Yunfeng Shi

List of Publications by Year
in descending order

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Version: 2024-02-01

98 papers	4,899 citations	117453 34 h-index	95083 68 g-index
101 all docs	101 docs citations	101 times ranked	7258 citing authors

#	Article	IF	Citations
1	Wetting transparency of graphene. Nature Materials, 2012, 11, 217-222.	13.3	971
2	Self-heatingâ€“induced healing of lithium dendrites. Science, 2018, 359, 1513-1516.	6.0	378
3	Strain Localization and Percolation of Stable Structure in Amorphous Solids. Physical Review Letters, 2005, 95, 095502.	2.9	258
4	Harvesting Energy from Water Flow over Graphene. Nano Letters, 2011, 11, 3123-3127.	4.5	206
5	Wetting of Mono and Few-Layered WS₂ and MoS₂ Films Supported on Si/SiO₂ Substrates. ACS Nano, 2015, 9, 3023-3031.	7.3	186
6	Modeling the structural evolution of carbide-derived carbons using quenched molecular dynamics. Carbon, 2010, 48, 1116-1123.	5.4	172
7	Evaluation of the Disorder Temperature and Free-Volume Formalisms via Simulations of Shear Banding in Amorphous Solids. Physical Review Letters, 2007, 98, 185505.	2.9	160
8	Atomic-scale simulations of strain localization in three-dimensional model amorphous solids. Physical Review B, 2006, 73, .	1.1	154
9	Stress-induced structural transformation and shear banding during simulated nanoindentation of a metallic glass. Acta Materialia, 2007, 55, 4317-4324.	3.8	140
10	Evaluation of individual and ensemble probabilistic forecasts of COVID-19 mortality in the United States. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2113561119.	3.3	136
11	Two-Dimensional van der Waals Epitaxy Kinetics in a Three-Dimensional Perovskite Halide. Crystal Growth and Design, 2015, 15, 4741-4749.	1.4	128
12	Protecting Silicon Film Anodes in Lithium-Ion Batteries Using an Atomically Thin Graphene Drape. ACS Nano, 2017, 11, 5051-5061.	7.3	113
13	Carrier lifetime enhancement in halide perovskite via remote epitaxy. Nature Communications, 2019, 10, 4145.	5.8	93
14	High Electrical Conductivity Antimony Selenide Nanocrystals and Assemblies. Nano Letters, 2010, 10, 4417-4422.	4.5	87
15	In situ healing of dendrites in a potassium metal battery. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5588-5594.	3.3	79
16	Structural transformation and localization during simulated nanoindentation of a noncrystalline metal film. Applied Physics Letters, 2005, 86, 011914.	1.5	77
17	Intrinsic ductility of glassy solids. Journal of Applied Physics, 2014, 115, .	1.1	70
18	A mimetic porous carbon model by quench molecular dynamics simulation. Journal of Chemical Physics, 2008, 128, 234707.	1.2	68

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19	Size-independent shear band formation in amorphous nanowires made from simulated casting. Applied Physics Letters, 2010, 96, .	1.5	65
20	A computational analysis of the deformation mechanisms of a nanocrystalâ€“metallic glass composite. Acta Materialia, 2008, 56, 995-1000.	3.8	55
21	Clean Nanotube Unzipping by Abrupt Thermal Expansion of Molecular Nitrogen: Graphene Nanoribbons with Atomically Smooth Edges. ACS Nano, 2012, 6, 2261-2272.	7.3	54
22	The normal-auxeticity mechanical phase transition in graphene. 2D Materials, 2017, 4, 021020.	2.0	49
23	Utilizing van der Waals Slippery Interfaces to Enhance the Electrochemical Stability of Silicon Film Anodes in Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2018, 10, 13442-13451.	4.0	48
24	Graphene Drape Minimizes the Pinning and Hysteresis of Water Drops on Nanotextured Rough Surfaces. ACS Nano, 2013, 7, 3512-3521.	7.3	46
25	A Tersoffâ€based interatomic potential for wurtzite AlN. Physica Status Solidi (A) Applications and Materials Science, 2011, 208, 1569-1572.	0.8	45
26	Facet-insensitive graphene growth on copper. Physical Review B, 2012, 85, .	1.1	45
27	Tensile fracture of metallic glasses via shear band cavitation. Acta Materialia, 2015, 82, 483-490.	3.8	39
28	Crack initiation in metallic glasses under nanoindentation. Acta Materialia, 2016, 115, 413-422.	3.8	39
29	Adhesion suppresses atomic wear in single-asperity sliding. Wear, 2016, 352-353, 31-41.	1.5	39
30	Highly Selective, Defect-Induced Photocatalytic CO₂ Reduction to Acetaldehyde by the Nb-Doped TiO₂ Nanotube Array under Simulated Solar Illumination. ACS Applied Materials & Interfaces, 2020, 12, 55982-55993.	4.0	39
31	Magic auxeticity angle of graphene. Carbon, 2019, 149, 350-354.	5.4	38
32	Low-cycle fatigue of metallic glass nanowires. Acta Materialia, 2015, 87, 225-232.	3.8	36
33	Size-dependent mechanical responses of metallic glasses. International Materials Reviews, 2019, 64, 163-180.	9.4	36
34	Jetting and Detonation Initiation in Shock Induced Collapse of Nanometer-Scale Voids. Journal of Physical Chemistry C, 2008, 112, 6263-6270.	1.5	34
35	Size- and Shape-Dependent Energetics of Nanocrystal Interfaces: Experiment and Simulation. Physical Review Letters, 2003, 90, 226104.	2.9	31
36	Suppression of shear banding in amorphous ZrCuAl nanopillars by irradiation. Journal of Applied Physics, 2013, 113, 083514.	1.1	30

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37	On measuring the fracture energy of model metallic glasses. Journal of Applied Physics, 2018, 124, .	1.1	30
38	Compression-compression fatigue study on model metallic glass nanowires by molecular dynamics simulations. Journal of Applied Physics, 2011, 110, .	1.1	26
39	Molecular simulation of tip wear in a single asperity sliding contact. Wear, 2013, 307, 150-154.	1.5	26
40	Silica Glass Toughened by Consolidation of Glassy Nanoparticles. Nano Letters, 2019, 19, 5222-5228.	4.5	26
41	Surface diffusion driven nanoshell formation by controlled sintering of mesoporous nanoparticle aggregates. Nanoscale, 2010, 2, 1423.	2.8	25
42	Structural transformation and embrittlement during lithiation and delithiation cycles in an amorphous silicon electrode. Acta Materialia, 2019, 175, 11-20.	3.8	22
43	Simulated thermal decomposition and detonation of nitrogen cubane by molecular dynamics. Journal of Chemical Physics, 2007, 127, 134503.	1.2	21
44	Molecular Simulation of the Influence of Interface Faceting on the Shock Sensitivity of a Model Plastic Bonded Explosive. Journal of Physical Chemistry B, 2008, 112, 14898-14904.	1.2	21
45	Nanocrystalline gold with small size: inverse Hallâ€“Petch between mixed regime and super-soft regime. Philosophical Magazine, 2020, 100, 2335-2351.	0.7	21
46	Simulations of nanoindentation in a thin amorphous metal film. Thin Solid Films, 2007, 515, 3179-3182.	0.8	20
47	Precursor to the Onset of the Bulk Oxidation of Cu(100). Physical Review Letters, 2012, 108, 176101.	2.9	20
48	Evaluating Mohrâ€“Coulomb yield criterion for plastic flow in model metallic glasses. Journal of Non-Crystalline Solids, 2012, 358, 3488-3494.	1.5	20
49	Detonation Initiation from Spontaneous Hotspots Formed During Cook-Off Observed in Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 2416-2422.	1.5	17
50	Impact of PEGDA photopolymerization in micro-stereolithography on 3D printed hydrogel structure and swelling. Soft Matter, 2021, 17, 7188-7195.	1.2	17
51	Single asperity friction in the wear regime. Friction, 2018, 6, 316-322.	3.4	16
52	Machine learning-based microstructure prediction during laser sintering of alumina. Scientific Reports, 2021, 11, 10724.	1.6	16
53	Computational study of nanometer-scale self-propulsion enabled by asymmetric chemical catalysis. Journal of Chemical Physics, 2009, 131, 014705.	1.2	14
54	Nanocasting of hierarchical nanostructured porous carbon in molecular dynamics simulation. Journal of Materials Chemistry A, 2013, 1, 3886.	5.2	14

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55	Comparison of chain-growth polymerization in solution versus on surface using reactive coarse-grained simulations. Polymer, 2017, 129, 105-116.	1.8	14
56	Commonalities in frequency-dependent viscoelastic damping in glasses in the MHz to THz regime. Journal of Applied Physics, 2017, 122, .	1.1	12
57	Heating-Rate and Particle-Size Effects on Melting Process of Au Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 7414-7420.	1.5	12
58	Mitigation of chemical wear by graphene platelets during diamond cutting of steel. Carbon, 2016, 108, 61-71.	5.4	11
59	A reactive coarse-grained model for polydisperse polymers. Polymer, 2016, 98, 88-99.	1.8	11
60	A model metallic glass exhibits size-independent tensile ductility. Acta Materialia, 2016, 103, 587-594.	3.8	11
61	The embrittlement and toughening of metallic glasses from nano-crystallization. Journal of Applied Physics, 2019, 125, .	1.1	11
62	Characterizing the Autonomous Motions of Linear Catalytic Nanomotors Using Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 19588-19597.	1.5	10
63	Molecular packing of fullerenes inside single-walled carbon nanotubes. Carbon, 2012, 50, 5450-5457.	5.4	10
64	Design ductile and work-hardenable composites with all brittle constituents. Acta Materialia, 2021, 208, 116770.	3.8	10
65	Engineering Faceted Nanoporosity by Reactions in Thin-Film Oxide Multilayers in Crystallographically Layered Calcium Cobaltate for Thermoelectrics. ACS Applied Nano Materials, 2021, 4, 9904-9911.	2.4	9
66	Topological defects in nanoporous carbon. Carbon, 2013, 60, 202-214.	5.4	8
67	Dynamic self-assembly of â€˜livingâ€™ polymeric chains. Chemical Physics Letters, 2017, 668, 14-18.	1.2	8
68	Solvent Effect on the Diffusion of Unentangled Linear Polymer Melts. Langmuir, 2017, 33, 11845-11850.	1.6	8
69	Frequency-dependent mechanical damping in alloys. Physical Review B, 2017, 95, .	1.1	8
70	Nanopores in nanocrystalline gold. Materialia, 2019, 5, 100195.	1.3	8
71	First principles and molecular dynamics study of Li wetting and diffusion on W surfaces. Journal of Nuclear Materials, 2020, 539, 152345.	1.3	8
72	Understanding the response of aluminosilicate and aluminoborate glasses to sharp contact loading using molecular dynamics simulation. Journal of Applied Physics, 2020, 128, .	1.1	8

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73	Towards damage resistant Al2O3â€“SiO2 glasses with structural and chemical heterogeneities through consolidation of glassy nanoparticles. Acta Materialia, 2021, 215, 117016.	3.8	8
74	Dominant shear bands observed in amorphous ZrCuAl nanowires under simulated compression. MRS Communications, 2012, 2, 13-16.	0.8	7
75	The local stress state of a running shear band in amorphous solids. Journal of Materials Research, 2015, 30, 1979-1987.	1.2	6
76	Interior Melting of Rapidly Heated Gold Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 8170-8177.	2.1	6
77	Hotspot Formation in Shock-Induced Void Collapse. Solid State Phenomena, 2008, 139, 77-82.	0.3	5
78	Elastic Properties of Mimetically Synthesized Model Nanoporous Carbon. Materials Research Society Symposia Proceedings, 2009, 1224, 1.	0.1	5
79	Dynamic self assembly of confined active nanoparticles. Chemical Physics Letters, 2013, 557, 76-79.	1.2	5
80	Shear-induced volumetric strain in CuZr metallic glass. International Journal of Engineering Science, 2014, 83, 99-106.	2.7	5
81	Creating Atomic Models of Brittle Glasses for In Silico Mechanical Tests. International Journal of Applied Glass Science, 2016, 7, 464-473.	1.0	5
82	Deformation and ductile fracture of nanocrystalline gold ultrathin nanoribbon: Width effect. Fatigue and Fracture of Engineering Materials and Structures, 2021, 44, 1850-1861.	1.7	5
83	Molecular dynamics study on the viscosity of glassâ€forming systems near and below the glass transition temperature. Journal of the American Ceramic Society, 2021, 104, 6227-6241.	1.9	5
84	Strain rate-dependent tensile response of glassy silicon nanowires studied by accelerated atomistic simulations. Journal of Applied Physics, 2021, 130, .	1.1	5
85	Melting of Nanocrystalline Gold. Journal of Physical Chemistry C, 2019, 123, 907-914.	1.5	4
86	Effect of voids on nanocrystalline gold ultrathin film. Computational Materials Science, 2021, 189, 110255.	1.4	4
87	Measuring the surface diffusivity of argon in nanoporous carbon. Physical Chemistry Chemical Physics, 2017, 19, 5855-5860.	1.3	3
88	The Effect of Strain Rate on the Deformation Processes of NC Gold with Small Grain Size. Crystals, 2020, 10, 858.	1.0	3
89	Tensile ductility and necking in consolidated amorphous alumina. Journal of the American Ceramic Society, 2022, 105, 958-965.	1.9	3
90	Strain Localization in a Molecular-Dynamics Model of a Metallic Glass. Materials Research Society Symposia Proceedings, 2002, 754, 1.	0.1	2

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91	Computational design of chemically propelled catalytic nanorotors. Journal of Chemical Physics, 2013, 139, 064707.	1.2	2
92	An in-silico walker. Chemical Physics Letters, 2016, 659, 6-9.	1.2	2
93	The nature of atomic wear from molecular simulations. Tribology International, 2022, 167, 107418.	3.0	2
94	Atomic-scale simulations of strain localization in a single-component three-dimensional model amorphous solid. Materials Research Society Symposia Proceedings, 2005, 903, 1.	0.1	1
95	The Effects of Annealing on Fatigue Behavior in Zr-based Bulk Metallic Glasses. Materials Research Society Symposia Proceedings, 2011, 1300, 1.	0.1	1
96	A minimalist's reactive potential for efficient molecular modelling of chemistry. Molecular Simulation, 2015, 41, 3-12.	0.9	1
97	Large-Area Uniaxial-Oriented Growth of Free-Standing Thin Films at the Liquidâ€“Air Interface with Millimeter-Sized Grains. ACS Nano, 2022, 16, 11802-11814.	7.3	1
98	Molecular Modeling on Artificial Molecular Motors. , 2016, , 2269-2274.		0