Qi An

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9497731/publications.pdf

Version: 2024-02-01

145 papers	4,141 citations	101496 36 h-index	143943 57 g-index
146 all docs	146 docs citations	146 times ranked	3810 citing authors

#	Article	IF	Citations
1	Ultrathin WO₃Â·0.33H₂O Nanotubes for CO₂ Photoreduction to Acetate with High Selectivity. Journal of the American Chemical Society, 2018, 140, 6474-6482.	6.6	233
2	Shock-induced plasticity in tantalum single crystals: Interatomic potentials and large-scale molecular-dynamics simulations. Physical Review B, 2013, 88, .	1.1	216
3	Efficient photocatalytic reduction of dinitrogen to ammonia on bismuth monoxide quantum dots. Journal of Materials Chemistry A, 2017, 5, 201-209.	5.2	160
4	Atomistic Explanation of Shear-Induced Amorphous Band Formation in Boron Carbide. Physical Review Letters, 2014, 113, 095501.	2.9	138
5	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. Journal of the American Chemical Society, 2018, 140, 6288-6297.	6.6	126
6	Fractal atomic-level percolation in metallic glasses. Science, 2015, 349, 1306-1310.	6.0	114
7	Atomistic Origin of Brittle Failure of Boron Carbide from Large-Scale Reactive Dynamics Simulations: Suggestions toward Improved Ductility. Physical Review Letters, 2015, 115, 105501.	2.9	109
8	Initial Steps of Thermal Decomposition of Dihydroxylammonium 5,5â€²-bistetrazole-1,1â€²-diolate Crystals from Quantum Mechanics. Journal of Physical Chemistry C, 2014, 118, 27175-27181.	1.5	101
9	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.	5.2	89
10	Elucidation of the dynamics for hot-spot initiation at nonuniform interfaces of highly shocked materials. Physical Review B, 2011, 84, .	1.1	85
11	Highly Shocked Polymer Bonded Explosives at a Nonplanar Interface: Hot-Spot Formation Leading to Detonation. Journal of Physical Chemistry C, 2013, 117, 26551-26561.	1.5	83
12	Aliovalent Doping Engineering for A- and B-Sites with Multiple Regulatory Mechanisms: A Strategy to Improve Energy Storage Properties of Sr_{0.7}Bi_{0.2}TiO₃-Based Lead-Free Relaxor Ferroelectric Ceramics. ACS Applied Materials & Interfaces, 2021, 13, 24833-24855.	4.0	79
13	Grain Boundary Sliding and Amorphization are Responsible for the Reverse Hall-Petch Relation in Superhard Nanocrystalline Boron Carbide. Physical Review Letters, 2018, 121, 145504.	2.9	73
14	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. Journal of Physical Chemistry C, 2012, 116, 10198-10206.	1.5	69
15	Compressive Shear Reactive Molecular Dynamics Studies Indicating That Cocrystals of TNT/CL-20 Decrease Sensitivity. Journal of Physical Chemistry C, 2014, 118, 30202-30208.	1.5	65
16	Superstrength through Nanotwinning. Nano Letters, 2016, 16, 7573-7579.	4.5	62
17	Brittle Failure Mechanism in Thermoelectric Skutterudite CoSb₃. Chemistry of Materials, 2015, 27, 6329-6336.	3.2	60
18	Atomic-Level Understanding of â€œAsymmetric Twinsâ€•in Boron Carbide. Physical Review Letters, 2015, 115, 175501.	2.9	56

#	Article	IF	Citations
19	Reactive molecular dynamics simulation of thermal decomposition for nano-aluminized explosives. Physical Chemistry Chemical Physics, 2018, 20, 29341-29350.	1.3	55
20	Ductile deformation mechanism in semiconductor Î±-Ag2S. Npj Computational Materials, 2018, 4, .	3.5	54
21	Superstrengthening <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><m through Nanotwinning. Physical Review Letters, 2017, 119, 085501.	2.9	53
22	Dislocation-mediated shear amorphization in boron carbide. Science Advances, 2021, 7, .	4.7	49
23	Enhanced ideal strength of thermoelectric half-Heusler TiNiSn by sub-structure engineering. Journal of Materials Chemistry A, 2016, 4, 14625-14636.	5.2	48
24	Microalloying Boron Carbide with Silicon to Achieve Dramatically Improved Ductility. Journal of Physical Chemistry Letters, 2014, 5, 4169-4174.	2.1	46
25	Enhanced Strength Through Nanotwinning in the Thermoelectric Semiconductor InSb. Physical Review Letters, 2017, 119, 215503.	2.9	45
26	New Ground-State Crystal Structure of Elemental Boron. Physical Review Letters, 2016, 117, 085501.	2.9	44
27	Nucleation of amorphous shear bands at nanotwins in boron suboxide. Nature Communications, 2016, 7, 11001.	5.8	43
28	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, 7053-7058.	3.3	43
29	Mechanism and kinetics of the electrocatalytic reaction responsible for the high cost of hydrogen fuel cells. Physical Chemistry Chemical Physics, 2017, 19, 2666-2673.	1.3	43
30	Bi2WO6 quantum dot-intercalated ultrathin montmorillonite nanostructure and its enhanced photocatalytic performance. Nano Research, 2014, 7, 1497-1506.	5.8	42
31	Boron Suboxide and Boron Subphosphide Crystals: Hard Ceramics That Shear without Brittle Failure. Chemistry of Materials, 2015, 27, 2855-2860.	3.2	42
32	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. Nano Letters, 2016, 16, 4236-4242.	4.5	42
33	Locating Si atoms in Si-doped boron carbide: A route to understand amorphization mitigation mechanism. Acta Materialia, 2018, 157, 106-113.	3.8	42
34	ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell. Journal of Physical Chemistry Letters, 2014, 5, 4039-4043.	2.1	40
35	Fracture toughness of thermoelectric materials. Materials Science and Engineering Reports, 2021, 144, 100607.	14.8	39
36	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.	5.2	38

#	Article	IF	Citations
37	Deformation and spallation of shocked Cu bicrystals with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î£</mml:mi></mml:math>3 coherent and symmetric incoherent twin boundaries. Physical Review B, 2012, 85, .	1.1	37
38	Prediction of the Chapmanâ€“Jouguet chemical equilibrium state in a detonation wave from first principles based reactive molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 2015-2022.	1.3	35
39	Shock response of a model structured nanofoam of Cu. Journal of Applied Physics, 2013, 113, .	1.1	34
40	Predicted Optimum Composition for the Glass-Forming Ability of Bulk Amorphous Alloys: Application to Cuâ€“Zrâ€“Al. Journal of Physical Chemistry Letters, 2012, 3, 3143-3148.	2.1	33
41	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. Journal of the American Chemical Society, 2018, 140, 17702-17710.	6.6	32
42	Breaking the icosahedra in boron carbide. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12012-12016.	3.3	31
43	Deformation mechanisms in high-efficiency thermoelectric layered Zintl compounds. Journal of Materials Chemistry A, 2017, 5, 9050-9059.	5.2	31
44	Nanotwins soften boron-rich boron carbide (B13C2). Applied Physics Letters, 2017, 110, .	1.5	30
45	Dramatically reduced lattice thermal conductivity of Mg2Si thermoelectric material from nanotwinning. Acta Materialia, 2019, 169, 9-14.	3.8	30
46	Structural origin of reversible martensitic transformation and reversible twinning in NiTi shape memory alloy. Acta Materialia, 2020, 199, 240-252.	3.8	29
47	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.	5.6	29
48	Atomistic explanation of brittle failure of thermoelectric skutterudite CoSb3. Acta Materialia, 2016, 103, 775-780.	3.8	28
49	Initial Decomposition of HMX Energetic Material from Quantum Molecular Dynamics and the Molecular Structure Transition of Î²-HMX to Î´-HMX. Journal of Physical Chemistry C, 2019, 123, 9231-9236.	1.5	28
50	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. Journal of the American Chemical Society, 2020, 142, 8223-8232.	6.6	28
51	Improved Ductility of Boron Carbide by Microalloying with Boron Suboxide. Journal of Physical Chemistry C, 2015, 119, 24649-24656.	1.5	27
52	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. Physical Chemistry Chemical Physics, 2019, 21, 11444-11454.	1.3	27
53	Mechanical properties in thermoelectric oxides: Ideal strength, deformation mechanism, and fracture toughness. Acta Materialia, 2018, 149, 341-349.	3.8	25
54	Prediction of the crystal packing of diâ€tetrazineâ€tetroxide (DTTO) energetic material. Journal of Computational Chemistry, 2016, 37, 163-167.	1.5	24

#	Article	IF	Citations
55	Synthesis of single-component metallic glasses by thermal spray of nanodroplets on amorphous substrates. Applied Physics Letters, 2012, 100, .	1.5	23
56	Nanotwinning and amorphization of boron suboxide. Acta Materialia, 2018, 147, 195-202.	3.8	23
57	Thermal Stability and Detonation Properties of Potassium 4,4â€²-Bis(dinitromethyl)-3,3â€²-azofurazanate, an Environmentally Friendly Energetic Three-Dimensional Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2019, 11, 1512-1519.	4.0	23
58	Formation of two glass phases in binary Cu-Ag liquid. Acta Materialia, 2020, 195, 274-281.	3.8	23
59	Reaction Mechanisms, Kinetics, and Improved Catalysts for Ammonia Synthesis from Hierarchical High Throughput Catalyst Design. Accounts of Chemical Research, 2022, 55, 1124-1134.	7.6	23
60	Shock-induced consolidation and spallation of Cu nanopowders. Journal of Applied Physics, 2012, 111, .	1.1	22
61	Inhibition of Hotspot Formation in Polymer Bonded Explosives Using an Interface Matching Low Density Polymer Coating at the Polymerâ€“Explosive Interface. Journal of Physical Chemistry C, 2014, 118, 19918-19928.	1.5	22
62	Grain boundary orientation effects on deformation of Ta bicrystal nanopillars under high strain-rate compression. Journal of Applied Physics, 2014, 115, .	1.1	21
63	Shear-Induced Brittle Failure along Grain Boundaries in Boron Carbide. ACS Applied Materials & Interfaces, 2018, 10, 5072-5080.	4.0	21
64	First-Order Phase Transition in Liquid Ag to the Heterogeneous G-Phase. Journal of Physical Chemistry Letters, 2020, 11, 632-645.	2.1	20
65	Solidâ€“liquid transitions of sodium chloride at high pressures. Journal of Chemical Physics, 2006, 125, 154510.	1.2	19
66	Enhanced fracture toughness of boron carbide from microalloying and nanotwinning. Scripta Materialia, 2019, 162, 306-310.	2.6	19
67	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.	5.2	18
68	Ductility in Crystalline Boron Subphosphide (B₁₂P₂) for Large Strain Indentation. Journal of Physical Chemistry C, 2017, 121, 16644-16649.	1.5	18
69	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, 119, 2290-2296.	1.5	17
70	Discovering Catalytic Reaction Networks Using Deep Reinforcement Learning from First-Principles. Journal of the American Chemical Society, 2021, 143, 16804-16812.	6.6	17
71	Dual Functions of Water in Stabilizing Metal-Pentazolate Hydrates [M(N₅)₂(H₂O)₄]Â·4H₂O (M = Mn, Fe, Co,) Tj ET Q q 1 1 0.784314 rg	1.5	17
72	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.	1.5	16

#	Article	IF	Citations
73	Light irradiation induced brittle-to-ductile and ductile-to-brittle transition in inorganic semiconductors. Physical Review B, 2019, 99, .	1.1	16
74	Shear induced deformation twinning evolution in thermoelectric InSb. Npj Computational Materials, 2021, 7, .	3.5	16
75	Left-right loading dependence of shock response of (111)//(112) Cu bicrystals: Deformation and spallation. Journal of Applied Physics, 2012, 111, .	1.1	15
76	Structure and Properties of Boron-Very-Rich Boron Carbides: B₁₂ Icosahedra Linked through Bent CBB Chains. Journal of Physical Chemistry C, 2018, 122, 2448-2453.	1.5	15
77	Prediction of superstrong Ï„ -boron carbide phase from quantum mechanics. Physical Review B, 2017, 95, .	1.1	14
78	Transgranular amorphous shear band formation in polycrystalline boron carbide. International Journal of Plasticity, 2019, 121, 218-226.	4.1	14
79	First principles predicting enhanced ductility of boride carbide through magnesium microalloying. Journal of the American Ceramic Society, 2019, 102, 5514-5523.	1.9	14
80	Strengthening boron carbide through lithium dopant. Journal of the American Ceramic Society, 2020, 103, 2012-2023.	1.9	14
81	Vacancy-induced densification of silica glass. Journal of Non-Crystalline Solids, 2006, 352, 3320-3325.	1.5	13
82	Improved Ductility of B₁₂ Icosahedra-based Superhard Materials through Icosahedral Slip. Journal of Physical Chemistry C, 2017, 121, 11831-11838.	1.5	13
83	Icosahedra clustering and short range order in Ni-Nb-Zr amorphous membranes. Scientific Reports, 2018, 8, 6084.	1.6	13
84	Mechanical softening of thermoelectric semiconductor Mg2Si from nanotwinning. Scripta Materialia, 2018, 157, 90-94.	2.6	13
85	Band-Gap Engineering in High-Temperature Boron-Rich Icosahedral Compounds. Journal of Physical Chemistry C, 2019, 123, 12505-12513.	1.5	13
86	Coordination and Thermophysical Properties of Transition Metal Chlorocomplexes in LiClâ€“KCl Eutectic. Journal of Physical Chemistry B, 2021, 125, 8876-8887.	1.2	13
87	An etÂal. Reply:. Physical Review Letters, 2017, 118, 089602.	2.9	12
88	Photomechanical effect leading to extraordinary ductility in covalent semiconductors. Physical Review B, 2019, 100, .	1.1	11
89	Spatiotemporal Temperature and Pressure in Thermoplasmonic Gold Nanosphereâ€“Water Systems. ACS Nano, 2021, 15, 6276-6288.	7.3	11
90	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.	7.3	11

#	Article	IF	Citations
91	Addressing amorphization and transgranular fracture of B₄C through Si doping and TiB₂ microparticle reinforcing. Journal of the American Ceramic Society, 2022, 105, 2959-2977.	1.9	11
92	Determining the Quality Factor of Dielectric Ceramic Mixtures with Dielectric Constants in the Microwave FrequencyÂRange. Scientific Reports, 2017, 7, 14120.	1.6	10
93	Determining ideal strength and failure mechanism of thermoelectric CuInTe2 through quantum mechanics. Journal of Materials Chemistry A, 2018, 6, 11743-11750.	5.2	10
94	Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide. Journal of Physical Chemistry C, 2020, 124, 9787-9794.	1.5	10
95	Models for the behavior of boron carbide in extreme dynamic environments. Journal of the American Ceramic Society, 2022, 105, 3043-3061.	1.9	10
96	Icosahedral superstrength at the nanoscale. Physical Review Materials, 2018, 2, .	0.9	10
97	Nanotwin-induced ductile mechanism in thermoelectric semiconductor PbTe. Matter, 2022, 5, 1839-1852.	5.0	10
98	Deformation Induced Solidâ€“Solid Phase Transitions in Gamma Boron. Chemistry of Materials, 2014, 26, 4289-4298.	3.2	9
99	Adsorption and decomposition of HMX and CLâ€20 on Al(111) surface by DFT investigation. Surface and Interface Analysis, 2017, 49, 441-449.	0.8	9
100	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.	1.5	9
101	Ordering and dimensional crossovers in metallic glasses and liquids. Physical Review B, 2017, 95, .	1.1	8
102	Brittle failure of Î²- and Ï„-boron: Amorphization under high pressure. Physical Review B, 2017, 95, .	1.1	8
103	The first order L-G phase transition in liquid Ag and Ag-Cu alloys is driven by deviatoric strain. Scripta Materialia, 2021, 194, 113695.	2.6	8
104	Mitigating the formation of amorphous shear band in boron carbide. Journal of Applied Physics, 2021, 129, .	1.1	8
105	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.	5.2	7
106	Shearâ€induced brittle failure of titanium carbide from quantum mechanics simulations. Journal of the American Ceramic Society, 2018, 101, 4184-4192.	1.9	7
107	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.	3.3	7
108	Enhanced strength and ductility of superhard boron carbide through injecting electrons. Journal of the European Ceramic Society, 2020, 40, 4428-4435.	2.8	7

#	Article	IF	Citations
109	Transition between Hall-Petch and inverse Hall-Petch behavior in nanocrystalline silicon carbide. Physical Review Materials, 2021, 5, .	0.9	7
110	Mitigating amorphization in superhard boron carbide by microalloying-induced stacking fault formation. Physical Review Materials, 2021, 5, .	0.9	7
111	Local amorphization in boron carbide at finite temperature: Strategies toward improved ductility. Physical Review B, 2021, 104, .	1.1	7
112	Shock compression and spallation of single crystal tantalum. AIP Conference Proceedings, 2012, , .	0.3	6
113	Stability of NNO and NPO Nanotube Crystals. Journal of Physical Chemistry Letters, 2014, 5, 485-489.	2.1	6
114	Shear-induced mechanical failure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi mathvariant="normal">G</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from quantum mechanics simulations. Physical Review B, 2017, 96, .	1.1	6
115	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.	3.2	6
116	Shearâ€induced amorphization in boron subphosphide (B₁₂P₂): Direct transition versus stacking fault mediation. Journal of the American Ceramic Society, 2022, 105, 6826-6838.	1.9	6
117	CCl Radicals As a Carbon Source for Diamond Thin Film Deposition. Journal of Physical Chemistry Letters, 2014, 5, 481-484.	2.1	5
118	Enhanced ductility of III-V covalent semiconductors from electrons and holes. Journal of Applied Physics, 2019, 126, .	1.1	5
119	Atomic structure and mechanical response of coincident stacking faults in boron suboxide. Materials Research Letters, 2019, 7, 75-81.	4.1	5
120	Intrinsic mechanical behavior of MgAgSb thermoelectric material: An ab initio study. Journal of Materiomics, 2020, 6, 24-32.	2.8	5
121	Convert Widespread Paraelectric Perovskite to Ferroelectrics. Physical Review Letters, 2022, 128, .	2.9	5
122	Asymmetric twins in boron rich boron carbide. Physical Chemistry Chemical Physics, 2018, 20, 13340-13347.	1.3	4
123	Nanotwinning induced decreased lattice thermal conductivity of high temperature thermoelectric boron subphosphide (B12P2) from deep learning potential simulations. Energy and AI, 2022, 8, 100135.	5.8	4
124	Modified Generalized Stacking Fault Energy Surface of IIâ€“VI Ionic Crystals from Excess Electrons and Holes. ACS Applied Electronic Materials, 2020, 2, 56-65.	2.0	3
125	Thermal decomposition and diffusion of methane in clathrate hydrates from quantum mechanics simulations. RSC Advances, 2020, 10, 14753-14760.	1.7	3
126	Characterizing local metallic bonding variation induced by external perturbation. Physical Chemistry Chemical Physics, 2020, 22, 2372-2378.	1.3	3

#	Article	IF	Citations
127	Strengthening boron carbide by doping Si into grain boundaries. Journal of the American Ceramic Society, 2022, 105, 2978-2989.	1.9	3
128	Shear band formation during nanoindentation of EuB6 rare-earth hexaboride. Communications Materials, 2022, 3, .	2.9	3
129	Li, An, and Morozov Reply:. Physical Review Letters, 2019, 123, 119602.	2.9	2
130	Bi-Doped Zirconium Alloys with Enhanced Water Oxidation Resistance. Journal of Physical Chemistry C, 2020, 124, 23116-23125.	1.5	2
131	Drastic Modification of Lattice Thermal Conductivity in Thermoelectrics Induced by Electronâ€“Hole Pairs. ACS Applied Materials & Interfaces, 2021, 13, 3911-3918.	4.0	2
132	The Lâ€“G phase transition in binary Cuâ€“Zr metallic liquids. Physical Chemistry Chemical Physics, 2021, 24, 497-506.	1.3	2
133	A Strong Two-Dimensional Semiconductor l-B₄C with High Carrier Mobility. Journal of Physical Chemistry C, 2022, 126, 6036-6046.	1.5	2
134	Structural failure of layered thermoelectric In4Se3-Î´ semiconductors is dominated by shear slippage. Acta Materialia, 2020, 187, 84-90.	3.8	1
135	Vacancy-driven shear localization in silicon nitride. Scripta Materialia, 2021, 190, 163-167.	2.6	1
136	First principles high-throughput screening to enhance the ductility of lightweight magnesium alloys. Physical Review Materials, 2019, 3, .	0.9	1
137	Locking of Screw Dislocations in Silicon due to Core Structure Transformation. Journal of Physical Chemistry C, 2021, 125, 24710-24718.	1.5	1
138	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.	1.5	1
139	Shear Banding in Binary Cu-Zr Metallic Glass: Comparison of the G-Phase With L-Phase. Frontiers in Materials, 2022, 9, .	1.2	1
140	Coordination and Thermophysical Properties of Select Trivalent Lanthanides in LiCl-KCl. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
141	Electronâ€“Hole Excitation Induced Softening in Boron Carbide-Based Superhard Materials. ACS Applied Materials & Interfaces, 0, , .	4.0	1
142	Brittle failure of orthorhombic borides from first-principles simulations. Physical Review B, 2018, 98, .	1.1	0
143	Modified Failure Mechanism of Silicon through Excess Electrons and Holes. Jom, 2020, 72, 3160-3169.	0.9	0
144	Electro-mechanical coupling in FCC metal rhodium from first-principles simulations. Journal of Materials Research, 2021, 36, 2662-2673.	1.2	0

#	Article	IF	Citations
145	Local Coordination Environment of 3d and 4d Transition Metal Ions in LiCl-KCl Eutectic Mixture. Materials, 2022, 15, 1478.	1.3	0