Michael Moseler

List of Publications by Year
in descending order

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120 papers	7,827 citations	61984 43 h-index	49909 87 g-index
124 all docs	124 docs citations	124 times ranked	7985 citing authors

#	Article	IF	Citations
1	Structural Relaxation Made Simple. Physical Review Letters, 2006, 97, 170201.	7.8	1,189
2	Bonding in Cu, Ag, and Au Clusters: Relativistic Effects, Trends, and Surprises. Physical Review Letters, 2002, 89, 033401.	7.8	611
3	Filling of micronâ€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
4	Molecular-dynamics simulation of thin-film growth by energetic cluster impact. Physical Review B, 1995, 51, 11061-11067.	3.2	315
5	The Ultrasmoothness of Diamond-like Carbon Surfaces. Science, 2005, 309, 1545-1548.	12.6	286
6	Anisotropic mechanical amorphization drives wear in diamond. Nature Materials, 2011, 10, 34-38.	27.5	282
7	Symmetry and Electronic Structure of Noble-Metal Nanoparticles and the Role of Relativity. Physical Review Letters, 2004, 93, 093401.	7.8	241
8	Atomic Scale Mechanisms of Friction Reduction and Wear Protection by Graphene. Nano Letters, 2014, 14, 7145-7152.	9.1	210
9	Size-Dependent Structural Evolution and Chemical Reactivity of Gold Clusters. ChemPhysChem, 2007, 8, 157-161.	2.1	197
10	Describing bond-breaking processes by reactive potentials: Importance of an environment-dependent interaction range. Physical Review B, 2008, 78, .	3.2	149
11	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
12	Atomistic Insights into the Running-in, Lubrication, and Failure of Hydrogenated Diamond-Like Carbon Coatings. Tribology Letters, 2010, 39, 49-61.	2.6	126
13	Polymorphisms in the IL 18 gene are associated with specific sensitization to common allergens and allergic rhinitis. Journal of Allergy and Clinical Immunology, 2003, 111, 117-122.	2.9	119
14	Mechano-chemical decomposition of organic friction modifiers with multiple reactive centres induces superlubricity of ta-C. Nature Communications, 2019, 10, 151.	12.8	118
15	Band Edge Engineering in BiVO₄/TiO₂ Heterostructure: Enhanced Photoelectrochemical Performance through Improved Charge Transfer. ACS Catalysis, 2016, 6, 5311-5318.	11.2	117
16	Hydrogen treated anatase TiO₂: a new experimental approach and further insights from theory. Journal of Materials Chemistry A, 2016, 4, 2670-2681.	10.3	117
17	Screened empirical bond-order potentials for Si-C. Physical Review B, 2013, 87, .	3.2	113
18	A Highly Selective and Selfâ€Powered Gas Sensor Via Organic Surface Functionalization of pâ€Si/nâ€ZnO Diodes. Advanced Materials, 2014, 26, 8017-8022.	21.0	103

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19	Ligand-Protected Gold Alloy Clusters: Doping the Superatom. Journal of Physical Chemistry C, 2009, 113, 15834-15837.	3.1	97
20	Structure Determination of Medium-Sized Sodium Clusters. Physical Review Letters, 2007, 98, 043401.	7.8	89
21	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. Tribology Letters, 2014, 53, 119-126.	2.6	89
22	Dynamic Catalyst Restructuring during Carbon Nanotube Growth. ACS Nano, 2010, 4, 7587-7595.	14.6	74
23	On the origin of surface smoothing by energetic cluster impact: Molecular dynamics simulation and mesoscopic modeling. Nuclear Instruments & Methods in Physics Research B, 2000, 164-165, 522-536.	1.4	71
24	Highly Selective SAMâ€“Nanowire Hybrid NO₂ Sensor: Insight into Charge Transfer Dynamics and Alignment of Frontier Molecular Orbitals. Advanced Functional Materials, 2014, 24, 595-602.	14.9	71
25	Effect of Different Particle Size Distributions on Solidâ€State Sintering: A Microscopic Simulation Approach. Journal of the American Ceramic Society, 2009, 92, 1428-1434.	3.8	68
26	Dynamic capillary wetting studied with dissipative particle dynamics. New Journal of Physics, 2008, 10, 043009.	2.9	67
27	Origins of Folding Instabilities on Polycrystalline Metal Surfaces. Physical Review Applied, 2014, 2, .	3.8	63
28	Friction Regimes of Water-Lubricated Diamond (111): Role of Interfacial Ether Groups and Tribo-Induced Aromatic Surface Reconstructions. Physical Review Letters, 2017, 119, 096101.	7.8	63
29	Liquid-Liquid Phase Coexistence in Gold Clusters: 2D or Not 2D?. Physical Review Letters, 2007, 98, 015701.	7.8	62
30	ENERGETIC CLUSTER IMPACT (ECI): A NEW METHOD FOR THIN-FILM FORMATION. Surface Review and Letters, 1996, 03, 887-890.	1.1	61
31	Activation and mechanochemical breaking of Câ€“C bonds initiate wear of diamond (110) surfaces in contact with silica. Carbon, 2016, 98, 474-483.	10.3	61
32	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
33	Ab initio study of CO2 hydrogenation mechanisms on inverse ZnO/Cu catalysts. Journal of Catalysis, 2018, 360, 168-174.	6.2	58
34	Oxidation of magnesia-supported Pd-clusters leads to the ultimate limit of epitaxy with a catalytic function. Nature Materials, 2006, 5, 44-47.	27.5	55
35	Plasma-chemical reduction of iron oxide photoanodes for efficient solar hydrogen production. International Journal of Hydrogen Energy, 2014, 39, 4828-4835.	7.1	54
36	Molecular dynamics simulation of thin film formation by energetic cluster impact (ECI). Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 229-231.	1.0	51

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37	Bond order potentials for fracture, wear, and plasticity. MRS Bulletin, 2012, 37, 493-503.	3.5	49
38	Fluorine-Terminated Diamond Surfaces as Dense Dipole Lattices: The Electrostatic Origin of Polar Hydrophobicity. Journal of the American Chemical Society, 2016, 138, 4018-4028.	13.7	47
39	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
40	A 58-electron superatom-complex model for the magic phosphine-protected gold clusters (Schmid-gold, NanogoldÂ®) of 1.4-nm dimension. Chemical Science, 2011, 2, 1583.	7.4	44
41	Friction and Wear Mechanisms of Tungstenâ€“Carbon Systems: A Comparison of Dry and Lubricated Conditions. ACS Applied Materials & Interfaces, 2013, 5, 6123-6135.	8.0	44
42	Nanoscale sliding friction phenomena at the interface of diamond-like carbon and tungsten. Acta Materialia, 2014, 67, 395-408.	7.9	44
43	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
44	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
45	Oxidation State and Symmetry of Magnesia-Supported Pd₁₃O_x Nanocatalysts Influence Activation Barriers of CO Oxidation. Journal of the American Chemical Society, 2012, 134, 7690-7699.	13.7	43
46	Interactions of polymers with reduced graphene oxide: van der Waals binding energies of benzene on graphene with defects. Physical Chemistry Chemical Physics, 2014, 16, 33-37.	2.8	43
47	Circadian Variation of Exhaled Nitric Oxide and Urinary Eosinophil Protein X in Asthmatic and Healthy Children. Pediatric Research, 2002, 51, 190-194.	2.3	42
48	Experimental and Numerical Atomistic Investigation of the Third Body Formation Process in Dry Tungsten/Tungsten-Carbide Tribo Couples. Tribology Letters, 2013, 50, 67-80.	2.6	42
49	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
50	Oxidation of Magnesia-Supported Pd₃₀ Nanoclusters and Catalyzed CO Combustion: Size-Selected Experiments and First-Principles Theory. Journal of Physical Chemistry C, 2012, 116, 9594-9607.	3.1	40
51	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
52	Progressive Shortening of sp-Hybridized Carbon Chains through Oxygen-Induced Cleavage. Journal of Physical Chemistry C, 2011, 115, 24653-24661.	3.1	38
53	Coarse Graining and Localized Plasticity between Sliding Nanocrystalline Metals. Physical Review Letters, 2014, 113, 036101.	7.8	37
54	Surface smoothing by energetic cluster impact. Journal of Applied Physics, 2001, 90, 3226-3231.	2.5	35

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55	Ultralow Friction of Steel Surfaces Using a 1,3-Diketone Lubricant in the Thin Film Lubrication Regime. Langmuir, 2015, 31, 11033-11039.	3.5	35
56	Penetration of thin C60 films by metal nanoparticles. Nature Nanotechnology, 2010, 5, 335-339.	31.5	34
57	Ageing of a Microscopic Sliding Gold Contact at Low Temperatures. Physical Review Letters, 2011, 107, 144303.	7.8	34
58	Photoelectron spectra of sodium clusters: The problem of interpreting Kohn-Sham eigenvalues. Physical Review B, 2006, 73, .	3.2	33
59	Die filling optimization using three-dimensional discrete element modeling. Powder Technology, 2009, 196, 169-179.	4.2	33
60	Contrast in nanoscale friction between rotational domains of graphene on Pt(111). Carbon, 2017, 113, 132-138.	10.3	33
61	Lithium Chalcogenidotetrelates: LiChTâ€”Synthesis and Characterization of New Li⁺ Ion Conducting Li/Sn/Se Compounds. Chemistry of Materials, 2013, 25, 2961-2969.	6.7	32
62	Influence of the potential range on the heat capacity of 13-atom Morse clusters. Physical Review B, 1999, 60, 11734-11737.	3.2	31
63	Charge-transfer model for carbonaceous electrodes in polar environments. Physical Review B, 2011, 83, .	3.2	30
64	Ultralow Friction Induced by Tribochemical Reactions: A Novel Mechanism of Lubrication on Steel Surfaces. Langmuir, 2013, 29, 5207-5213.	3.5	30
65	Surface passivation and boundary lubrication of self-mated tetrahedral amorphous carbon asperities under extreme tribological conditions. Friction, 2014, 2, 193-208.	6.4	29
66	Influence of hydrodynamic drag model on shear stress in the simulation of magnetorheological fluids. Journal of Non-Newtonian Fluid Mechanics, 2015, 218, 16-26.	2.4	29
67	Integrated Strategy toward Self-Powering and Selectivity Tuning of Semiconductor Gas Sensors. ACS Sensors, 2016, 1, 1256-1264.	7.8	28
68	55-Atom clusters of silver and gold: Symmetry breaking by relativistic effects. Computational Materials Science, 2006, 35, 332-336.	3.0	27
69	Oxidation of small gas phase Pd clusters: A density functional study. Computational Materials Science, 2006, 35, 371-374.	3.0	26
70	Quaternary Diamondâ€Like Chalcogenidometalate Networks as Efficient Anode Material in Lithiumâ€Ion Batteries. Advanced Functional Materials, 2013, 23, 5693-5699.	14.9	26
71	Shear melting of silicon and diamond and the disappearance of the polyamorphic transition under shear. Physical Review Materials, 2018, 2, .	2.4	26
72	Insights into Interfacial Changes and Photoelectrochemical Stability of In_xGa_{1â€“x}N (0001) Photoanode Surfaces in Liquid Environments. ACS Applied Materials & Interfaces, 2016, 8, 8232-8238.	8.0	23

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73	Surface Softening in Metalâ€“Ceramic Sliding Contacts: An Experimental and Numerical Investigation. ACS Nano, 2015, 9, 1478-1491.	14.6	22
74	Facile and Efficient Atomic Hydrogenation Enabled Black TiO₂ with Enhanced Photoâ€Electrochemical Activity via a Favorably Lowâ€Energyâ€Barrier Pathway. Advanced Energy Materials, 2019, 9, 1900725.	19.5	21
75	Continuum concepts in nanoscale capillary impregnation. New Journal of Physics, 2008, 10, 113022.	2.9	20
76	Solution of boundary-element problems using the fast-inertial-relaxation-engine method. Physical Review B, 2019, 99, .	3.2	20
77	Structural evolution of the sodium cluster anions<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Na</mml:mtext></mml:mrow><mml:mrow><mml:mn>20</mml:mn></mml:mrow> Physical Review B, 2009, 80, .	3.2	19
78	Discrete element study of viscous flow in magnetorheological fluids. Rheologica Acta, 2014, 53, 417-443.	2.4	19
79	Density functional theory and chromium: Insights from the dimers. Journal of Chemical Physics, 2015, 142, 124316.	3.0	18
80	Electronically Coupled Uranium and Iron Oxide Heterojunctions as Efficient Water Oxidation Catalysts. Advanced Functional Materials, 2019, 29, 1905005.	14.9	18
81	1,3-Diketone Fluids and Their Complexes with Iron. Journal of Physical Chemistry A, 2013, 117, 3369-3376.	2.5	17
82	Effects of Gas-Phase Conditions and Particle Size on the Properties of Cu(111)-Supported Zn_yO_x Particles Revealed by Global Optimization and Ab Initio Thermodynamics. Journal of Physical Chemistry C, 2019, 123, 30903-30916.	3.1	17
83	Ab Initio Wavelength-Dependent Raman Spectra: Placzek Approximation and Beyond. Journal of Chemical Theory and Computation, 2020, 16, 576-586.	5.3	17
84	Role of oxygen functional groups in the friction of water-lubricated low-index diamond surfaces. Physical Review Materials, 2018, 2, .	2.4	17
85	Molecular Dynamic Simulation of Collision-Induced Third-Body Formation in Hydrogen-Free Diamond-Like Carbon Asperities. Tribology Letters, 2016, 63, 26.	2.6	16
86	Contact mechanics of graphene-covered metal surfaces. Applied Physics Letters, 2018, 112, .	3.3	16
87	In Situ Synthesis of Graphene Nitride Nanolayers on Glycerol-Lubricated Si₃N₄ for Superlubricity Applications. ACS Applied Nano Materials, 2021, 4, 2721-2732.	5.0	16
88	Nonempirical Free Volume Viscosity Model for Alkane Lubricants under Severe Pressures. Physical Review Letters, 2020, 124, 105501.	7.8	15
89	Steric Effects Control Dry Friction of H- and F-Terminated Carbon Surfaces. ACS Applied Materials & Interfaces, 2020, 12, 8805-8816.	8.0	15
90	Offset-corrected<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">Î”</mml:mi></mml:math>-Kohn-Sham scheme for semiempirical prediction of absolute x-ray photoelectron energies in molecules and solids. Physical Review B, 2016, 94, .	3.2	14

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91	Slipping domains in water-lubricated microsystems for improved load support. Tribology International, 2018, 120, 269-279.	5.9	14
92	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
93	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
94	Energetic impact of Cu-clusters on Cu-surfaces. Radiation Effects and Defects in Solids, 1997, 142, 27-38.	1.2	12
95	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. Physical Chemistry Chemical Physics, 2019, 21, 6651-6661.	2.8	12
96	The growth dynamics of energetic cluster impact films. Computational Materials Science, 1998, 10, 452-456.	3.0	11
97	Understanding the microscopic processes that govern the charge-induced deformation of carbon nanotubes. Physical Review B, 2009, 80, .	3.2	11
98	Decay Kinetics of Cluster-Beam-Deposited Metal Particles. Journal of Physical Chemistry C, 2012, 116, 19327-19334.	3.1	10
99	Li+ adsorption at prismatic graphite surfaces enhances interlayer cohesion. Journal of Power Sources, 2013, 239, 321-325.	7.8	10
100	Simple models for film growth by energetic cluster impact. Radiation Effects and Defects in Solids, 1997, 142, 39-50.	1.2	9
101	Relating Dry Friction to Interdigitation of Surface Passivation Species: A Molecular Dynamics Study on Amorphous Carbon. Materials, 2022, 15, 3247.	2.9	8
102	Predicting experimental signatures for the oxidation of magnesia supported palladium clusters by density functional theory. European Physical Journal D, 2007, 45, 485-489.	1.3	7
103	Charging properties of gold clusters in different environments. Physical Review B, 2013, 87, .	3.2	7
104	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
105	Ab Initio Modeling of the ZnO-Cu(111) Interface. Journal of Physical Chemistry C, 2022, 126, 764-771.	3.1	7
106	Preventive effect of 2 and 10â€‰mg of sodium cromoglycate on exercise-induced bronchoconstriction. European Journal of Pediatrics, 2000, 159, 759-763.	2.7	6
107	Solid-Phase Silicon Homoepitaxy via Shear-Induced Amorphization and Recrystallization. Physical Review Letters, 2021, 127, 126101.	7.8	5
108	Molecular dynamics simulation of gold solid film lubrication. International Journal of Materials Research, 2010, 101, 981-988.	0.3	4

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109	How to observe the oxidation of magnesiaâ€supported Pd clusters by scanning tunnelling microscopy. Physica Status Solidi (B): Basic Research, 2010, 247, 1016-1022.	1.5	4
110	Atomistic Insights Into Lubricated Tungsten/Diamond Sliding Contacts. Frontiers in Mechanical Engineering, 2019, 5, .	1.8	4
111	Constitutive relations for plasticity of amorphous carbon. JPhys Materials, 2020, 3, 035005.	4.2	4
112	Ab initiothermodynamics study of ambient gases reacting with amorphous carbon. Physical Review B, 2019, 99, .	3.2	3
113	On the Influence of Microtopography on the Sliding Performance of Cross Country Skis. Frontiers in Mechanical Engineering, 2021, 7, .	1.8	3
114	Taming the Untamable-The Art and Science of Diamond Polishing. , 2014, , 81-98.		2
115	Carbon nanotubes as fillers for composites with enhanced thermal conductivity. Physical Review Materials, 2021, 5, .	2.4	2
116	Sensors: Highly Selective SAMâ€“Nanowire Hybrid NO₂ Sensor: Insight into Charge Transfer Dynamics and Alignment of Frontier Molecular Orbitals (Adv. Funct. Mater. 5/2014). Advanced Functional Materials, 2014, 24, 566-566.	14.9	1
117	Reply to â€œComment on 'Dynamic Catalyst Restructuring during Carbon Nanotube Growth'â€• ACS Nano, 2011, 5, 686-687.	14.6	0
118	Adaptive molecular decomposition: Large-scale quantum chemistry for liquids. Journal of Chemical Physics, 2013, 138, 104108.	3.0	0
119	European Symposium on Friction, Wear, and Wear Protection. Conference Papers in Science, 2015, 2015, 1-1.	0.3	0
120	Shear Induced Dynamic Grain-Refinement in Sliding Polycrystalline Metal Surfaces. , 2021, , 169-183.		0