chemical Ordering in Nanoparticles: Exact Solution of a Model for Ag-Au Clusters. Physical Review Letters, 2018, 120, 256101.	2.9	15
49	Computer simulations of nanoindentation in Mgâ€“Cu and Cuâ€“Zr metallic glasses. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 055006.	0.8	14
50	Longitudinal domain wall formation in elongated assemblies of ferromagnetic nanoparticles. Scientific Reports, 2015, 5, 14536.	1.6	10
51	H₂/D₂ exchange reaction on mono-disperse Pt clusters: enhanced activity from minute O₂ concentrations. Catalysis Science and Technology, 2016, 6, 6893-6900.	2.1	9
52	Roughness in flatland. Nature Materials, 2017, 16, 1059-1060.	13.3	9
53	Is the water/Pt(111) interface ordered at room temperature?. Journal of Chemical Physics, 2021, 155, 224701.	1.2	9
54	Simulations of super-structure domain walls in two dimensional assemblies of magnetic nanoparticles. Journal of Applied Physics, 2015, 118, .	1.1	8

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55	Structure and energetics of liquid waterâ€“hydroxyl layers on Pt(111). Physical Chemistry Chemical Physics, 2022, 24, 9885-9890.	1.3	8
56	Modeling of Dislocation Generation and Interaction During High-Speed Deformation of Metals. Radiation Effects and Defects in Solids, 2002, 157, 193-200.	0.4	7
57	Site Specificity in Femtosecond Laser Desorption of Neutral H Atoms from Graphite(0001). Physical Review Letters, 2010, 104, 256102.	2.9	7
58	Desorption of H atoms from graphite (0001) using XUV free electron laser pulses. Chemical Physics Letters, 2010, 500, 291-294.	1.2	6
59	Initiation and Progression of Anisotropic Galvanic Replacement Reactions in a Single Ag Nanowire: Implications for Nanostructure Synthesis. ACS Applied Nano Materials, 2021, 4, 12346-12355.	2.4	6
60	Memory effects in nonadiabatic molecular dynamics at metal surfaces. Journal of Chemical Physics, 2010, 133, 134109.	1.2	5
61	Calculation of elastic Greenâ€™s functions for lattices with cavities. Physical Review B, 1997, 56, 2292-2294.	1.1	4
62	EIS Characterization of Ultra High Purity, Float Zone Single Crystal Silicon. ECS Transactions, 2009, 16, 331-342.	0.3	4
63	Reversible and concerted atom diffusion on supported gold nanoparticles. JPhys Materials, 2020, 3, 024009.	1.8	4
64	Quantum corrected Langevin dynamics for adsorbates on metal surfaces interacting with hot electrons. Journal of Chemical Physics, 2010, 133, 034115.	1.2	3
65	Identifying Atoms in High Resolution Transmission Electron Micrographs Using a Deep Convolutional Neural Net. Microscopy and Microanalysis, 2018, 24, 512-513.	0.2	3
66	Effect of Crack Blunting on Subsequent Crack Propagation. Materials Research Society Symposia Proceedings, 1995, 408, 237.	0.1	2
67	Atomic-Scale Modeling of the Deformation of Nanocrystalline Metals. Materials Research Society Symposia Proceedings, 1998, 538, 299.	0.1	2
68	Vibrationally mediated control of single-electron transmission in weakly coupled molecule-metal junctions. Physical Review B, 2010, 81, .	1.1	2
69	Using Neural Networks to Identify Atoms in HRTEM Images. Microscopy and Microanalysis, 2019, 25, 216-217.	0.2	2
70	Transformations of Supported Gold Nanoparticles Observed by In Situ Electron Microscopy. Microscopy and Microanalysis, 2020, 26, 2406-2407.	0.2	1
71	Reconstructing the exit wave in high-resolution transmission electron microscopy using machine learning. Microscopy and Microanalysis, 2021, 27, 254-256.	0.2	1
72	Computer Simulations of the Mechanical Properties of Metals. Science Progress, 1999, 82, 313-325.	1.0	0

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73	Spatio-temporally resolved in situ transmission electron microscopy of the dynamics of nanostructured materials. Microscopy and Microanalysis, 2017, 23, 902-903.	0.2	0
74	Approaches to Quantifying the Dynamics of Nanostructures using in situ Electron Microscopy. Microscopy and Microanalysis, 2018, 24, 1938-1939.	0.2	0
75	In situ Probing of Nanostructure Surfaces. Microscopy and Microanalysis, 2019, 25, 2080-2081.	0.2	0
76	In Situ Study of the Motion of Supported Gold Nanoparticles. Microscopy and Microanalysis, 2020, 26, 3040-3042.	0.2	0
77	Superior Neural Network for Distinguishing Between Atomic Species. Microscopy and Microanalysis, 2021, 27, 466-468.	0.2	0
78	Interaction of electron beam and gold nanoparticles. Microscopy and Microanalysis, 2021, 27, 3350-3352.	0.2	0
79	Electron beam effects in high-resolution transmission electron microscopy investigations of catalytic nanoparticles. Microscopy and Microanalysis, 2021, 27, 3348-3349.	0.2	0
80	Surface dynamics of catalytic nanoparticles in non-vacuum conditions. Microscopy and Microanalysis, 2021, 27, 1316-1317.	0.2	0
81	Competing Deformation Mechanisms in Nanocrystalline Metals. Solid Mechanics and Its Applications, 2004, , 355-363.	0.1	0