

# Hao Zhang

## List of Publications by Year in descending order

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121  
papers

3,398  
citations

147726

31  
h-index

189801

50  
g-index

122  
all docs

122  
docs citations

122  
times ranked

2752  
citing authors

#	ARTICLE	IF	CITATIONS
1	Grain boundaries exhibit the dynamics of glass-forming liquids. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 7735-7740.	3.3	164
2	Stabilization mechanism and chemical demulsification of water-in-oil and oil-in-water emulsions in petroleum industry: A review. Fuel, 2021, 286, 119390.	3.4	143
3	Computer simulation of the elastically driven migration of a flat grain boundary. Acta Materialia, 2004, 52, 2569-2576.	3.8	115
4	Curvature driven grain boundary migration in aluminum: molecular dynamics simulations. Acta Materialia, 2005, 53, 79-86.	3.8	106
5	Role of string-like collective atomic motion on diffusion and structural relaxation in glass forming Cu-Zr alloys. Journal of Chemical Physics, 2015, 142, 164506.	1.2	97
6	Single-atomic Pt sites anchored on defective TiO <sub>2</sub> nanosheets as a superior photocatalyst for hydrogen evolution. Journal of Energy Chemistry, 2021, 62, 1-10.	7.1	70
7	String-like cooperative motion in homogeneous melting. Journal of Chemical Physics, 2013, 138, 12A538.	1.2	69
8	Interaction Mechanisms between Air Bubble and Molybdenite Surface: Impact of Solution Salinity and Polymer Adsorption. Langmuir, 2017, 33, 2353-2361.	1.6	67
9	Wetting at the nanoscale: A molecular dynamics study. Journal of Chemical Physics, 2017, 146, 114704.	1.2	64
10	Grain boundary energy and grain growth in Al films: Comparison of experiments and simulations. Scripta Materialia, 2006, 54, 1059-1063.	2.6	63
11	Localization model description of diffusion and structural relaxation in glass-forming Cu-Zr alloys. Journal of Statistical Mechanics: Theory and Experiment, 2016, 2016, 054048.	0.9	62
12	Characterization of atomic motion governing grain boundary migration. Physical Review B, 2006, 74, .	1.1	59
13	Stretchable, compressible, and conductive hydrogel for sensitive wearable soft sensors. Journal of Colloid and Interface Science, 2022, 618, 111-120.	5.0	59
14	Temperature-dependent structure evolution in liquid gallium. Acta Materialia, 2017, 128, 304-312.	3.8	57
15	Mapping the Nanoscale Heterogeneity of Surface Hydrophobicity on the Sphalerite Mineral. Journal of Physical Chemistry C, 2017, 121, 5620-5628.	1.5	55
16	Effects of boundary inclination and boundary type on shear-driven grain boundary migration. Philosophical Magazine, 2008, 88, 243-256.	0.7	52
17	The size-dependent non-localized deformation in a metallic alloy. Scripta Materialia, 2015, 101, 48-51.	2.6	50
18	String-like collective atomic motion in the interfacial dynamics of nanoparticles. Soft Matter, 2010, 6, 5944.	1.2	49

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19	Corrosion fatigue crack growth behavior of pipeline steel under underload-type variable amplitude loading schemes. <i>Acta Materialia</i> , 2015, 96, 159-169.	3.8	49
20	Probing Surface Interactions of Electrochemically Active Galena Mineral Surface Using Atomic Force Microscopy. <i>Journal of Physical Chemistry C</i> , 2016, 120, 22433-22442.	1.5	48
21	On the critical thickness for non-localized to localized plastic flow transition in metallic glasses: A molecular dynamics study. <i>Scripta Materialia</i> , 2016, 114, 93-97.	2.6	48
22	Self-Assembled Mesoporous Carbon Nitride with Tunable Texture for Enhanced Visible-Light Photocatalytic Hydrogen Evolution. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 8291-8299.	3.2	48
23	Surface interaction mechanisms in mineral flotation: Fundamentals, measurements, and perspectives. <i>Advances in Colloid and Interface Science</i> , 2021, 295, 102491.	7.0	47
24	Simulation and analysis of the migration mechanism of $\sim 5^\circ$ tilt grain boundaries in an fcc metal. <i>Acta Materialia</i> , 2006, 54, 623-633.	3.8	46
25	Selective flotation separation of molybdenite and talc by humic substances. <i>Minerals Engineering</i> , 2018, 117, 34-41.	1.8	46
26	Atomic motion during the migration of general $[001]$ tilt grain boundaries in Ni. <i>Acta Materialia</i> , 2007, 55, 4527-4533.	3.8	40
27	Effect of Annealing Treatment on Mechanical Properties of Nanocrystalline $\alpha$ -iron: an Atomistic Study. <i>Scientific Reports</i> , 2015, 5, 8459.	1.6	37
28	Mobility of $75^\circ$ tilt grain boundaries: Inclination dependence. <i>Scripta Materialia</i> , 2005, 52, 1193-1198.	2.6	36
29	Role of molecular architecture in the modulation of hydrophobic interactions. <i>Current Opinion in Colloid and Interface Science</i> , 2020, 47, 58-69.	3.4	36
30	Non-localized deformation in Cu-Zr multi-layer amorphous films under tension. <i>Journal of Alloys and Compounds</i> , 2016, 678, 410-420.	2.8	35
31	Atomistic simulation of hydrogen-assisted ductile-to-brittle transition in $\alpha$ -iron. <i>Computational Materials Science</i> , 2017, 127, 211-221.	1.4	34
32	Interfacial Free Energy Controlling Glass-Forming Ability of Cu-Zr Alloys. <i>Scientific Reports</i> , 2014, 4, 5167.	1.6	33
33	Deformation behavior of metallic glasses with shear band like atomic structure: a molecular dynamics study. <i>Scientific Reports</i> , 2016, 6, 30935.	1.6	33
34	Atomistic study of hydrogen embrittlement during cyclic loading: Quantitative model of hydrogen accumulation effects. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 4571-4578.	3.8	33
35	Effects of grain boundary and boundary inclination on hydrogen diffusion in $\alpha$ -iron. <i>Journal of Materials Research</i> , 2011, 26, 2735-2743.	1.2	32
36	A size-dependent structural evolution of ZnS nanoparticles. <i>Scientific Reports</i> , 2015, 5, 14267.	1.6	32

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37	Fast dynamics in a model metallic glass-forming material. <i>Journal of Chemical Physics</i> , 2021, 154, 084505.	1.2	32
38	Coacervate-Based Instant and Repeatable Underwater Adhesive with Anticancer and Antibacterial Properties. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 48239-48251.	4.0	32
39	Glassy interfacial dynamics of Ni nanoparticles: part I Colored noise, dynamic heterogeneity and collective atomic motion. <i>Soft Matter</i> , 2013, 9, 1254-1265.	1.2	31
40	Plastic deformation of nanocrystalline aluminum at high temperatures and strain rate. <i>Acta Materialia</i> , 2010, 58, 2176-2185.	3.8	30
41	String-Like Collective Atomic Motion in the Melting and Freezing of Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14068-14076.	1.2	30
42	Universal nature of dynamic heterogeneity in glass-forming liquids: A comparative study of metallic and polymeric glass-forming liquids. <i>Journal of Chemical Physics</i> , 2019, 151, 184503.	1.2	30
43	Coacervation-driven instant paintable underwater adhesives with tunable optical and electrochromic properties. <i>Journal of Materials Chemistry A</i> , 2021, 9, 12988-13000.	5.2	30
44	Properties and determination of the interface stiffness. <i>Acta Materialia</i> , 2007, 55, 467-471.	3.8	29
45	Anisotropic Polymer Adsorption on Molybdenite Basal and Edge Surfaces and Interaction Mechanism With Air Bubbles. <i>Frontiers in Chemistry</i> , 2018, 6, 361.	1.8	29
46	High pH stress corrosion cracking initiation and crack evolution in buried steel pipelines: A review. <i>Engineering Failure Analysis</i> , 2021, 120, 105013.	1.8	29
47	Grain boundary self-diffusion in Ni: Effect of boundary inclination. <i>Journal of Materials Research</i> , 2005, 20, 1146-1153.	1.2	28
48	Superionic $\text{UO}_2$ : A model anharmonic crystalline material. <i>Journal of Chemical Physics</i> , 2019, 150, 174506.	1.2	28
49	Glassy interfacial dynamics of Ni nanoparticles: Part II Discrete breathers as an explanation of two-level energy fluctuations. <i>Soft Matter</i> , 2013, 9, 1266-1280.	1.2	25
50	Influence of string-like cooperative atomic motion on surface diffusion in the (110) interfacial region of crystalline Ni. <i>Journal of Chemical Physics</i> , 2015, 142, 084704.	1.2	25
51	Size distribution of shear transformation zones and their evolution towards the formation of shear bands in metallic glasses. <i>Journal of Non-Crystalline Solids</i> , 2016, 445-446, 61-68.	1.5	24
52	Recent advances in bubble-based technologies: Underlying interaction mechanisms and applications. <i>Applied Physics Reviews</i> , 2021, 8, .	5.5	24
53	Dynamic heterogeneity, cooperative motion, and Johariâ€“Goldstein $\beta$ -relaxation in a metallic glass-forming material exhibiting a fragile-to-strong transition. <i>European Physical Journal E</i> , 2021, 44, 56.	0.7	24
54	Hydrogen-Bonding-Driven Multifunctional Polymer Hydrogel Networks Based on Tannic Acid. <i>ACS Applied Polymer Materials</i> , 2022, 4, 1836-1845.	2.0	24

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55	String-like collective motion and diffusion in the interfacial region of ice. <i>Journal of Chemical Physics</i> , 2017, 147, 194508.	1.2	23
56	Nanomechanical Insights into Versatile Polydopamine Wet Adhesive Interacting with Liquid-Infused and Solid Slippery Surfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 6941-6950.	4.0	23
57	Size-dependent deformation mechanisms in hollow silicon nanoparticles. <i>AIP Advances</i> , 2015, 5, 077162.	0.6	22
58	Atomic picture of elastic deformation in a metallic glass. <i>Scientific Reports</i> , 2015, 5, 9184.	1.6	22
59	Probing the Reversible Fe <sup>3+</sup> –DOPA-Mediated Bridging Interaction in Mussel Foot Protein-1. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21670-21677.	1.5	22
60	Hydrogen hardening effect in heavily deformed single crystal $\alpha$ -Fe. <i>Computational Materials Science</i> , 2011, 50, 3397-3402.	1.4	21
61	Prediction of crack propagation under cyclic loading based on hydrogen diffusion. <i>Materials Letters</i> , 2015, 152, 86-89.	1.3	21
62	Probing interactions between sphalerite and hydrophobic/hydrophilic surfaces: Effect of water chemistry. <i>Powder Technology</i> , 2017, 320, 511-518.	2.1	21
63	Defect generation in nano-twinned, nano-grained and single crystal Cu systems caused by wear: A molecular dynamics study. <i>Scripta Materialia</i> , 2010, 63, 1116-1119.	2.6	20
64	Effects of misorientation and inclination on mechanical response of $\alpha$ -Fe tilt grain boundaries in $\alpha$ -Fe to external stresses. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2014, 22, 065016.	0.8	20
65	Local piezoelectric response of ZnO nanoparticles embedded in a photosensitive polymer. <i>Physica Status Solidi - Rapid Research Letters</i> , 2012, 6, 77-79.	1.2	19
66	Origin and Nature of Spontaneous Shape Fluctuations in $\alpha$ -Fe Nanoparticles. <i>ACS Nano</i> , 2014, 8, 7465-7477.	7.3	19
67	Mechanistic Understanding and Nanomechanics of Multiple Hydrogen-Bonding Interactions in Aqueous Environment. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4540-4548.	1.5	19
68	Structural evolution and atomic dynamics in Ni–Nb metallic glasses: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2017, 147, 144503.	1.2	18
69	Effects of Thickness and Adsorption of Airborne Hydrocarbons on Wetting Properties of MoS <sub>2</sub> : An Atomistic Simulation Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6737-6747.	1.5	18
70	Localization model description of diffusion and structural relaxation in superionic crystalline UO <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2019, 151, 071101.	1.2	18
71	Flame normalizing-induced robust and oriented metallic layer for stable Zn anode. <i>Chemical Engineering Journal</i> , 2022, 437, 135246.	6.6	18
72	Hydrogen diffusion and vacancy clusterization in iron. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 15378-15385.	3.8	17

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73	Localization model description of the interfacial dynamics of crystalline Cu and Cu <sub>64</sub> Zr <sub>36</sub> metallic glass films. <i>Journal of Chemical Physics</i> , 2020, 153, 124508.	1.2	16
74	A size effect in grain boundary migration: A molecular dynamics study of bicrystal thin films. <i>Acta Materialia</i> , 2005, 53, 5273-5279.	3.8	15
75	Molecular dynamics study on structure evolution of monocarboxylic acid intercalated layered double hydroxides. <i>RSC Advances</i> , 2016, 6, 98804-98811.	1.7	15
76	Hydrogen inhibited phase transition near crack tip – An atomistic mechanism of hydrogen embrittlement. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 17146-17153.	3.8	15
77	A Novel Method to Improve Crystallinity of Supported Nanoparticles Using Low Melting Point Metals. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14591-14597.	1.5	13
78	A Sensitive Ammonia Sensor Using Long Period Fiber Grating Coated With Graphene Oxide/Cellulose Acetate. <i>IEEE Sensors Journal</i> , 2021, 21, 16691-16700.	2.4	13
79	The initiation of shear band formation in deformed metallic glasses from soft localized domains. <i>Journal of Chemical Physics</i> , 2021, 155, 204504.	1.2	13
80	A closer look at the local responses of twin and grain boundaries in Cu to stress at the nanoscale with possible transition from the P-H to the inverse P-H relation. <i>Acta Materialia</i> , 2010, 58, 2677-2684.	3.8	12
81	On the atomistic mechanisms of grain boundary migration in [001] twist boundaries: Molecular dynamics simulations. <i>Computational Materials Science</i> , 2010, 48, 773-782.	1.4	12
82	Molecular dynamics simulation of Bauschinger's effect in deformed copper single crystal in different strain ranges. <i>Journal of Applied Physics</i> , 2011, 110, 124911.	1.1	12
83	Influence of Nanotwin Boundary on the Bauschinger's Effect in Cu: A Molecular Dynamics Simulation Study. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2013, 44, 4207-4217.	1.1	12
84	Comparative Study of the Collective Dynamics of Proteins and Inorganic Nanoparticles. <i>Scientific Reports</i> , 2017, 7, 41671.	1.6	12
85	Quantification of Temperature Dependence of Hydrogen Embrittlement in Pipeline Steel. <i>Materials</i> , 2019, 12, 585.	1.3	12
86	Effects of Loading Spectra on High pH Crack Growth Behavior of X65 Pipeline Steel. <i>Corrosion</i> , 2020, 76, 601-615.	0.5	12
87	Size effect on atomic structure in low-dimensional Cu-Zr amorphous systems. <i>Scientific Reports</i> , 2017, 7, 7291.	1.6	11
88	Study of Thermal Stability of Hydrotalcite and Carbon Dioxide Adsorption Behavior on Hydrotalcite-Derived Mixed Oxides Using Atomistic Simulations. <i>ACS Omega</i> , 2018, 3, 12041-12051.	1.6	11
89	Atomistic simulation of sliding of [1010] tilt grain boundaries in Mg. <i>Journal of Materials Research</i> , 2009, 24, 3446-3453.	1.2	10
90	Effects of Location of Twin Boundaries and Grain Size on Plastic Deformation of Nanocrystalline Copper. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2012, 43, 3547-3555.	1.1	10

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91	Effects of nano-scale grain boundaries in Cu on its Bauschinger's effect and response to cyclic deformation. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2013, 583, 140-150.	2.6	10
92	Structural Evolutions of ZnS Nanoparticles in Hydrated and Bare States. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7870-7884.	1.5	10
93	Bulk and surface properties of gypsum: A comparison between classical force fields and dispersion-corrected DFT calculations. <i>Computational Materials Science</i> , 2019, 164, 8-16.	1.4	10
94	Effects of load interactions on the onset of stage two of high pH stress corrosion cracking. <i>Journal of Pipeline Science and Engineering</i> , 2021, 1, 122-136.	2.4	10
95	Determination of grain boundary stiffness from molecular dynamics simulation. <i>Applied Physics Letters</i> , 2006, 88, 121927.	1.5	9
96	Anisotropic Deformation in the Compressions of Single Crystalline Copper Nanoparticles. <i>Crystals</i> , 2018, 8, 116.	1.0	9
97	A comparison of different empirical potentials in ZnS. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2014, 22, 085014.	0.8	8
98	Atomistic deformation mechanisms in twinned copper nanospheres. <i>Nanoscale Research Letters</i> , 2014, 9, 335.	3.1	8
99	Atomistic simulation of Cu-Ni precipitates hardening in $\alpha$ -iron. <i>Journal Physics D: Applied Physics</i> , 2015, 48, 115302.	1.3	8
100	Probing the Interactions between Pickering Emulsion Droplets Stabilized with pH-Responsive Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7320-7331.	1.2	8
101	Unraveling the Interaction of Water-in-Oil Emulsion Droplets via Molecular Simulations and Surface Force Measurements. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7556-7567.	1.2	8
102	Molecular dynamics simulation of cluster beam Al deposition on Si (100) substrate. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2000, 160, 372-376.	0.6	7
103	Size-dependent concentrations of thermal vacancies in solid films. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22661-22667.	1.3	7
104	Structure and CO <sub>2</sub> physisorption capacity of hydrotalcite-derived oxide. <i>Journal of CO<sub>2</sub> Utilization</i> , 2020, 36, 64-75.	3.3	7
105	Molecular Dynamics Studies of Hydrogen Effect on Intergranular Fracture in $\alpha$ -Iron. <i>Materials</i> , 2020, 13, 4949.	1.3	7
106	Crack Growth Sensitivity to the Magnitude and Frequency of Load Fluctuation in Stage 1b of High-pH Stress Corrosion Cracking. <i>Corrosion</i> , 2021, 77, 618-631.	0.5	7
107	Comparative investigation of a newly optimized modified embedded atom method potential with other potentials for silicon. <i>Computational Materials Science</i> , 2015, 109, 277-286.	1.4	6
108	Molecular Dynamics Study of the Role of Water in the Carbon Dioxide Intercalation in Chloride Ions Bearing Hydrotalcite. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9507-9514.	1.5	6

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109	Localization model description of the interfacial dynamics of crystalline Cu and $\text{Cu}_{64}\text{Zr}_{36}$ metallic glass nanoparticles. European Physical Journal E, 2021, 44, 33.	0.7	6
110	Development of a second-nearest-neighbor modified embedded atom method potential for silicon-phosphorus binary system. Computational Materials Science, 2016, 120, 1-12.	1.4	5
111	Deposition of an energetic Al cluster on Si(111) substrate: a molecular dynamics simulation. Modelling and Simulation in Materials Science and Engineering, 1998, 6, 709-716.	0.8	4
112	Topological correlations of grain faces in polycrystal with experimental verification. Europhysics Letters, 2013, 104, 56006.	0.7	4
113	Ultrasound driven aggregation—A novel method to assemble ceramic nanoparticles. Extreme Mechanics Letters, 2016, 7, 71-77.	2.0	4
114	High pH Crack Growth Sensitivity to Underload-Type of Pressure Fluctuations. , 2018, , .		4
115	Probing Hydrophobic Interactions between Polymer Surfaces and Air Bubbles or Oil Droplets: Effects of Molecular Weight and Surfactants. Langmuir, 2022, 38, 5257-5268.	1.6	4
116	Design of high $T_g$ Zr-based metallic glasses using atomistic simulation and experiment. Philosophical Magazine, 2011, 91, 3393-3405.	0.7	3
117	Microbubble-Enhanced Cell Membrane Permeability in High Gravity Field. Cellular and Molecular Bioengineering, 2013, 6, 266-278.	1.0	3
118	Interactions of model airborne particulate matter with dipalmitoyl phosphatidylcholine and a clinical surfactant Calsurf. Journal of Colloid and Interface Science, 2022, 607, 1993-2009.	5.0	3
119	Vacancy enhanced formation and phase transition of Cu-rich precipitates in $\text{Fe}$ -iron under neutron irradiation. AIP Advances, 2016, 6, 045004.	0.6	2
120	Surface compressive and softening effect on deformation mode transition in Ni-Nb metallic glassy thin films: A molecular dynamics study. Journal of Applied Physics, 2018, 124, 205304.	1.1	1
121	Warm hydrogen direct adsorptive separation and purification with highly CO/H <sub>2</sub> S-tolerant rare earth alloys. Applications in Energy and Combustion Science, 2020, 1-4, 100004.	0.9	1