

Michael Moseler

List of Publications by Year in descending order

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120
papers

7,827
citations

61984

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49909

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124
all docs

124
docs citations

124
times ranked

7985
citing authors

#	ARTICLE	IF	CITATIONS
1	Ab Initio Modeling of the ZnO-Cu(111) Interface. Journal of Physical Chemistry C, 2022, 126, 764-771.	3.1	7
2	Relating Dry Friction to Interdigitation of Surface Passivation Species: A Molecular Dynamics Study on Amorphous Carbon. Materials, 2022, 15, 3247.	2.9	8
3	<i>In Situ</i> Synthesis of Graphene Nitride Nanolayers on Glycerol-Lubricated Si ₃ N ₄ for Superlubricity Applications. ACS Applied Nano Materials, 2021, 4, 2721-2732.	5.0	16
4	On the Influence of Microtopography on the Sliding Performance of Cross Country Skis. Frontiers in Mechanical Engineering, 2021, 7, .	1.8	3
5	Multiscale Friction Simulation of Dry Polymer Contacts: Reaching Experimental Length Scales by Coupling Molecular Dynamics and Contact Mechanics. Tribology Letters, 2021, 69, 1.	2.6	7
6	Interplay of mechanics and chemistry governs wear of diamond-like carbon coatings interacting with ZDDP-additivated lubricants. Nature Communications, 2021, 12, 4550.	12.8	42
7	Carbon nanotubes as fillers for composites with enhanced thermal conductivity. Physical Review Materials, 2021, 5, .	2.4	2
8	Superlow Friction of a-C:H Coatings in Vacuum: Passivation Regimes and Structural Characterization of the Sliding Interfaces. Coatings, 2021, 11, 1069.	2.6	14
9	A Combined Experimental and Atomistic Investigation of PTFE Double Transfer Film Formation and Lubrication in Rolling Point Contacts. Tribology Letters, 2021, 69, 1.	2.6	13
10	Solid-Phase Silicon Homoepitaxy via Shear-Induced Amorphization and Recrystallization. Physical Review Letters, 2021, 127, 126101.	7.8	5
11	Shear Induced Dynamic Grain-Refinement in Sliding Polycrystalline Metal Surfaces. , 2021, , 169-183.		0
12	Ab Initio Wavelength-Dependent Raman Spectra: Placzek Approximation and Beyond. Journal of Chemical Theory and Computation, 2020, 16, 576-586.	5.3	17
13	Constitutive relations for plasticity of amorphous carbon. JPhys Materials, 2020, 3, 035005.	4.2	4
14	Nonempirical Free Volume Viscosity Model for Alkane Lubricants under Severe Pressures. Physical Review Letters, 2020, 124, 105501.	7.8	15
15	Steric Effects Control Dry Friction of H- and F-Terminated Carbon Surfaces. ACS Applied Materials & Interfaces, 2020, 12, 8805-8816.	8.0	15
16	Facile and Efficient Atomic Hydrogenation Enabled Black TiO ₂ with Enhanced Photoelectrochemical Activity via a Favorably Low Energy Barrier Pathway. Advanced Energy Materials, 2019, 9, 1900725.	19.5	21
17	Electronically Coupled Uranium and Iron Oxide Heterojunctions as Efficient Water Oxidation Catalysts. Advanced Functional Materials, 2019, 29, 1905005.	14.9	18
18	Atomistic Insights Into Lubricated Tungsten/Diamond Sliding Contacts. Frontiers in Mechanical Engineering, 2019, 5, .	1.8	4

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19	Experimental and theoretical 2p core-level spectra of size-selected gas-phase aluminum and silicon cluster cations: chemical shifts, geometric structure, and coordination-dependent screening. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6651-6661.	2.8	12
20	Solution of boundary-element problems using the fast-inertial-relaxation-engine method. <i>Physical Review B</i> , 2019, 99, .	3.2	20
21	Ab initio thermodynamics study of ambient gases reacting with amorphous carbon. <i>Physical Review B</i> , 2019, 99, .	3.2	3
22	Effects of Gas-Phase Conditions and Particle Size on the Properties of Cu(111)-Supported Zn _y O _x Particles Revealed by Global Optimization and Ab Initio Thermodynamics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30903-30916.	3.1	17
23	Mechano-chemical decomposition of organic friction modifiers with multiple reactive centres induces superlubricity of ta-C. <i>Nature Communications</i> , 2019, 10, 151.	12.8	118
24	Ab initio study of CO ₂ hydrogenation mechanisms on inverse ZnO/Cu catalysts. <i>Journal of Catalysis</i> , 2018, 360, 168-174.	6.2	58
25	Contact mechanics of graphene-covered metal surfaces. <i>Applied Physics Letters</i> , 2018, 112, .	3.3	16
26	Slipping domains in water-lubricated microsystems for improved load support. <i>Tribology International</i> , 2018, 120, 269-279.	5.9	14
27	Role of oxygen functional groups in the friction of water-lubricated low-index diamond surfaces. <i>Physical Review Materials</i> , 2018, 2, .	2.4	17
28	Shear melting of silicon and diamond and the disappearance of the polyamorphic transition under shear. <i>Physical Review Materials</i> , 2018, 2, .	2.4	26
29	Friction Regimes of Water-Lubricated Diamond (111): Role of Interfacial Ether Groups and Tribo-Induced Aromatic Surface Reconstructions. <i>Physical Review Letters</i> , 2017, 119, 096101.	7.8	63
30	Contrast in nanoscale friction between rotational domains of graphene on Pt(111). <i>Carbon</i> , 2017, 113, 132-138.	10.3	33
31	Integrated Strategy toward Self-Powering and Selectivity Tuning of Semiconductor Gas Sensors. <i>ACS Sensors</i> , 2016, 1, 1256-1264.	7.8	28
32	Offset-corrected \hat{I} -Kohn-Sham scheme for semiempirical prediction of absolute x-ray photoelectron energies in molecules and solids. <i>Physical Review B</i> , 2016, 94, .	3.2	14
33	Molecular Dynamic Simulation of Collision-Induced Third-Body Formation in Hydrogen-Free Diamond-Like Carbon Asperities. <i>Tribology Letters</i> , 2016, 63, 26.	2.6	16
34	Band Edge Engineering in BiVO ₄ /TiO ₂ Heterostructure: Enhanced Photoelectrochemical Performance through Improved Charge Transfer. <i>ACS Catalysis</i> , 2016, 6, 5311-5318.	11.2	117
35	Hydrogen treated anatase TiO ₂ : a new experimental approach and further insights from theory. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2670-2681.	10.3	117
36	Activation and mechanochemical breaking of C-C bonds initiate wear of diamond (110) surfaces in contact with silica. <i>Carbon</i> , 2016, 98, 474-483.	10.3	61

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37	Fluorine-Terminated Diamond Surfaces as Dense Dipole Lattices: The Electrostatic Origin of Polar Hydrophobicity. <i>Journal of the American Chemical Society</i> , 2016, 138, 4018-4028.	13.7	47
38	Insights into Interfacial Changes and Photoelectrochemical Stability of In _x Ga _{1-x} N (0001) Photoanode Surfaces in Liquid Environments. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 8232-8238.	8.0	23
39	Density functional theory and chromium: Insights from the dimers. <i>Journal of Chemical Physics</i> , 2015, 142, 124316.	3.0	18
40	European Symposium on Friction, Wear, and Wear Protection. <i>Conference Papers in Science</i> , 2015, 2015, 1-1.	0.3	0
41	Surface Softening in Metal-Ceramic Sliding Contacts: An Experimental and Numerical Investigation. <i>ACS Nano</i> , 2015, 9, 1478-1491.	14.6	22
42	Influence of hydrodynamic drag model on shear stress in the simulation of magnetorheological fluids. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2015, 218, 16-26.	2.4	29
43	Ultralow Friction of Steel Surfaces Using a 1,3-Diketone Lubricant in the Thin Film Lubrication Regime. <i>Langmuir</i> , 2015, 31, 11033-11039.	3.5	35
44	Origins of Folding Instabilities on Polycrystalline Metal Surfaces. <i>Physical Review Applied</i> , 2014, 2, .	3.8	63
45	Taming the Untamable-The Art and Science of Diamond Polishing. , 2014, , 81-98.		2
46	Nanoscale sliding friction phenomena at the interface of diamond-like carbon and tungsten. <i>Acta Materialia</i> , 2014, 67, 395-408.	7.9	44
47	Highly Selective SAM-Nanowire Hybrid NO ₂ Sensor: Insight into Charge Transfer Dynamics and Alignment of Frontier Molecular Orbitals. <i>Advanced Functional Materials</i> , 2014, 24, 595-602.	14.9	71
48	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. <i>Tribology Letters</i> , 2014, 53, 119-126.	2.6	89
49	Interactions of polymers with reduced graphene oxide: van der Waals binding energies of benzene on graphene with defects. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 33-37.	2.8	43
50	Atomic Scale Mechanisms of Friction Reduction and Wear Protection by Graphene. <i>Nano Letters</i> , 2014, 14, 7145-7152.	9.1	210
51	A Highly Selective and Self-Powered Gas Sensor Via Organic Surface Functionalization of p-Si/n-ZnO Diodes. <i>Advanced Materials</i> , 2014, 26, 8017-8022.	21.0	103
52	Coarse Graining and Localized Plasticity between Sliding Nanocrystalline Metals. <i>Physical Review Letters</i> , 2014, 113, 036101.	7.8	37
53	Discrete element study of viscous flow in magnetorheological fluids. <i>Rheologica Acta</i> , 2014, 53, 417-443.	2.4	19
54	Surface passivation and boundary lubrication of self-mated tetrahedral amorphous carbon asperities under extreme tribological conditions. <i>Friction</i> , 2014, 2, 193-208.	6.4	29

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55	Plasma-chemical reduction of iron oxide photoanodes for efficient solar hydrogen production. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 4828-4835.	7.1	54
56	Sensors: Highly Selective SAM-Modified Nanowire Hybrid NO ₂ Sensor: Insight into Charge Transfer Dynamics and Alignment of Frontier Molecular Orbitals (<i>Adv. Funct. Mater.</i> 5/2014). <i>Advanced Functional Materials</i> , 2014, 24, 566-566.	14.9	1
57	Experimental and Numerical Atomistic Investigation of the Third Body Formation Process in Dry Tungsten/Tungsten-Carbide Tribo Couples. <i>Tribology Letters</i> , 2013, 50, 67-80.	2.6	42
58	Lithium Chalcogenidotetrelates: LiChTâ€”Synthesis and Characterization of New Li ⁺ Ion Conducting Li/Sn/Se Compounds. <i>Chemistry of Materials</i> , 2013, 25, 2961-2969.	6.7	32
59	Friction and Wear Mechanisms of Tungsten-Modified Carbon Systems: A Comparison of Dry and Lubricated Conditions. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 6123-6135.	8.0	44
60	Screened empirical bond-order potentials for Si-C. <i>Physical Review B</i> , 2013, 87, .	3.2	113
61	Charging properties of gold clusters in different environments. <i>Physical Review B</i> , 2013, 87, .	3.2	7
62	Li ⁺ adsorption at prismatic graphite surfaces enhances interlayer cohesion. <i>Journal of Power Sources</i> , 2013, 239, 321-325.	7.8	10
63	Quaternary Diamond-Like Chalcogenidometalate Networks as Efficient Anode Material in Lithium-Ion Batteries. <i>Advanced Functional Materials</i> , 2013, 23, 5693-5699.	14.9	26
64	1,3-Diketone Fluids and Their Complexes with Iron. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3369-3376.	2.5	17
65	Ultralow Friction Induced by Tribochemical Reactions: A Novel Mechanism of Lubrication on Steel Surfaces. <i>Langmuir</i> , 2013, 29, 5207-5213.	3.5	30
66	Adaptive molecular decomposition: Large-scale quantum chemistry for liquids. <i>Journal of Chemical Physics</i> , 2013, 138, 104108.	3.0	0
67	Oxidation of Magnesia-Supported Pd ₃₀ Nanoclusters and Catalyzed CO Combustion: Size-Selected Experiments and First-Principles Theory. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9594-9607.	3.1	40
68	Oxidation State and Symmetry of Magnesia-Supported Pd ₁₃ O ₃ Nanocatalysts Influence Activation Barriers of CO Oxidation. <i>Journal of the American Chemical Society</i> , 2012, 134, 7690-7699.	13.7	43
69	Decay Kinetics of Cluster-Beam-Deposited Metal Particles. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19327-19334.	3.1	10
70	Bond order potentials for fracture, wear, and plasticity. <i>MRS Bulletin</i> , 2012, 37, 493-503.	3.5	49
71	A 58-electron superatom-complex model for the magic phosphine-protected gold clusters (Schmid-gold, Nanogold®) of 1.4-nm dimension. <i>Chemical Science</i> , 2011, 2, 1583.	7.4	44
72	Reply to â€œComment on 'Dynamic Catalyst Restructuring during Carbon Nanotube Growth'â€•. <i>ACS Nano</i> , 2011, 5, 686-687.	14.6	0

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73	Progressive Shortening of sp-Hybridized Carbon Chains through Oxygen-Induced Cleavage. Journal of Physical Chemistry C, 2011, 115, 24653-24661.	3.1	38
74	Anisotropic mechanical amorphization drives wear in diamond. Nature Materials, 2011, 10, 34-38.	27.5	282
75	Formation and Oxidation of Linear Carbon Chains and Their Role in the Wear of Carbon Materials. Tribology Letters, 2011, 44, 355-365.	2.6	43
76	Ageing of a Microscopic Sliding Gold Contact at Low Temperatures. Physical Review Letters, 2011, 107, 144303.	7.8	34
77	Charge-transfer model for carbonaceous electrodes in polar environments. Physical Review B, 2011, 83, .	3.2	30
78	Molecular dynamics simulation of gold solid film lubrication. International Journal of Materials Research, 2010, 101, 981-988.	0.3	4
79	Atomistic Insights into the Running-in, Lubrication, and Failure of Hydrogenated Diamond-Like Carbon Coatings. Tribology Letters, 2010, 39, 49-61.	2.6	126
80	How to observe the oxidation of magnesia-supported Pd clusters by scanning tunnelling microscopy. Physica Status Solidi (B): Basic Research, 2010, 247, 1016-1022.	1.5	4
81	Penetration of thin C60 films by metal nanoparticles. Nature Nanotechnology, 2010, 5, 335-339.	31.5	34
82	Dynamic Catalyst Restructuring during Carbon Nanotube Growth. ACS Nano, 2010, 4, 7587-7595.	14.6	74
83	Structural evolution of the sodium cluster anions Na_{20}^{19-} . Physical Review B, 2009, 80, .	3.2	19
84	Die filling optimization using three-dimensional discrete element modeling. Powder Technology, 2009, 196, 169-179.	4.2	33
85	Surface amorphization, sputter rate, and intrinsic stresses of silicon during low energy Ga ⁺ focused-ion beam milling. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3072-3075.	1.4	44
86	Effect of Different Particle Size Distributions on Solid-state Sintering: A Microscopic Simulation Approach. Journal of the American Ceramic Society, 2009, 92, 1428-1434.	3.8	68
87	Three-dimensional discrete element models for the granular statics and dynamics of powders in cavity filling. Journal of the Mechanics and Physics of Solids, 2009, 57, 10-31.	4.8	145
88	Ligand-Protected Gold Alloy Clusters: Doping the Superatom. Journal of Physical Chemistry C, 2009, 113, 15834-15837.	3.1	97
89	Understanding the microscopic processes that govern the charge-induced deformation of carbon nanotubes. Physical Review B, 2009, 80, .	3.2	11
90	Continuum concepts in nanoscale capillary impregnation. New Journal of Physics, 2008, 10, 113022.	2.9	20

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91	Dynamic capillary wetting studied with dissipative particle dynamics. <i>New Journal of Physics</i> , 2008, 10, 043009.	2.9	67
92	Describing bond-breaking processes by reactive potentials: Importance of an environment-dependent interaction range. <i>Physical Review B</i> , 2008, 78, .	3.2	149
93	Liquid-Liquid Phase Coexistence in Gold Clusters: 2D or Not 2D?. <i>Physical Review Letters</i> , 2007, 98, 015701.	7.8	62
94	Structure Determination of Medium-Sized Sodium Clusters. <i>Physical Review Letters</i> , 2007, 98, 043401.	7.8	89
95	Size-Dependent Structural Evolution and Chemical Reactivity of Gold Clusters. <i>ChemPhysChem</i> , 2007, 8, 157-161.	2.1	197
96	Predicting experimental signatures for the oxidation of magnesia supported palladium clusters by density functional theory. <i>European Physical Journal D</i> , 2007, 45, 485-489.	1.3	7
97	Structural Relaxation Made Simple. <i>Physical Review Letters</i> , 2006, 97, 170201.	7.8	1,189
98	55-Atom clusters of silver and gold: Symmetry breaking by relativistic effects. <i>Computational Materials Science</i> , 2006, 35, 332-336.	3.0	27
99	Oxidation of small gas phase Pd clusters: A density functional study. <i>Computational Materials Science</i> , 2006, 35, 371-374.	3.0	26
100	Oxidation of magnesia-supported Pd-clusters leads to the ultimate limit of epitaxy with a catalytic function. <i>Nature Materials</i> , 2006, 5, 44-47.	27.5	55
101	Photoelectron spectra of sodium clusters: The problem of interpreting Kohn-Sham eigenvalues. <i>Physical Review B</i> , 2006, 73, .	3.2	33
102	The Ultrasmoothness of Diamond-like Carbon Surfaces. <i>Science</i> , 2005, 309, 1545-1548.	12.6	286
103	Symmetry and Electronic Structure of Noble-Metal Nanoparticles and the Role of Relativity. <i>Physical Review Letters</i> , 2004, 93, 093401.	7.8	241
104	Polymorphisms in the IL 18 gene are associated with specific sensitization to common allergens and allergic rhinitis. <i>Journal of Allergy and Clinical Immunology</i> , 2003, 111, 117-122.	2.9	119
105	Circadian Variation of Exhaled Nitric Oxide and Urinary Eosinophil Protein X in Asthmatic and Healthy Children. <i>Pediatric Research</i> , 2002, 51, 190-194.	2.3	42
106	Bonding in Cu, Ag, and Au Clusters: Relativistic Effects, Trends, and Surprises. <i>Physical Review Letters</i> , 2002, 89, 033401.	7.8	611
107	Surface smoothing by energetic cluster impact. <i>Journal of Applied Physics</i> , 2001, 90, 3226-3231.	2.5	35
108	On the origin of surface smoothing by energetic cluster impact: Molecular dynamics simulation and mesoscopic modeling. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2000, 164-165, 522-536.	1.4	71

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109	Preventive effect of 2 and 10µmg of sodium cromoglycate on exercise-induced bronchoconstriction. European Journal of Pediatrics, 2000, 159, 759-763.	2.7	6
110	Influence of the potential range on the heat capacity of 13-atom Morse clusters. Physical Review B, 1999, 60, 11734-11737.	3.2	31
111	The growth dynamics of energetic cluster impact films. Computational Materials Science, 1998, 10, 452-456.	3.0	11
112	Reduction of the reflected pressure wave in the molecular-dynamics simulation of energetic particle-solid collisions. Physical Review B, 1997, 56, 15439-15445.	3.2	58
113	Simple models for film growth by energetic cluster impact. Radiation Effects and Defects in Solids, 1997, 142, 39-50.	1.2	9
114	Energetic impact of Cu-clusters on Cu-surfaces. Radiation Effects and Defects in Solids, 1997, 142, 27-38.	1.2	12
115	ENERGETIC CLUSTER IMPACT (ECI): A NEW METHOD FOR THIN-FILM FORMATION. Surface Review and Letters, 1996, 03, 887-890.	1.1	61
116	Molecular-dynamics simulation of thin-film growth by energetic cluster impact. Physical Review B, 1995, 51, 11061-11067.	3.2	315
117	Filling of micron-sized contact holes with copper by energetic cluster impact. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1994, 12, 2925-2930.	2.1	364
118	Thin film growth by energetic cluster impact (ECI): comparison between experiment and molecular dynamics simulations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1993, 19, 31-36.	3.5	39
119	Thin films from energetic cluster impact; experiment and molecular dynamics simulations. Nuclear Instruments & Methods in Physics Research B, 1993, 80-81, 1320-1323.	1.4	43
120	Molecular dynamics simulation of thin film formation by energetic cluster impact (ECI). Zeitschrift für Physik D-Atoms Molecules and Clusters, 1993, 26, 229-231.	1.0	51