Bu Wang

List of Publications by Year in descending order

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201385 276539 1,813 61 27 41 citations h-index g-index papers 61 61 61 1813 citing authors all docs docs citations times ranked

#	Article	IF	CITATIONS
1	A new transferable interatomic potential for molecular dynamics simulations of borosilicate glasses. Journal of Non-Crystalline Solids, 2018, 498, 294-304.	1.5	121
2	Cooling rate effects in sodium silicate glasses: Bridging the gap between molecular dynamics simulations and experiments. Journal of Chemical Physics, 2017, 147, 074501.	1.2	107
3	Revisiting silica with ReaxFF: Towards improved predictions of glass structure and properties via reactive molecular dynamics. Journal of Non-Crystalline Solids, 2016, 443, 148-154.	1.5	97
4	Fracture toughness anomalies: Viewpoint of topological constraint theory. Acta Materialia, 2016, 121, 234-239.	3.8	84
5	The durability of cementitious composites containing microencapsulated phase change materials. Cement and Concrete Composites, 2017, 81, 66-76.	4.6	83
6	Intrinsic Nano-Ductility of Glasses: The Critical Role of Composition. Frontiers in Materials, 2015, 2, .	1.2	55
7	Clinkering-free cementation by fly ash carbonation. Journal of CO2 Utilization, 2018, 23, 117-127.	3.3	55
8	Stretched Exponential Relaxation of Glasses at Low Temperature. Physical Review Letters, 2015, 115, 165901.	2.9	53
9	Topological Control on the Structural Relaxation of Atomic Networks under Stress. Physical Review Letters, 2017, 119, 035502.	2.9	51
10	Computer simulations of large-scale defect clustering and nanodomain structure in gadolinia-doped ceria. Acta Materialia, 2011, 59, 2035-2045.	3.8	49
11	Nanoductility in silicate glasses is driven by topological heterogeneity. Physical Review B, 2016, 93, .	1.1	47
12	Direct Experimental Evidence for Differing Reactivity Alterations of Minerals following Irradiation: The Case of Calcite and Quartz. Scientific Reports, 2016, 6, 20155.	1.6	46
13	Reactive Molecular Dynamics Simulations of Sodium Silicate Glasses — Toward an Improved Understanding of the Structure. International Journal of Applied Glass Science, 2017, 8, 276-284.	1.0	44
14	Confined Water in Layered Silicates: The Origin of Anomalous Thermal Expansion Behavior in Calcium-Silicate-Hydrates. ACS Applied Materials & Samp; Interfaces, 2016, 8, 35621-35627.	4.0	43
15	Irradiation-induced topological transition in SiO2: Structural signature of networks' rigidity. Journal of Non-Crystalline Solids, 2017, 463, 25-30.	1.5	43
16	Revealing the Effect of Irradiation on Cement Hydrates: Evidence of a Topological Self-Organization. ACS Applied Materials & Samp; Interfaces, 2017, 9, 32377-32385.	4.0	40
17	Modeling and characterization of two-phase composites by Voronoi diagram in the Laguerre geometry based on random close packing of spheres. Computational Materials Science, 2010, 47, 951-961.	1.4	39
18	Chemical Strain and Point Defect Configurations in Reduced Ceria. Chemistry of Materials, 2014, 26, 3687-3692.	3.2	38

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19	Nature of radiation-induced defects in quartz. Journal of Chemical Physics, 2015, 143, 024505.	1.2	38
20	A printability index for linking slurry rheology to the geometrical attributes of 3D-printed components. Cement and Concrete Composites, 2019, 101, 32-43.	4.6	38
21	lon exchange strengthening and thermal expansion of glasses: Common origin and critical role of network connectivity. Journal of Non-Crystalline Solids, 2017, 455, 70-74.	1.5	36
22	Direct observation of pitting corrosion evolutions on carbon steel surfaces at the nano-to-microscales. Scientific Reports, 2018, 8, 7990.	1.6	36
23	Irradiation- vs. vitrification-induced disordering: The case of <i>?</i> -quartz and glassy silica. Journal of Chemical Physics, 2017, 146, 204502.	1.2	35
24	Effect of Surface Nanotopography on Immunoaffinity Cell Capture in Microfluidic Devices. Langmuir, 2011, 27, 11229-11237.	1.6	33
25	Electronic Origin of Doping-Induced Enhancements of Reactivity: Case Study of Tricalcium Silicate. Journal of Physical Chemistry C, 2015, 119, 25991-25999.	1.5	32
26	Luminescence of delafossite-type CuAlO ₂ fibers with Eu substitution for Al cations. Science and Technology of Advanced Materials, 2016, 17, 200-209.	2.8	31
27	Misfit Stresses Caused by Atomic Size Mismatch: The Origin of Doping-Induced Destabilization of Dicalcium Silicate. Crystal Growth and Design, 2016, 16, 3124-3132.	1.4	31
28	Recycled concrete aggregate in base course applications: Review of field and laboratory investigations of leachate pH. Journal of Hazardous Materials, 2020, 385, 121562.	6.5	28
29	Enthalpy Landscape Dictates the Irradiation-Induced Disordering of Quartz. Physical Review X, 2017, 7, .	2.8	27
30	Irradiation-driven amorphous-to-glassy transition in quartz: The crucial role of the medium-range order in crystallization. Physical Review Materials, 2017, 1 , .	0.9	27
31	Atomic picture of structural relaxation in silicate glasses. Applied Physics Letters, 2019, 114, .	1.5	26
32	Selective sulfur removal from semi-dry flue gas desulfurization coal fly ash for concrete and carbon dioxide capture applications. Waste Management, 2021, 121, 117-126.	3.7	23
33	Maintenance and Neuronal Cell Differentiation of Neural Stem Cells C17.2 Correlated to Medium Availability Sets Design Criteria in Microfluidic Systems. PLoS ONE, 2014, 9, e109815.	1.1	21
34	Crucial effect of angular flexibility on the fracture toughness and nano-ductility of aluminosilicate glasses. Journal of Non-Crystalline Solids, 2016, 454, 46-51.	1.5	20
35	Anisotropic Molecular Organization at a Liquid/Vapor Interface Promotes Crystal Nucleation with Polymorph Selection. Journal of the American Chemical Society, 2022, 144, 11638-11645.	6.6	18
36	The effect of irradiation on the atomic structure and chemical durability of calcite and dolomite. Npj Materials Degradation, $2019, 3, .$	2.6	17

#	Article	IF	Citations
37	Rate controls on silicate dissolution in cementitious environments. RILEM Technical Letters, 0, 2, 67-73.	0.0	16
38	Direct Air Capture and Sequestration of CO ₂ by Accelerated Indirect Aqueous Mineral Carbonation under Ambient Conditions. ACS Sustainable Chemistry and Engineering, 2022, 10, 7852-7861.	3.2	16
39	Investigating the microstructure of high-calcium fly ash-based alkali-activated material for aqueous Zn sorption. Environmental Research, 2021, 198, 110484.	3.7	15
40	Strain Modulation of Defect Structure in Gadolinia-Doped Ceria. Journal of Physical Chemistry C, 2013, 117, 146-151.	1.5	13
41	Surface Diffusion Is Controlled by Bulk Fragility across All Glass Types. Physical Review Letters, 2022, 128, 075501.	2.9	13
42	Theoretical analysis and experiment on Eu reduction in alumina optical materials. Optical Materials Express, 2016, 6, 2404.	1.6	12
43	The local structure of Fe in Li(Al, Fe)Si2O6 glasses from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2016, 444, 16-22.	1.5	11
44	New insights into the atomic structure of amorphous TiO2 using tight-binding molecular dynamics. Journal of Chemical Physics, 2018, 149, 094501.	1.2	11
45	Atomistic simulation of B-type–fluorite structural relationship and B-type large defect clusters in gadolinia-doped ceria. Solid State Ionics, 2011, 182, 8-12.	1.3	10
46	Fracture Toughness of Silicate Glasses: Insights from Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2015, 1757, 47.	0.1	9
47	Formation and stability of gismondineâ€type zeolite in cementitious systems. Journal of the American Ceramic Society, 2021, 104, 1513-1525.	1.9	9
48	Molecular dynamics simulations of Mg-doped beta″-alumina with potential models fitted for accurate structural response to thermal vibrations. Solid State Ionics, 2014, 263, 9-14.	1.3	8
49	Enhancement of binding kinetics on affinity substrates by laser point heating induced transport. Analyst, The, 2016, 141, 1807-1813.	1.7	8
50	Calcination-free production of calcium hydroxide at sub-boiling temperatures. RSC Advances, 2021, 11, 1762-1772.	1.7	8
51	Simulations of ceria nanoparticles. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2015, 471, 20150218.	1.0	7
52	Structural signatures for thermodynamic stability in vitreous silica: Insight from machine learning and molecular dynamics simulations. Physical Review Materials, 2021, 5, .	0.9	7
53	Understanding the Fragile-to-Strong Transition in Silica from Microscopic Dynamics. Physical Review Letters, 2022, 129, .	2.9	7
54	Implementation of Ion Exchange Processes for Carbon Dioxide Mineralization Using Industrial Waste Streams. Frontiers in Energy Research, 2020, 8, .	1.2	6

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55	Understanding Oxygen Nonstoichiometry in Mayenite: From Electride to Oxygen Radical Clathrate. Journal of Physical Chemistry C, 2019, 123, 11982-11992.	1.5	5
56	Comparison of Biotite Elastic Properties Recovered by Spherical Nanoindentations and Atomistic Simulations — Influence of Nanoâ€Scale Defects in Phyllosilicates. Journal of Geophysical Research: Solid Earth, 2021, 126, e2021JB021902.	1.4	3
57	Process Simulations Reveal the Carbon Dioxide Removal Potential of a Process That Mineralizes Industrial Waste Streams via an Ion Exchange-Based Regenerable pH Swing. ACS Sustainable Chemistry and Engineering, 2022, 10, 6255-6264.	3.2	3
58	Formation and Transport Mechanisms of Hydrogenous Species in Mayenite. Journal of Physical Chemistry C, 2020, 124, 11150-11157.	1.5	2
59	Preparation of Pb(Zr,Ti)O3–Pb(Mg1/3Nb2/3)O3 piezoelectric ceramics by dry–dry method. Journal of Materials Science, 2007, 42, 221-227.	1.7	1
60	Rapid Elemental Extraction from Ordered and Disordered Solutes by Acoustically-Stimulated Dissolution. ACS Engineering Au, 0, , .	2.3	1
61	Particle Breakage and Fines Generation of Recycled Concrete Aggregates Subjected to Compaction. , 2020, , .		O