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	Structure and energetics of liquid waterâ€“hydroxyl layers on Pt(111). Physical Chemistry Chemical Physics, 2022, 24, 9885-9890.	1.3	8
2	Superior Neural Network for Distinguishing Between Atomic Species. Microscopy and Microanalysis, 2021, 27, 466-468.	0.2	0
3	Reconstructing the exit wave in high-resolution transmission electron microscopy using machine learning. Microscopy and Microanalysis, 2021, 27, 254-256.	0.2	1
4	Interaction of electron beam and gold nanoparticles. Microscopy and Microanalysis, 2021, 27, 3350-3352.	0.2	0
5	Electron beam effects in high-resolution transmission electron microscopy investigations of catalytic nanoparticles. Microscopy and Microanalysis, 2021, 27, 3348-3349.	0.2	0
6	Surface dynamics of catalytic nanoparticles in non-vacuum conditions. Microscopy and Microanalysis, 2021, 27, 1316-1317.	0.2	0
7	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
8	Is the water/Pt(111) interface ordered at room temperature?. Journal of Chemical Physics, 2021, 155, 224701.	1.2	9
9	Transformations of Supported Gold Nanoparticles Observed by In Situ Electron Microscopy. Microscopy and Microanalysis, 2020, 26, 2406-2407.	0.2	1
10	In Situ Study of the Motion of Supported Gold Nanoparticles. Microscopy and Microanalysis, 2020, 26, 3040-3042.	0.2	0
11	Reversible and concerted atom diffusion on supported gold nanoparticles. JPhys Materials, 2020, 3, 024009.	1.8	4
12	Using Neural Networks to Identify Atoms in HRTEM Images. Microscopy and Microanalysis, 2019, 25, 216-217.	0.2	2
13	In situ Probing of Nanostructure Surfaces. Microscopy and Microanalysis, 2019, 25, 2080-2081.	0.2	0
14	Sizeâ€Đependence of the Melting Temperature of Individual Au Nanoparticles. Particle and Particle Systems Characterization, 2019, 36, 1800480.	1.2	35
15	Transformations of supported gold nanoparticles observed by in situ electron microscopy. Nanoscale, 2019, 11, 11885-11891.	2.8	19
16	Approaches to Quantifying the Dynamics of Nanostructures using in situ Electron Microscopy. Microscopy and Microanalysis, 2018, 24, 1938-1939.	0.2	0
17	Identifying Atoms in High Resolution Transmission Electron Micrographs Using a Deep Convolutional Neural Net. Microscopy and Microanalysis, 2018, 24, 512-513.	0.2	3
18	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

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19	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
20	New Platinum Alloy Catalysts for Oxygen Electroreduction Based on Alkaline Earth Metals. Electrocatalysis, 2017, 8, 594-604.	1.5	23
21	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	0.7	1,933
22	Roughness in flatland. Nature Materials, 2017, 16, 1059-1060.	13.3	9
23	Spatio-temporally resolved in situ transmission electron microscopy of the dynamics of nanostructured materials. Microscopy and Microanalysis, 2017, 23, 902-903.	0.2	0
24	Accuracy of surface strain measurements from transmission electron microscopy images of nanoparticles. Advanced Structural and Chemical Imaging, 2017, 3, 14.	4.0	16
25	Tuning the activity of Pt alloy electrocatalysts by means of the lanthanide contraction. Science, 2016, 352, 73-76.	6.0	783
26	Robust structural identification via polyhedral template matching. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 055007.	0.8	580
27	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
28	Pt Gd alloy formation on Pt(111): Preparation and structural characterization. Surface Science, 2016, 652, 114-122.	0.8	16
29	Correlation between diffusion barriers and alloying energy in binary alloys. Physical Chemistry Chemical Physics, 2016, 18, 3302-3307.	1.3	33
30	Longitudinal domain wall formation in elongated assemblies of ferromagnetic nanoparticles. Scientific Reports, 2015, 5, 14536.	1.6	10
31	Simulations of super-structure domain walls in two dimensional assemblies of magnetic nanoparticles. Journal of Applied Physics, 2015, 118, .	1.1	8
32	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
33	Understanding the catalytic activity of gold nanoparticles through multi-scale simulations. Journal of Catalysis, 2011, 284, 34-41.	3.1	68
34	Desorption of H atoms from graphite (0001) using XUV free electron laser pulses. Chemical Physics Letters, 2010, 500, 291-294.	1.2	6
35	Site Specificity in Femtosecond Laser Desorption of Neutral H Atoms from Graphite(0001). Physical Review Letters, 2010, 104, 256102.	2.9	7
36	Vibrationally mediated control of single-electron transmission in weakly coupled molecule-metal junctions. Physical Review B, 2010, 81, .	1.1	2

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37	Memory effects in nonadiabatic molecular dynamics at metal surfaces. Journal of Chemical Physics, 2010, 133, 134109.	1.2	5
38	Quantum corrected Langevin dynamics for adsorbates on metal surfaces interacting with hot electrons. Journal of Chemical Physics, 2010, 133, 034115.	1.2	3
39	Electrochemical control of quantum interference in anthraquinone-based molecular switches. Journal of Chemical Physics, 2010, 132, 224104.	1.2	98
40	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
41	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
42	Hot-electron-mediated desorption rates calculated from excited-state potential energy surfaces. Physical Review B, 2009, 79, .	1.1	59
43	Origin of Power Laws for Reactions at Metal Surfaces Mediated by Hot Electrons. Physical Review Letters, 2009, 103, 238301.	2.9	41
44	Long time scale simulation of a grain boundary in copper. New Journal of Physics, 2009, 11, 073034.	1.2	20
45	EIS Characterization of Ultra High Purity, Float Zone Single Crystal Silicon. ECS Transactions, 2009, 16, 331-342.	0.3	4
46	Hot-electron-assisted femtochemistry at surfaces: A time-dependent density functional theory approach. Physical Review B, 2009, 79, .	1.1	18
47	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î”</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
48	Structure and reactivity of ruthenium nanoparticles. Physical Review B, 2008, 77, .	1.1	49
49	Avalanche Size Scaling in Sheared Three-Dimensional Amorphous Solid. Physical Review Letters, 2007, 98, 095501.	2.9	97
50	An Interatomic Potential for Studying CuZr Bulk Metallic Glasses. Advanced Engineering Materials, 2007, 9, 505-508.	1.6	26
51	Simulations of boundary migration during recrystallization using molecular dynamics. Acta Materialia, 2007, 55, 6383-6391.	3.8	49
52	Atomistic simulation study of the shear-band deformation mechanism in Mg-Cu metallic glasses. Physical Review B, 2006, 73, .	1.1	82
53	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
54	Simulation of Cu-Mg metallic glass: Thermodynamics and structure. Physical Review B, 2004, 69, .	1.1	57

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55	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
56	Atomic-scale modeling of plastic deformation of nanocrystalline copper. Scripta Materialia, 2004, 51, 837-841.	2.6	142
57	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
58	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
59	Simulations of intergranular fracture in nanocrystalline molybdenum. Acta Materialia, 2004, 52, 5019-5029.	3.8	69
60	Nano-scale effects in electrochemistry. Chemical Physics Letters, 2004, 390, 440-444.	1.2	126
61	Competing Deformation Mechanisms in Nanocrystalline Metals. Solid Mechanics and Its Applications, 2004, , 355-363.	0.1	0
62	A Maximum in the Strength of Nanocrystalline Copper. Science, 2003, 301, 1357-1359.	6.0	1,296
63	MATERIALS SCIENCE: Nanocrystals Get Twins. Science, 2003, 300, 1244-1245.	6.0	19
64	Atomic-Scale Structure of Dislocations Revealed by Scanning Tunneling Microscopy and Molecular Dynamics. Physical Review Letters, 2002, 88, 206106.	2.9	34
65	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
66	Nanoscale plasticity. Nature Materials, 2002, 1, 15-16.	13.3	48
67	Dislocation nucleation and vacancy formation during high-speed deformation of fcc metals. Philosophical Magazine Letters, 2001, 81, 301-309.	0.5	30
68	Computer Simulations of the Mechanical Properties of Metals. Science Progress, 1999, 82, 313-325.	1.0	0
69	Atomic-scale simulations of the mechanical deformation of nanocrystalline metals. Physical Review B, 1999, 60, 11971-11983.	1.1	569
70	Softening of nanocrystalline metals at very small grain sizes. Nature, 1998, 391, 561-563.	13.7	1,558
71	Atomic-Scale Modeling of the Deformation of Nanocrystalline Metals. Materials Research Society Symposia Proceedings, 1998, 538, 299.	0.1	2
72	Calculation of elastic Greenâ€™s functions for lattices with cavities. Physical Review B, 1997, 56, 2292-2294.	1.1	4

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73	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
74	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
75	Mechanical deformation of nanocrystalline materials. Philosophical Magazine Letters, 1996, 74, 339-344.	0.5	28
76	Effect of Crack Blunting on Subsequent Crack Propagation. Materials Research Society Symposia Proceedings, 1995, 408, 237.	0.1	2
77	Quantized conductance in atom-sized wires between two metals. Physical Review B, 1995, 52, 8499-8514.	1.1	307
78	Olesenet al.Reply:. Physical Review Letters, 1995, 74, 2147-2147.	2.9	73
79	Kinematic generation of dislocations. Philosophical Magazine Letters, 1995, 72, 245-250.	0.5	23
80	Quantized conductance in an atom-sized point contact. Physical Review Letters, 1994, 72, 2251-2254.	2.9	414
81	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