

Qi An

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

130
papers

2,825
citations

30
h-index

47
g-index

146
ext. papers

3,526
ext. citations

7
avg, IF

5.72
L-index

#	Paper	IF	Citations
130	Nanotwinning induced decreased lattice thermal conductivity of high temperature thermoelectric boron subphosphide (B12P2) from deep learning potential simulations. <i>Energy and AI</i> , 2022 , 8, 100135	12.6	0
129	A Strong Two-Dimensional Semiconductor l-B4C with High Carrier Mobility. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 6036-6046	3.8	0
128	The L-G phase transition in binary Cu-Zr metallic liquids.. <i>Physical Chemistry Chemical Physics</i> , 2021 , 24, 497-506	3.6	0
127	Mitigating amorphization in superhard boron carbide by microalloying-induced stacking fault formation. <i>Physical Review Materials</i> , 2021 , 5,	3.2	1
126	Discovering Catalytic Reaction Networks Using Deep Reinforcement Learning from First-Principles. <i>Journal of the American Chemical Society</i> , 2021 , 143, 16804-16812	16.4	4
125	Controlling the Shapes of Nanoparticles by Dopant-Induced Enhancement of Chemisorption and Catalytic Activity: Application to Fe-Based Ammonia Synthesis. <i>ACS Nano</i> , 2021 , 15, 1675-1684	16.7	3
124	The first order L-G phase transition in liquid Ag and Ag-Cu alloys is driven by deviatoric strain. <i>Scripta Materialia</i> , 2021 , 194, 113695	5.6	4
123	Fracture toughness of thermoelectric materials. <i>Materials Science and Engineering Reports</i> , 2021 , 144, 100607	30.9	7
122	Mitigating the formation of amorphous shear band in boron carbide. <i>Journal of Applied Physics</i> , 2021 , 129, 140902	2.5	2
121	Aliovalent Doping Engineering for A- and B-Sites with Multiple Regulatory Mechanisms: A Strategy to Improve Energy Storage Properties of SrBiTiO-Based Lead-Free Relaxor Ferroelectric Ceramics. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 24833-24855	9.5	16
120	Shear induced deformation twinning evolution in thermoelectric InSb. <i>Npj Computational Materials</i> , 2021 , 7,	10.9	4
119	Coordination and Thermophysical Properties of Transition Metal Chlorocomplexes in LiCl-KCl Eutectic. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 8876-8887	3.4	3
118	Vacancy-driven shear localization in silicon nitride. <i>Scripta Materialia</i> , 2021 , 190, 163-167	5.6	0
117	Drastic Modification of Lattice Thermal Conductivity in Thermoelectrics Induced by Electron-Hole Pairs. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 3911-3918	9.5	0
116	Spatiotemporal Temperature and Pressure in Thermoplasmonic Gold Nanosphere-Water Systems. <i>ACS Nano</i> , 2021 , 15, 6276-6288	16.7	3
115	Electro-mechanical coupling in FCC metal rhodium from first-principles simulations. <i>Journal of Materials Research</i> , 2021 , 36, 2662-2673	2.5	
114	Dislocation-mediated shear amorphization in boron carbide. <i>Science Advances</i> , 2021 , 7,	14.3	14

113	Microstructure evolution and mechanical property of Cu-15Ni-8Sn-0.2Nb alloy during aging treatment. <i>Journal of Materials Science and Technology</i> , 2021 , 86, 227-236	9.1	5
112	Vibrational Spectroscopy Signatures of Catalytically Relevant Configurations for N ₂ Reduction to NH ₃ on Fe Surfaces via Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 27919-27930	3.8	0
111	Formation of two glass phases in binary Cu-Ag liquid. <i>Acta Materialia</i> , 2020 , 195, 274-281	8.4	15
110	Thermal decomposition and diffusion of methane in clathrate hydrates from quantum mechanics simulations.. <i>RSC Advances</i> , 2020 , 10, 14753-14760	3.7	3
109	Enhanced strength and ductility of superhard boron carbide through injecting electrons. <i>Journal of the European Ceramic Society</i> , 2020 , 40, 4428-4435	6	3
108	Modified Failure Mechanism of Silicon through Excess Electrons and Holes. <i>Jom</i> , 2020 , 72, 3160-3169	2.1	
107	Structural failure of layered thermoelectric In ₄ Se ₃ -based semiconductors is dominated by shear slippage. <i>Acta Materialia</i> , 2020 , 187, 84-90	8.4	1
106	Characterizing local metallic bonding variation induced by external perturbation. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 2372-2378	3.6	3
105	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8223-8232	16.4	14
104	Intrinsic mechanical behavior of MgAgSb thermoelectric material: An ab initio study. <i>Journal of Materiomics</i> , 2020 , 6, 24-32	6.7	1
103	Strengthening boron carbide through lithium dopant. <i>Journal of the American Ceramic Society</i> , 2020 , 103, 2012-2023	3.8	5
102	First-Order Phase Transition in Liquid Ag to the Heterogeneous G-Phase. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 632-645	6.4	15
101	Modified Generalized Stacking Fault Energy Surface of III-V Ionic Crystals from Excess Electrons and Holes. <i>ACS Applied Electronic Materials</i> , 2020 , 2, 56-65	4	1
100	Bi-Doped Zirconium Alloys with Enhanced Water Oxidation Resistance. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 23116-23125	3.8	0
99	Structural origin of reversible martensitic transformation and reversible twinning in NiTi shape memory alloy. <i>Acta Materialia</i> , 2020 , 199, 240-252	8.4	10
98	Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe(211) Surface. <i>Chemistry of Materials</i> , 2020 , 32, 9914-9924	9.6	3
97	Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 9787-9794	3.8	4
96	Li, An, and Morozov Reply. <i>Physical Review Letters</i> , 2019 , 123, 119602	7.4	1

95	Photomechanical effect leading to extraordinary ductility in covalent semiconductors. <i>Physical Review B</i> , 2019 , 100,	3.3	6
94	Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from Quantum-Mechanics-Based Hierarchical High-Throughput Catalyst Screening. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 17375-17383	3.8	9
93	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 11444-11454	3.6	17
92	Band-Gap Engineering in High-Temperature Boron-Rich Icosahedral Compounds. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 12505-12513	3.8	5
91	Dramatically reduced lattice thermal conductivity of Mg ₂ Si thermoelectric material from nanotwinning. <i>Acta Materialia</i> , 2019 , 169, 9-14	8.4	17
90	Initial Decomposition of HMX Energetic Material from Quantum Molecular Dynamics and the Molecular Structure Transition of HMX to HMX. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 9231-9236	3.8	21
89	Light irradiation induced brittle-to-ductile and ductile-to-brittle transition in inorganic semiconductors. <i>Physical Review B</i> , 2019 , 99,	3.3	12
88	First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 18193-18201	11.5	6
87	Transgranular amorphous shear band formation in polycrystalline boron carbide. <i>International Journal of Plasticity</i> , 2019 , 121, 218-226	7.6	6
86	First principles high-throughput screening to enhance the ductility of lightweight magnesium alloys. <i>Physical Review Materials</i> , 2019 , 3,	3.2	1
85	First principles predicting enhanced ductility of boride carbide through magnesium microalloying. <i>Journal of the American Ceramic Society</i> , 2019 , 102, 5514-5523	3.8	5
84	Enhanced ductility of III-V covalent semiconductors from electrons and holes. <i>Journal of Applied Physics</i> , 2019 , 126, 195105	2.5	4
83	Atomic structure and mechanical response of coincident stacking faults in boron suboxide. <i>Materials Research Letters</i> , 2019 , 7, 75-81	7.4	5
82	Enhanced fracture toughness of boron carbide from microalloying and nanotwinning. <i>Scripta Materialia</i> , 2019 , 162, 306-310	5.6	9
81	Thermal Stability and Detonation Properties of Potassium 4,4-Bis(dinitromethyl)-3,3-azofurazanate, an Environmentally Friendly Energetic Three-Dimensional Metal-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 1512-1519	9.5	14
80	Mechanical properties in thermoelectric oxides: Ideal strength, deformation mechanism, and fracture toughness. <i>Acta Materialia</i> , 2018 , 149, 341-349	8.4	16
79	Asymmetric twins in boron rich boron carbide. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 13340-13347	7.6	3
78	Nanotwinning and amorphization of boron suboxide. <i>Acta Materialia</i> , 2018 , 147, 195-202	8.4	15

77	Shear-Induced Brittle Failure along Grain Boundaries in Boron Carbide. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 5072-5080	9.5	16
76	Structure and Properties of Boron-Very-Rich Boron Carbides: B ₁₂ Icosahedra Linked through Bent CBB Chains. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 2448-2453	3.8	12
75	Shear-induced brittle failure of titanium carbide from quantum mechanics simulations. <i>Journal of the American Ceramic Society</i> , 2018 , 101, 4184-4192	3.8	7
74	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6288-6297	16.4	78
73	Ultrathin WO ₃ /H ₂ O Nanotubes for CO Photoreduction to Acetate with High Selectivity. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6474-6482	16.4	148
72	Icosahedra clustering and short range order in Ni-Nb-Zr amorphous membranes. <i>Scientific Reports</i> , 2018 , 8, 6084	4.9	9
71	Locating Si atoms in Si-doped boron carbide: A route to understand amorphization mitigation mechanism. <i>Acta Materialia</i> , 2018 , 157, 106-113	8.4	27
70	Ductile deformation mechanism in semiconductor α -Ag ₂ S. <i>Npj Computational Materials</i> , 2018 , 4,	10.9	28
69	Dual Functions of Water in Stabilizing Metal-Pentazolate Hydrates [M(N ₅) ₂ (H ₂ O) ₄] _n H ₂ O (M = Mn, Fe, Co, and Zn) High-Energy-Density Materials. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 21192-21201	3.8	11
68	Mechanical softening of thermoelectric semiconductor Mg ₂ Si from nanotwinning. <i>Scripta Materialia</i> , 2018 , 157, 90-94	5.6	10
67	Icosahedral superstrength at the nanoscale. <i>Physical Review Materials</i> , 2018 , 2,	3.2	8
66	Reactive molecular dynamics simulation of thermal decomposition for nano-aluminized explosives. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 29341-29350	3.6	29
65	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. <i>Journal of the American Chemical Society</i> , 2018 , 140, 17702-17710	16.4	21
64	Grain Boundary Sliding and Amorphization are Responsible for the Reverse Hall-Petch Relation in Superhard Nanocrystalline Boron Carbide. <i>Physical Review Letters</i> , 2018 , 121, 145504	7.4	41
63	Influence of Silicon on the Detonation Performance of Energetic Materials from First-Principles Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 24481-24487	3.8	6
62	Determining ideal strength and failure mechanism of thermoelectric CuInTe ₂ through quantum mechanics. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 11743-11750	13	7
61	Ordering and dimensional crossovers in metallic glasses and liquids. <i>Physical Review B</i> , 2017 , 95,	3.3	7
60	An et al. Reply. <i>Physical Review Letters</i> , 2017 , 118, 089602	7.4	10

59	Prediction of superstrong Boron carbide phase from quantum mechanics. <i>Physical Review B</i> , 2017 , 95,	3.3	11
58	Improved Ductility of B12 Icosahedra-based Superhard Materials through Icosahedral Slip. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 11831-11838	3.8	8
57	Nanotwins soften boron-rich boron carbide (B13C2). <i>Applied Physics Letters</i> , 2017 , 110, 111902	3.4	21
56	Adsorption and decomposition of HMX and CL-20 on Al(111) surface by DFT investigation. <i>Surface and Interface Analysis</i> , 2017 , 49, 441-449	1.5	5
55	Deformation mechanisms in high-efficiency thermoelectric layered Zintl compounds. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 9050-9059	13	27
54	Brittle failure of Boron: Amorphization under high pressure. <i>Physical Review B</i> , 2017 , 95,	3.3	5
53	Mechanism and kinetics of the electrocatalytic reaction responsible for the high cost of hydrogen fuel cells. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 2666-2673	3.6	38
52	Determining the Quality Factor of Dielectric Ceramic Mixtures with Dielectric Constants in the Microwave Frequency Range. <i>Scientific Reports</i> , 2017 , 7, 14120	4.9	5
51	Superstrengthening Bi ₂ Te ₃ through Nanotwinning. <i>Physical Review Letters</i> , 2017 , 119, 085501	7.4	39
50	Ductility in Crystalline Boron Subphosphide (B12P2) for Large Strain Indentation. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 16644-16649	3.8	11
49	Enhanced Strength Through Nanotwinning in the Thermoelectric Semiconductor InSb. <i>Physical Review Letters</i> , 2017 , 119, 215503	7.4	31
48	Shear-induced mechanical failure of Ga ₂ O ₃ from quantum mechanics simulations. <i>Physical Review B</i> , 2017 , 96,	3.3	4
47	Efficient photocatalytic reduction of dinitrogen to ammonia on bismuth monoxide quantum dots. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 201-209	13	127
46	New Ground-State Crystal Structure of Elemental Boron. <i>Physical Review Letters</i> , 2016 , 117, 085501	7.4	38
45	Breaking the icosahedra in boron carbide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 12012-12016	11.5	22
44	Superstrength through Nanotwinning. <i>Nano Letters</i> , 2016 , 16, 7573-7579	11.5	44
43	Nucleation of amorphous shear bands at nanotwins in boron suboxide. <i>Nature Communications</i> , 2016 , 7, 11001	17.4	30
42	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. <i>Nano Letters</i> , 2016 , 16, 4236-42	11.5	35

41	The quantum mechanics derived atomistic mechanism underlying the acceleration of catalytic CO oxidation on Pt(110) by surface acoustic waves. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 12036-12045	13	6
40	How the toughness in metallic glasses depends on topological and chemical heterogeneity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 7053-8	11.5	38
39	Prediction of the crystal packing of di-tetrazine-tetroxide (DTTO) energetic material. <i>Journal of Computational Chemistry</i> , 2016 , 37, 163-7	3.5	15
38	Atomistic explanation of brittle failure of thermoelectric skutterudite CoSb ₃ . <i>Acta Materialia</i> , 2016 , 103, 775-780	8.4	25
37	Prediction of the Chapman-Jouguet chemical equilibrium state in a detonation wave from first principles based reactive molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 2015-22	3.6	23
36	Enhanced ideal strength of thermoelectric half-Heusler TiNiSn by sub-structure engineering. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 14625-14636	13	39
35	The co-crystal of TNT/CL-20 leads to decreased sensitivity toward thermal decomposition from first principles based reactive molecular dynamics. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 5409-5419	13	66
34	Reaction mechanism from quantum molecular dynamics for the initial thermal decomposition of 2,4,6-triamino-1,3,5-triazine-1,3,5-trioxide (MTO) and 2,4,6-trinitro-1,3,5-triazine-1,3,5-trioxide (MTO3N), promising green energetic materials. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 12044-12050	13	14
33	Boron Suboxide and Boron Subphosphide Crystals: Hard Ceramics That Shear without Brittle Failure. <i>Chemistry of Materials</i> , 2015 , 27, 2855-2860	9.6	33
32	Improved Ductility of Boron Carbide by Microalloying with Boron Suboxide. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24649-24656	3.8	23
31	Brittle Failure Mechanism in Thermoelectric Skutterudite CoSb ₃ . <i>Chemistry of Materials</i> , 2015 , 27, 6329-6336	9.3	46
30	Fractal atomic-level percolation in metallic glasses. <i>Science</i> , 2015 , 349, 1306-10	33.3	93
29	Initial decomposition reaction of di-tetrazine-tetroxide (DTTO) from quantum molecular dynamics: implications for a promising energetic material. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 1972-1978	13	31
28	Atomic-Level Understanding of "Asymmetric Twins" in Boron Carbide. <i>Physical Review Letters</i> , 2015 , 115, 175501	7.4	39
27	Atomistic Origin of Brittle Failure of Boron Carbide from Large-Scale Reactive Dynamics Simulations: Suggestions toward Improved Ductility. <i>Physical Review Letters</i> , 2015 , 115, 105501	7.4	76
26	Initial Decomposition Reactions of Bicyclo-HMX [BCHMX or cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole] from Quantum Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2015 , 150123143703008	3.8	13
25	ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 4039-43	6.4	25
24	Grain boundary orientation effects on deformation of Ta bicrystal nanopillars under high strain-rate compression. <i>Journal of Applied Physics</i> , 2014 , 115, 053528	2.5	18

23	Initial Steps of Thermal Decomposition of Dihydroxylammonium 5,5?-bistetrazole-1,1?-diolate Crystals from Quantum Mechanics. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 27175-27181	3.8	74
22	Inhibition of Hotspot Formation in Polymer Bonded Explosives Using an Interface Matching Low Density Polymer Coating at the PolymerExplosive Interface. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 19918-19928	3.8	18
21	Deformation Induced SolidSolid Phase Transitions in Gamma Boron. <i>Chemistry of Materials</i> , 2014 , 26, 4289-4298	9.6	8
20	Atomistic explanation of shear-induced amorphous band formation in boron carbide. <i>Physical Review Letters</i> , 2014 , 113, 095501	7.4	108
19	Bi2WO6 quantum dot-intercalated ultrathin montmorillonite nanostructure and its enhanced photocatalytic performance. <i>Nano Research</i> , 2014 , 7, 1497-1506	10	40
18	CCl Radicals As a Carbon Source for Diamond Thin Film Deposition. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 481-4	6.4	3
17	Stability of NNO and NPO Nanotube Crystals. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 485-9	6.4	5
16	Compressive Shear Reactive Molecular Dynamics Studies Indicating That Cocrystals of TNT/CL-20 Decrease Sensitivity. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 30202-30208	3.8	51
15	Microalloying Boron Carbide with Silicon to Achieve Dramatically Improved Ductility. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 4169-74	6.4	36
14	Shock response of a model structured nanofoam of Cu. <i>Journal of Applied Physics</i> , 2013 , 113, 063516	2.5	27
13	Shock-induced plasticity in tantalum single crystals: Interatomic potentials and large-scale molecular-dynamics simulations. <i>Physical Review B</i> , 2013 , 88,	3.3	173
12	Highly Shocked Polymer Bonded Explosives at a Nonplanar Interface: Hot-Spot Formation Leading to Detonation. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 26551-26561	3.8	71
11	Deformation and spallation of shocked Cu bicrystals with B coherent and symmetric incoherent twin boundaries. <i>Physical Review B</i> , 2012 , 85,	3.3	34
10	Predicted Optimum Composition for the Glass-Forming Ability of Bulk Amorphous Alloys: Application to Cu-Zr-Al. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3143-8	6.4	29
9	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 10198-10206	3.8	64
8	Left-right loading dependence of shock response of (111)/(112) Cu bicrystals: Deformation and spallation. <i>Journal of Applied Physics</i> , 2012 , 111, 053525	2.5	13
7	Shock compression and spallation of single crystal tantalum 2012 ,		5
6	Shock-induced consolidation and spallation of Cu nanopowders. <i>Journal of Applied Physics</i> , 2012 , 111, 013508	2.5	19

5	Synthesis of single-component metallic glasses by thermal spray of nanodroplets on amorphous substrates. <i>Applied Physics Letters</i> , 2012 , 100, 041909	3.4	17
4	Elucidation of the dynamics for hot-spot initiation at nonuniform interfaces of highly shocked materials. <i>Physical Review B</i> , 2011 , 84,	3.3	78
3	Solid-liquid transitions of sodium chloride at high pressures. <i>Journal of Chemical Physics</i> , 2006 , 125, 15454	3.0	16
2	Vacancy-induced densification of silica glass. <i>Journal of Non-Crystalline Solids</i> , 2006 , 352, 3320-3325	3.9	11
1	Addressing amorphization and transgranular fracture of B4C through Si doping and TiB2 microparticle reinforcing. <i>Journal of the American Ceramic Society</i> ,	3.8	0