Qi An

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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	Shock-induced plasticity in tantalum single crystals: Interatomic potentials and large-scale molecular-dynamics simulations. *Physical Review B*, **2013**, 88,	3.3	173
129	Ultrathin WO□0.33HO Nanotubes for CO Photoreduction to Acetate with High Selectivity. *Journal of the American Chemical Society*, **2018**, 140, 6474-6482	16.4	148
128	Efficient photocatalytic reduction of dinitrogen to ammonia on bismuth monoxide quantum dots. *Journal of Materials Chemistry A*, **2017**, 5, 201-209	13	127
127	Atomistic explanation of shear-induced amorphous band formation in boron carbide. *Physical Review Letters*, **2014**, 113, 095501	7.4	108
126	Fractal atomic-level percolation in metallic glasses. *Science*, **2015**, 349, 1306-10	33.3	93
125	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. *Journal of the American Chemical Society*, **2018**, 140, 6288-6297	16.4	78
124	Elucidation of the dynamics for hot-spot initiation at nonuniform interfaces of highly shocked materials. *Physical Review B*, **2011**, 84,	3.3	78
123	Atomistic Origin of Brittle Failure of Boron Carbide from Large-Scale Reactive Dynamics Simulations: Suggestions toward Improved Ductility. *Physical Review Letters*, **2015**, 115, 105501	7.4	76
122	Initial Steps of Thermal Decomposition of Dihydroxylammonium 5,5?-bistetrazole-1,1?-diolate Crystals from Quantum Mechanics. *Journal of Physical Chemistry C*, **2014**, 118, 27175-27181	3.8	74
121	Highly Shocked Polymer Bonded Explosives at a Nonplanar Interface: Hot-Spot Formation Leading to Detonation. *Journal of Physical Chemistry C*, **2013**, 117, 26551-26561	3.8	71
120	The co-crystal of TNT/CL-20 leads to decreased sensitivity toward thermal decomposition from first principles based reactive molecular dynamics. *Journal of Materials Chemistry A*, **2015**, 3, 5409-5419	13	66
119	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. *Journal of Physical Chemistry C*, **2012**, 116, 10198-10206	3.8	64
118	Compressive Shear Reactive Molecular Dynamics Studies Indicating That Cocrystals of TNT/CL-20 Decrease Sensitivity. *Journal of Physical Chemistry C*, **2014**, 118, 30202-30208	3.8	51
117	Brittle Failure Mechanism in Thermoelectric Skutterudite CoSb3. *Chemistry of Materials*, **2015**, 27, 6329-6336	9.6	46
116	Superstrength through Nanotwinning. *Nano Letters*, **2016**, 16, 7573-7579	11.5	44
115	Grain Boundary Sliding and Amorphization are Responsible for the Reverse Hall-Petch Relation in Superhard Nanocrystalline Boron Carbide. *Physical Review Letters*, **2018**, 121, 145504	7.4	41
114	Bi2WO6 quantum dot-intercalated ultrathin montmorillonite nanostructure and its enhanced photocatalytic performance. *Nano Research*, **2014**, 7, 1497-1506	10	40

113	Superstrengthening Bi_{2}Te_{3} through Nanotwinning. *Physical Review Letters*, **2017**, 119, 085501	7.4	39
112	Atomic-Level Understanding of "Asymmetric Twins" in Boron Carbide. *Physical Review Letters*, **2015**, 115, 175501	7.4	39
111	Enhanced ideal strength of thermoelectric half-Heusler TiNiSn by sub-structure engineering. *Journal of Materials Chemistry A*, **2016**, 4, 14625-14636	13	39
110	Mechanism and kinetics of the electrocatalytic reaction responsible for the high cost of hydrogen fuel cells. *Physical Chemistry Chemical Physics*, **2017**, 19, 2666-2673	3.6	38
109	New Ground-State Crystal Structure of Elemental Boron. *Physical Review Letters*, **2016**, 117, 085501	7.4	38
108	How the toughness in metallic glasses depends on topological and chemical heterogeneity. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 7053-8	11.5	38
107	Microalloying Boron Carbide with Silicon to Achieve Dramatically Improved Ductility. *Journal of Physical Chemistry Letters*, **2014**, 5, 4169-74	6.4	36
106	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. *Nano Letters*, **2016**, 16, 4236-42	11.5	35
105	Deformation and spallation of shocked Cu bicrystals with coherent and symmetric incoherent twin boundaries. *Physical Review B*, **2012**, 85,	3.3	34
104	Boron Suboxide and Boron Subphosphide Crystals: Hard Ceramics That Shear without Brittle Failure. *Chemistry of Materials*, **2015**, 27, 2855-2860	9.6	33
103	Initial decomposition reaction of di-tetrazine-tetroxide (DTTO) from quantum molecular dynamics: implications for a promising energetic material. *Journal of Materials Chemistry A*, **2015**, 3, 1972-1978	13	31
102	Enhanced Strength Through Nanotwinning in the Thermoelectric Semiconductor InSb. *Physical Review Letters*, **2017**, 119, 215503	7.4	31
101	Nucleation of amorphous shear bands at nanotwins in boron suboxide. *Nature Communications*, **2016**, 7, 11001	17.4	30
100	Predicted Optimum Composition for the Glass-Forming Ability of Bulk Amorphous Alloys: Application to Cu-Zr-Al. *Journal of Physical Chemistry Letters*, **2012**, 3, 3143-8	6.4	29
99	Reactive molecular dynamics simulation of thermal decomposition for nano-aluminized explosives. *Physical Chemistry Chemical Physics*, **2018**, 20, 29341-29350	3.6	29
98	Ductile deformation mechanism in semiconductor Ag2S. *Npj Computational Materials*, **2018**, 4,	10.9	28
97	Deformation mechanisms in high-efficiency thermoelectric layered Zintl compounds. *Journal of Materials Chemistry A*, **2017**, 5, 9050-9059	13	27
96	Locating Si atoms in Si-doped boron carbide: A route to understand amorphization mitigation mechanism. *Acta Materialia*, **2018**, 157, 106-113	8.4	27

95	Shock response of a model structured nanofoam of Cu. *Journal of Applied Physics*, **2013**, 113, 063516	2.5	27
94	Atomistic explanation of brittle failure of thermoelectric skutterudite CoSb3. *Acta Materialia*, **2016**, 103, 775-780	8.4	25
93	ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell. *Journal of Physical Chemistry Letters*, **2014**, 5, 4039-43	6.4	25
92	Improved Ductility of Boron Carbide by Microalloying with Boron Suboxide. *Journal of Physical Chemistry C*, **2015**, 119, 24649-24656	3.8	23
91	Prediction of the Chapman-Jouguet chemical equilibrium state in a detonation wave from first principles based reactive molecular dynamics. *Physical Chemistry Chemical Physics*, **2016**, 18, 2015-22	3.6	23
90	Breaking the icosahedra in boron carbide. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12012-12016	11.5	22
89	Nanotwins soften boron-rich boron carbide (B13C2). *Applied Physics Letters*, **2017**, 110, 111902	3.4	21
88	Initial Decomposition of HMX Energetic Material from Quantum Molecular Dynamics and the Molecular Structure Transition of β-HMX to δ-HMX. *Journal of Physical Chemistry C*, **2019**, 123, 9231-9236	3.8	21
87	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. *Journal of the American Chemical Society*, **2018**, 140, 17702-17710	16.4	21
86	Shock-induced consolidation and spallation of Cu nanopowders. *Journal of Applied Physics*, **2012**, 111, 013508	2.5	19
85	Grain boundary orientation effects on deformation of Ta bicrystal nanopillars under high strain-rate compression. *Journal of Applied Physics*, **2014**, 115, 053528	2.5	18
84	Inhibition of Hotspot Formation in Polymer Bonded Explosives Using an Interface Matching Low Density Polymer Coating at the Polymer-Explosive Interface. *Journal of Physical Chemistry C*, **2014**, 118, 19918-19928	3.8	18
83	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 11444-11454	3.6	17
82	Dramatically reduced lattice thermal conductivity of Mg2Si thermoelectric material from nanotwinning. *Acta Materialia*, **2019**, 169, 9-14	8.4	17
81	Synthesis of single-component metallic glasses by thermal spray of nanodroplets on amorphous substrates. *Applied Physics Letters*, **2012**, 100, 041909	3.4	17
80	Mechanical properties in thermoelectric oxides: Ideal strength, deformation mechanism, and fracture toughness. *Acta Materialia*, **2018**, 149, 341-349	8.4	16
79	Shear-Induced Brittle Failure along Grain Boundaries in Boron Carbide. *ACS Applied Materials & Interfaces*, **2018**, 10, 5072-5080	9.5	16
78	Solid-liquid transitions of sodium chloride at high pressures. *Journal of Chemical Physics*, **2006**, 125, 154510	3.9	16

77	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. *ACS Applied Materials & Interfaces*, **2021**, 13, 24833-24855	9.5	16
76	Formation of two glass phases in binary Cu-Ag liquid. *Acta Materialia*, **2020**, 195, 274-281	8.4	15
75	Nanotwinning and amorphization of boron suboxide. *Acta Materialia*, **2018**, 147, 195-202	8.4	15
74	Prediction of the crystal packing of di-tetrazine-tetroxide (DTTO) energetic material. *Journal of Computational Chemistry*, **2016**, 37, 163-7	3.5	15
73	First-Order Phase Transition in Liquid Ag to the Heterogeneous G-Phase. *Journal of Physical Chemistry Letters*, **2020**, 11, 632-645	6.4	15
72	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. *Journal of Materials Chemistry A*, **2015**, 3, 12044-12050	13	14
71	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. *Journal of the American Chemical Society*, **2020**, 142, 8223-8232	16.4	14
70	Thermal Stability and Detonation Properties of Potassium 4,4Q-Bis(dinitromethyl)-3,3Q-azofurazanate, an Environmentally Friendly Energetic Three-Dimensional Metal-Organic Framework. *ACS Applied Materials & Interfaces*, **2019**, 11, 1512-1519	9.5	14
69	Dislocation-mediated shear amorphization in boron carbide. *Science Advances*, **2021**, 7,	14.3	14
68	Initial Decomposition Reactions of Bicyclo-HMX [BCHMX or cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole] from Quantum Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2015**, 150123143703008	3.8	13
67	Left-right loading dependence of shock response of (111)//(112) Cu bicrystals: Deformation and spallation. *Journal of Applied Physics*, **2012**, 111, 053525	2.5	13
66	Light irradiation induced brittle-to-ductile and ductile-to-brittle transition in inorganic semiconductors. *Physical Review B*, **2019**, 99,	3.3	12
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64	Prediction of superstrong □boron carbide phase from quantum mechanics. *Physical Review B*, **2017**, 95,	3.3	11
63	Dual Functions of Water in Stabilizing Metal-Pentazolate Hydrates [M(N5)2(H2O)4]□4H2O (M = Mn, Fe, Co, and Zn) High-Energy-Density Materials. *Journal of Physical Chemistry C*, **2018**, 122, 21192-21201	3.8	11
62	Ductility in Crystalline Boron Subphosphide (B12P2) for Large Strain Indentation. *Journal of Physical Chemistry C*, **2017**, 121, 16644-16649	3.8	11
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60	An et□al. Reply. *Physical Review Letters*, **2017**, 118, 089602	7.4	10

59	Mechanical softening of thermoelectric semiconductor Mg2Si from nanotwinning. *Scripta Materialia*, **2018**, 157, 90-94	5.6	10
58	Structural origin of reversible martensitic transformation and reversible twinning in NiTi shape memory alloy. *Acta Materialia*, **2020**, 199, 240-252	8.4	10
57	Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from Quantum-Mechanics-Based Hierarchical High-Throughput Catalyst Screening. *Journal of Physical Chemistry C*, **2019**, 123, 17375-17383	3.8	9
56	Icosahedra clustering and short range order in Ni-Nb-Zr amorphous membranes. *Scientific Reports*, **2018**, 8, 6084	4.9	9
55	Enhanced fracture toughness of boron carbide from microalloying and nanotwinning. *Scripta Materialia*, **2019**, 162, 306-310	5.6	9
54	Improved Ductility of B12 Icosahedra-based Superhard Materials through Icosahedral Slip. *Journal of Physical Chemistry C*, **2017**, 121, 11831-11838	3.8	8
53	Deformation Induced Solid–Solid Phase Transitions in Gamma Boron. *Chemistry of Materials*, **2014**, 26, 4289-4298	9.6	8
52	Icosahedral superstrength at the nanoscale. *Physical Review Materials*, **2018**, 2,	3.2	8
51	Ordering and dimensional crossovers in metallic glasses and liquids. *Physical Review B*, **2017**, 95,	3.3	7
50	Shear-induced brittle failure of titanium carbide from quantum mechanics simulations. *Journal of the American Ceramic Society*, **2018**, 101, 4184-4192	3.8	7
49	Fracture toughness of thermoelectric materials. *Materials Science and Engineering Reports*, **2021**, 144, 100607	30.9	7
48	Determining ideal strength and failure mechanism of thermoelectric CuInTe2 through quantum mechanics. *Journal of Materials Chemistry A*, **2018**, 6, 11743-11750	13	7
47	Photomechanical effect leading to extraordinary ductility in covalent semiconductors. *Physical Review B*, **2019**, 100,	3.3	6
46	The quantum mechanics derived atomistic mechanism underlying the acceleration of catalytic CO oxidation on Pt(110) by surface acoustic waves. *Journal of Materials Chemistry A*, **2016**, 4, 12036-12045	13	6
45	First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18193-18201	11.5	6
44	Transgranular amorphous shear band formation in polycrystalline boron carbide. *International Journal of Plasticity*, **2019**, 121, 218-226	7.6	6
43	Influence of Silicon on the Detonation Performance of Energetic Materials from First-Principles Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 24481-24487	3.8	6
42	Adsorption and decomposition of HMX and CL-20 on Al(111) surface by DFT investigation. *Surface and Interface Analysis*, **2017**, 49, 441-449	1.5	5

41	Brittle failure of □and □boron: Amorphization under high pressure. *Physical Review B*, **2017**, 95,	3.3	5
40	Determining the Quality Factor of Dielectric Ceramic Mixtures with Dielectric Constants in the Microwave Frequency□Range. *Scientific Reports*, **2017**, 7, 14120	4.9	5
39	Band-Gap Engineering in High-Temperature Boron-Rich Icosahedral Compounds. *Journal of Physical Chemistry C*, **2019**, 123, 12505-12513	3.8	5
38	Stability of NNO and NPO Nanotube Crystals. *Journal of Physical Chemistry Letters*, **2014**, 5, 485-9	6.4	5
37	Shock compression and spallation of single crystal tantalum **2012**,		5
36	Strengthening boron carbide through lithium dopant. *Journal of the American Ceramic Society*, **2020** , 103, 2012-2023	3.8	5
35	First principles predicting enhanced ductility of boride carbide through magnesium microalloying. *Journal of the American Ceramic Society*, **2019**, 102, 5514-5523	3.8	5
34	Atomic structure and mechanical response of coincident stacking faults in boron suboxide. *Materials Research Letters*, **2019**, 7, 75-81	7.4	5
33	Microstructure evolution and mechanical property of Cu-15Ni-8Sn-0.2Nb alloy during aging treatment. *Journal of Materials Science and Technology*, **2021**, 86, 227-236	9.1	5
32	Shear-induced mechanical failure of □a2O3 from quantum mechanics simulations. *Physical Review B*, **2017**, 96,	3.3	4
31	Discovering Catalytic Reaction Networks Using Deep Reinforcement Learning from First-Principles. *Journal of the American Chemical Society*, **2021**, 143, 16804-16812	16.4	4
30	The first order L-G phase transition in liquid Ag and Ag-Cu alloys is driven by deviatoric strain. *Scripta Materialia*, **2021**, 194, 113695	5.6	4
29	Shear induced deformation twinning evolution in thermoelectric InSb. *Npj Computational Materials*, **2021**, 7,	10.9	4
28	Enhanced ductility of III-V covalent semiconductors from electrons and holes. *Journal of Applied Physics*, **2019**, 126, 195105	2.5	4
27	Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide. *Journal of Physical Chemistry C*, **2020**, 124, 9787-9794	3.8	4
26	Thermal decomposition and diffusion of methane in clathrate hydrates from quantum mechanics simulations.. *RSC Advances*, **2020**, 10, 14753-14760	3.7	3
25	Enhanced strength and ductility of superhard boron carbide through injecting electrons. *Journal of the European Ceramic Society*, **2020**, 40, 4428-4435	6	3
24	Characterizing local metallic bonding variation induced by external perturbation. *Physical Chemistry Chemical Physics*, **2020**, 22, 2372-2378	3.6	3

23	Asymmetric twins in boron rich boron carbide. *Physical Chemistry Chemical Physics*, **2018**, 20, 13340-13347	3.6	3
22	CCl Radicals As a Carbon Source for Diamond Thin Film Deposition. *Journal of Physical Chemistry Letters*, **2014**, 5, 481-4	6.4	3
21	Controlling the Shapes of Nanoparticles by Dopant-Induced Enhancement of Chemisorption and Catalytic Activity: Application to Fe-Based Ammonia Synthesis. *ACS Nano*, **2021**, 15, 1675-1684	16.7	3
20	Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe(211) Surface. *Chemistry of Materials*, **2020**, 32, 9914-9924	9.6	3
19	Coordination and Thermophysical Properties of Transition Metal Chlorocomplexes in LiCl-KCl Eutectic. *Journal of Physical Chemistry B*, **2021**, 125, 8876-8887	3.4	3
18	Spatiotemporal Temperature and Pressure in Thermoplasmonic Gold Nanosphere-Water Systems. *ACS Nano*, **2021**, 15, 6276-6288	16.7	3
17	Mitigating the formation of amorphous shear band in boron carbide. *Journal of Applied Physics*, **2021**, 129, 140902	2.5	2
16	Li, An, and Morozov Reply. *Physical Review Letters*, **2019**, 123, 119602	7.4	1
15	Structural failure of layered thermoelectric In4Se3-δ semiconductors is dominated by shear slippage. *Acta Materialia*, **2020**, 187, 84-90	8.4	1
14	First principles high-throughput screening to enhance the ductility of lightweight magnesium alloys. *Physical Review Materials*, **2019**, 3,	3.2	1
13	Mitigating amorphization in superhard boron carbide by microalloying-induced stacking fault formation. *Physical Review Materials*, **2021**, 5,	3.2	1
12	Intrinsic mechanical behavior of MgAgSb thermoelectric material: An ab initio study. *Journal of Materiomics*, **2020**, 6, 24-32	6.7	1
11	Modified Generalized Stacking Fault Energy Surface of III-VI Ionic Crystals from Excess Electrons and Holes. *ACS Applied Electronic Materials*, **2020**, 2, 56-65	4	1
10	The L-G phase transition in binary Cu-Zr metallic liquids.. *Physical Chemistry Chemical Physics*, **2021**, 24, 497-506	3.6	0
9	Nanotwinning induced decreased lattice thermal conductivity of high temperature thermoelectric boron subphosphide (B12P2) from deep learning potential simulations. *Energy and AI*, **2022**, 8, 100135	12.6	0
8	Addressing amorphization and transgranular fracture of B4C through Si doping and TiB2 microparticle reinforcing. *Journal of the American Ceramic Society*,	3.8	0
7	Bi-Doped Zirconium Alloys with Enhanced Water Oxidation Resistance. *Journal of Physical Chemistry C*, **2020**, 124, 23116-23125	3.8	0
6	Vacancy-driven shear localization in silicon nitride. *Scripta Materialia*, **2021**, 190, 163-167	5.6	0

5	Drastic Modification of Lattice Thermal Conductivity in Thermoelectrics Induced by Electron-Hole Pairs. *ACS Applied Materials & Interfaces*, **2021**, 13, 3911-3918	9.5	0
4	A Strong Two-Dimensional Semiconductor l-B4C with High Carrier Mobility. *Journal of Physical Chemistry C*, **2022**, 126, 6036-6046	3.8	0
3	Vibrational Spectroscopy Signatures of Catalytically Relevant Configurations for N2 Reduction to NH3 on Fe Surfaces via Density Functional Theory. *Journal of Physical Chemistry C*, **2021**, 125, 27919-27930	3.8	0
2	Modified Failure Mechanism of Silicon through Excess Electrons and Holes. *Jom*, **2020**, 72, 3160-3169	2.1	
1	Electro-mechanical coupling in FCC metal rhodium from first-principles simulations. *Journal of Materials Research*, **2021**, 36, 2662-2673	2.5	