Alejandro Strachan

List of Publications by Year
in descending order

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204	7,647	70961	62479
papers	citations	41	80
		h-index	g-index

207	207	207	6280
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. Journal of Physical Chemistry A, 2003, 107, 3803-3811.	1.1	821
2	Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX. Physical Review Letters, 2003, 91, 098301.	2.9	495
3	Thermal decomposition of RDX from reactive molecular dynamics. Journal of Chemical Physics, 2005, 122, 054502.	1.2	366
4	Molecular dynamics predictions of thermal and mechanical properties of thermoset polymer EPON862/DETDA. Polymer, 2011, 52, 2920-2928.	1.8	244
5	Maximum superheating and undercooling: Systematics, molecular dynamics simulations, and dynamic experiments. Physical Review B, 2003, 68, .	1.1	234
6	Molecular simulations of crosslinking process of thermosetting polymers. Polymer, 2010, 51, 6058-6070.	1.8	222
7	Molecular scale simulations on thermoset polymers: A review. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 103-122.	2.4	179
8	Atomic origin of ultrafast resistance switching in nanoscale electrometallization cells. Nature Materials, 2015, 14, 440-446.	13.3	172
9	Nonequilibrium melting and crystallization of a model Lennard-Jones system. Journal of Chemical Physics, 2004, 120, 11640-11649.	1.2	163
10	Molecular dynamics simulations and experimental studies of the thermomechanical response of an epoxy thermoset polymer. Polymer, 2012, 53, 4222-4230.	1.8	131
11	Atomistic simulations on multilayer graphene reinforced epoxy composites. Composites Part A: Applied Science and Manufacturing, 2012, 43, 1293-1300.	3.8	116
12	Role of strain on electronic and mechanical response of semiconducting transition-metal dichalcogenide monolayers: An ab-initio study. Journal of Applied Physics, 2014, 115, .	1.1	111
13	Ultrafast Chemistry under Nonequilibrium Conditions and the Shock to Deflagration Transition at the Nanoscale. Journal of Physical Chemistry C, 2015, 119, 22008-22015.	1.5	110
14	Coupled Thermal and Electromagnetic Induced Decomposition in the Molecular Explosive Î±HMX; A Reactive Molecular Dynamics Study. Journal of Physical Chemistry A, 2014, 118, 885-895.	1.1	109
15	Thermal Decomposition of Condensed-Phase Nitromethane from Molecular Dynamics from ReaxFF Reactive Dynamics. Journal of Physical Chemistry B, 2011, 115, 6534-6540.	1.2	105
16	Roadmap on multiscale materials modeling. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 043001.	0.8	100
17	Tailored Reactivity of Ni+Al Nanocomposites: Microstructural Correlations. Journal of Physical Chemistry C, 2012, 116, 21027-21038.	1.5	97
18	Critical behavior in spallation failure of metals. Physical Review B, 2001, 63, .	1.1	92

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19	Atomic-level view of inelastic deformation in a shock loaded molecular crystal. Physical Review B, 2007, 76, .	1.1	88
20	Atomistic simulations of shock-induced alloying reactions in Niâˆ•Al nanolaminates. Journal of Chemical Physics, 2006, 125, 164707.	1.2	83
21	Density functional theory and molecular dynamics studies of the energetics and kinetics of electroactive polymers: PVDF and P(VDF-TrFE). Physical Review B, 2004, 70, .	1.1	82
22	Phase diagram of MgO from density-functional theory and molecular-dynamics simulations. Physical Review B, 1999, 60, 15084-15093.	1.1	77
23	Normal modes and frequencies from covariances in molecular dynamics or Monte Carlo simulations. Journal of Chemical Physics, 2004, 120, 1-4.	1.2	73
24	Novel doping alternatives for single-layer transition metal dichalcogenides. Journal of Applied Physics, 2017, 122, .	1.1	61
25	Material property prediction of thermoset polymers by molecular dynamics simulations. Acta Mechanica, 2014, 225, 1187-1196.	1.1	58
26	Prediction of the chemical and thermal shrinkage in a thermoset polymer. Composites Part A: Applied Science and Manufacturing, 2014, 66, 35-43.	3.8	57
27	Separation of aleatory and epistemic uncertainty in probabilistic model validation. Reliability Engineering and System Safety, 2016, 147, 49-59.	5.1	56
28	Energy Exchange between Mesoparticles and Their Internal Degrees of Freedom. Physical Review Letters, 2005, 94, 014301.	2.9	55
29	Phase stability and transformations in NiTi from density functional theory calculations. Acta Materialia, 2010, 58, 745-752.	3.8	53
30	Vibrational density of states and Lindemann melting law. Journal of Chemical Physics, 2005, 122, 194709.	1.2	52
31	First-Principles Investigation of Low Energy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>E</mml:mi><mml:mo>â€²</mml:mo></mml:msup></mml:math>Center Precursors in Amorphous Silica. Physical Review Letters, 2011, 106, 206402.	2.9	52
32	Molecular dynamics simulations of 1/2 aã€ˆ1 1 1ã€‰ screw dislocation in Ta. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2001, 309-310, 133-137.	2.6	50
33	Cohesive energy density and solubility parameter evolution during the curing of thermoset. Polymer, 2018, 135, 162-170.	1.8	50
34	Thermal transport in SiGe superlattice thin films and nanowires: Effects of specimen and periodic lengths. Physical Review B, 2013, 87, .	1.1	47
35	Shock Loading of Granular Ni/Al Composites. Part 1: Mechanics of Loading. Journal of Physical Chemistry C, 2014, 118, 26377-26386.	1.5	47
36	Voltage equilibration for reactive atomistic simulations of electrochemical processes. Journal of Chemical Physics, 2015, 143, 054109.	1.2	46

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37	Phonon thermal conductivity in nanolaminated composite metals via molecular dynamics. Journal of Chemical Physics, 2007, 127, 184702.	1.2	45
38	Ab initioand finite-temperature molecular dynamics studies of lattice resistance in tantalum. Physical Review B, 2003, 68, .	1.1	44
39	Hotspot formation due to shock-induced pore collapse in 1,3,5,7-tetranitro-1,3,5,7-tetrazoctane (HMX): Role of pore shape and shock strength in collapse mechanism and temperature. Journal of Applied Physics, 2020, 127, .	1.1	44
40	Effects of water on epoxy cure kinetics and glass transition temperature utilizing molecular dynamics simulations. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 1150-1159.	2.4	43
41	Melting and alloying of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ni</mml:mi><mml:mo>âˆ•</mml:mo><mml:mi mathvariant="normal">Al</mml:mi></mml:mrow></mml:math>nanolaminates induced by shock loading: A molecular dynamics simulation study. Physical Review B, 2007, 76, .	1.1	42
42	Decomposition and Reaction of Polyvinyl Nitrate under Shock and Thermal Loading: A ReaxFF Reactive Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 22452-22464.	1.5	42
43	Unsupervised Learning-Based Multiscale Model of Thermochemistry in 1,3,5-Trinitro-1,3,5-triazinane (RDX). Journal of Physical Chemistry A, 2020, 124, 9141-9155.	1.1	41
44	Fragment recognition in molecular dynamics. Physical Review C, 1997, 56, 995-1001.	1.1	40
45	Molecular dynamics simulation of dynamical response of perfect and porousNiâˆ•Alnanolaminates under shock loading. Physical Review B, 2007, 76, .	1.1	39
46	Uncertainty propagation in a multiscale model of nanocrystalline plasticity. Reliability Engineering and System Safety, 2011, 96, 1161-1170.	5.1	39
47	Neural network reactive force field for C, H, N, and O systems. Npj Computational Materials, 2021, 7, .	3.5	39
48	Energy-based yield criterion for PMMA from large-scale molecular dynamics simulations. Physical Review B, 2012, 85, .	1.1	38
49	Free volume evolution in the process of epoxy curing and its effect on mechanical properties. Polymer, 2016, 97, 456-464.	1.8	38
50	Continuum and molecular dynamics simulations of pore collapse in shocked Î²-tetramethylene tetranitramine (Î²-HMX) single crystals. Journal of Applied Physics, 2021, 129, .	1.1	38
51	Effect of Thickness on the Thermo-Mechanical Response of Free-Standing Thermoset Nanofilms from Molecular Dynamics. Macromolecules, 2011, 44, 9448-9454.	2.2	36
52	Mechanisms of Plastic Deformation of Metalâ€“Organic Framework-5. Journal of Physical Chemistry C, 2015, 119, 25845-25852.	1.5	36
53	Opportunities and challenges of 2D materials in back-end-of-line interconnect scaling. Journal of Applied Physics, 2020, 128, .	1.1	36
54	Evolution of network topology of bifunctional epoxy thermosets during cure and its relationship to thermo-mechanical properties: A molecular dynamics study. Polymer, 2015, 75, 151-160.	1.8	35

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55	Shock Loading of Granular Ni/Al Composites. Part 2: Shock-Induced Chemistry. Journal of Physical Chemistry C, 2016, 120, 6804-6813.	1.5	35
56	Sensitivity of the Shock Initiation Threshold of 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) to Nuclear Quantum Effects. Journal of Physical Chemistry C, 2019, 123, 21969-21981.	1.5	35
57	First principles force field for metallic tantalum. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S445-S459.	0.8	34
58	Role of nanostructure on reaction and transport in Ni/Al intermolecular reactive composites. Physical Review B, 2012, 86, .	1.1	33
59	Molecular dynamics simulations of the reaction mechanism in Ni/Al reactive intermetallics. Acta Materialia, 2015, 96, 1-9.	3.8	33
60	Structures and energetics of silicon nanotubes from molecular dynamics and density functional theory. Physical Review B, 2008, 78, .	1.1	32
61	A multiscale approach for modeling crystalline solids. Journal of Computer-Aided Materials Design, 2001, 8, 127-149.	0.7	31
62	Calculating the Peierls energy and Peierls stress from atomistic simulations of screw dislocation dynamics: application to bcc tantalum. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S371-S389.	0.8	31
63	Deducing solidâ€“liquid interfacial energy from superheating or supercooling: application to H2O at high pressures. Modelling and Simulation in Materials Science and Engineering, 2005, 13, 321-328.	0.8	31
64	Effect of topological disorder on structural, mechanical, and electronic properties of amorphous silicon nitride: An atomistic study. Physical Review B, 2012, 85, .	1.1	31
65	Shockwave Energy Dissipation in Metalâ€“Organic Framework MOF-5. Journal of Physical Chemistry C, 2016, 120, 12463-12471.	1.5	31
66	Reactive Molecular Dynamics Simulations to Investigate the Shock Response of Liquid Nitromethane. Journal of Physical Chemistry C, 2019, 123, 2613-2626.	1.5	31
67	Time scales in fragmentation. Physical Review C, 1997, 55, 775-787.	1.1	30
68	Temperature and energy partition in fragmentation. Physical Review C, 1999, 59, 285-294.	1.1	30
69	Atomistic simulations of kinks in1/2aã€ˆ111ã€‰screw dislocations in bcc tantalum. Physical Review B, 2003, 68, .	1.1	30
70	Cyber-Enabled Simulations in Nanoscale Science and Engineering. Computing in Science and Engineering, 2010, 12, 12-17.	1.2	30
71	Effect of core energy on mobility in a continuum dislocation model. Physical Review B, 2011, 83, .	1.1	30
72	Defect level distributions and atomic relaxations induced by charge trapping in amorphous silica. Applied Physics Letters, 2012, 100, .	1.5	30

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73	Molecular dynamics simulations on cyclic deformation of an epoxy thermoset. Polymer, 2013, 54, 881-890.	1.8	30
74	A Hotspotâ€™s Better Half: Non-Equilibrium Intra-Molecular Strain in Shock Physics. Journal of Physical Chemistry Letters, 2021, 12, 2756-2762.	2.1	30
75	Role of grain size on the martensitic transformation and ultra-fast superelasticity in shape memory alloys. Acta Materialia, 2015, 95, 37-43.	3.8	28
76	Role of core polarization curvature of screw dislocations in determining the Peierls stress in bcc Ta:â€ƒA criterion for designing high-performance materials. Physical Review B, 2003, 67, .	1.1	27
77	PUQ: A code for non-intrusive uncertainty propagation in computer simulations. Computer Physics Communications, 2015, 194, 97-107.	3.0	27
78	Role of Molecular Disorder on the Reactivity of RDX. Journal of Physical Chemistry C, 2018, 122, 27032-27043.	1.5	27
79	Pulse Dynamics of Electric Double Layer Formation on All-Solid-State Graphene Field-Effect Transistors. ACS Applied Materials & Interfaces, 2018, 10, 43166-43176.	4.0	25
80	Chemistry Under Shock Conditions. Annual Review of Materials Research, 2021, 51, 101-130.	4.3	25
81	Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCC Ni. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2001, 309-310, 156-159.	2.6	24
82	Stability and migration of small copper clusters in amorphous dielectrics. Journal of Applied Physics, 2015, 117, .	1.1	24
83	Exothermic Self-Sustained Waves with Amorphous Nickel. Journal of Physical Chemistry C, 2016, 120, 5827-5838.	1.5	23
84	Error correction in multi-fidelity molecular dynamics simulations using functional uncertainty quantification. Journal of Computational Physics, 2017, 334, 207-220.	1.9	23
85	Prediction of PEKK properties related to crystallization by molecular dynamics simulations with a united-atom model. Polymer, 2019, 174, 25-32.	1.8	23
86	Size effects in NiTi from density functional theory calculations. Physical Review B, 2012, 85, .	1.1	22
87	High-temperature emissivity of silica, zirconia and samaria from ab initio simulations: role of defects and disorder. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 075004.	0.8	22
88	Atomistic simulations of electrochemical metallization cells: mechanisms of ultra-fast resistance switching in nanoscale devices. Nanoscale, 2016, 8, 14037-14047.	2.8	22
89	Molecular dynamics modeling of stishovite. Earth and Planetary Science Letters, 2002, 202, 147-157.	1.8	21
90	Melting dynamics of superheated argon: Nucleation and growth. Journal of Chemical Physics, 2007, 126, 034505.	1.2	21

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91	Molecular modeling of the microstructure evolution during carbon fiber processing. Journal of Chemical Physics, 2017, 147, 224705.	1.2	21
92	Uncertainties in the predictions of thermo-physical properties of thermoplastic polymers via molecular dynamics. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 065007.	0.8	21
93	Atomistic Insights on the Full Operation Cycle of a HfO₂-Based Resistive Random Access Memory Cell from Molecular Dynamics. ACS Nano, 2021, 15, 12945-12954.	7.3	21
94	Caloric curve in fragmentation. Physical Review C, 1998, 58, R632-R636.	1.1	20
95	Coarse grain modeling of spall failure in molecular crystals: role of intra-molecular degrees of freedom. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 015007.	0.8	20
96	Ab-initio studies of pressure induced phase transitions in BaO. Journal of Computer-Aided Materials Design, 2001, 8, 193-202.	0.7	19
97	Estimating the In-Plane Young's Modulus of Polycrystalline Films in MEMS. Journal of Microelectromechanical Systems, 2012, 21, 840-849.	1.7	19
98	Role of atomic variability and mechanical constraints on the martensitic phase transformation of a model disordered shape memory alloy via molecular dynamics. Acta Materialia, 2014, 69, 30-36.	3.8	19
99	Modeling resistive switching materials and devices across scales. Journal of Electroceramics, 2017, 39, 39-60.	0.8	19
100	Role of dynamical compressive and shear loading on hotspot criticality in RDX via reactive molecular dynamics. Journal of Applied Physics, 2020, 128, .	1.1	19
101	Predicted Reaction Mechanisms, Product Speciation, Kinetics, and Detonation Properties of the Insensitive Explosive 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105). Journal of Physical Chemistry A, 2021, 125, 1766-1777.	1.1	19
102	Mesodynamics with implicit degrees of freedom. Journal of Chemical Physics, 2014, 141, 064107.	1.2	18
103	Fourier-like Thermal Relaxation of Nanoscale Explosive Hot Spots. Journal of Physical Chemistry C, 2021, 125, 20570-20582.	1.5	18
104	Role of energy distribution in contacts on thermal transport in Si: A molecular dynamics study. Journal of Applied Physics, 2016, 120, .	1.1	17
105	First-principles study of elastic mechanical responses to applied deformation of metal-organic frameworks. Journal of Chemical Physics, 2017, 146, .	1.2	17
106	Crystalline and pseudo-crystalline phases of polyacrylonitrile from molecular dynamics: Implications for carbon fiber precursors. Polymer, 2018, 155, 13-26.	1.8	17
107	Insight into the Chemistry of PETN Under Shock Compression Through Ultrafast Broadband Mid-Infrared Absorption Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 7031-7046.	1.1	17
108	The Potential Energy Hotspot: Effects of Impact Velocity, Defect Geometry, and Crystallographic Orientation. Journal of Physical Chemistry C, 2022, 126, 3743-3755.	1.5	17

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109	Amorphous Ni/Al nanoscale laminates as high-energy intermolecular reactive composites. Physical Review B, 2012, 85, .	1.1	16
110	Nitromethane Decomposition via Automated Reaction Discovery and an Ab Initio Corrected Kinetic Model. Journal of Physical Chemistry A, 2021, 125, 1447-1460.	1.1	16
111	Thermodynamic Properties of Asphaltenes Through Computer Assisted Structure Elucidation and Atomistic Simulations. 1. Bulk Arabian Light Asphaltenes. Petroleum Science and Technology, 2004, 22, 877-899.	0.7	15
112	Strain relaxation in Si/Ge/Si nanoscale bars from molecular dynamics simulations. Journal of Applied Physics, 2009, 106, 034304.	1.1	15
113	Shape memory metamaterials with tunable thermo-mechanical response via hetero-epitaxial integration: A molecular dynamics study. Journal of Applied Physics, 2013, 113, 103503.	1.1	15
114	Extemporaneous Mechanochemistry: Shock-Wave-Induced Ultrafast Chemical Reactions Due to Intramolecular Strain Energy. Journal of Physical Chemistry Letters, 2022, 13, 6657-6663.	2.1	15
115	Large electrostrictive strain at gigahertz frequencies in a polymer nanoactuator: Computational device design. Applied Physics Letters, 2005, 86, 083103.	1.5	14
116	Nanoscale Metal-Metal Contact Physics from Molecular Dynamics: The Strongest Contact Size. Physical Review Letters, 2010, 104, 215504.	2.9	14
117	Coarse grain model for coupled thermo-mechano-chemical processes and its application to pressure-induced endothermic chemical reactions. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 025027.	0.8	14
118	Mesoscale simulations of shockwave energy dissipation via chemical reactions. Journal of Chemical Physics, 2015, 142, 084108.	1.2	14
119	Tunability of martensitic transformation in Mg-Sc shape memory alloys: A DFT study. Acta Materialia, 2020, 189, 1-9.	3.8	14
120	Parsimonious neural networks learn interpretable physical laws. Scientific Reports, 2021, 11, 12761.	1.6	14
121	Reply to â€œComment on â€˜Phase diagram of MgO from density-functional theory and molecular- dynamics simulationsâ€™ â€• Physical Review B, 2001, 63, .	1.1	13
122	An Active Learning Approach for the Design of Doped LLZO Ceramic Garnets for Battery Applications. Integrating Materials and Manufacturing Innovation, 2021, 10, 299-310.	1.2	13
123	Onset of fragment formation in periodic expanding systems. Physical Review B, 1996, 54, 236-243.	1.1	12
124	Role of atomic variability in dielectric charging: A first-principles-based multiscale modeling study. Physical Review B, 2013, 88, .	1.1	12
125	Nonequilibrium Reaction Kinetics in Molecular Solids. Journal of Physical Chemistry C, 2016, 120, 542-552.	1.5	12
126	Accurate calculations of the Peierls stress in small periodic cells. Journal of Computer-Aided Materials Design, 2001, 8, 161-172.	0.7	11

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127	Thermal conduction in molecular materials using coarse grain dynamics: Role of mass diffusion and quantum corrections for molecular dynamics simulations. Journal of Chemical Physics, 2009, 131, 234113.	1.2	11
128	Molecular dynamics study of dynamical contact between a nanoscale tip and substrate for atomic force microscopy experiments. Journal of Applied Physics, 2012, 112, .	1.1	11
129	Harnessing mechanical instabilities at the nanoscale to achieve ultra-low stiffness metals. Nature Communications, 2017, 8, 1137.	5.8	11
130	Reactive Force Fields Based on Quantum Mechanics for Applications to Materials at Extreme Conditions. AIP Conference Proceedings, 2006, , .	0.3	10
131	Heteroepitaxial integration of metallic nanowires: transition from coherent to defective interfaces via molecular dynamics. Nanotechnology, 2007, 18, 345705.	1.3	10
132	Functional derivatives for uncertainty quantification and error estimation and reduction via optimal high-fidelity simulations. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 065009.	0.8	10
133	Micro-RVE modeling of mechanistic response in porous intermetallics subject to weak and moderate impact loading. International Journal of Plasticity, 2013, 51, 1-32.	4.1	10
134	Multiscale contact mechanics model for RFâ€“MEMS switches with quantified uncertainties. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 085002.	0.8	10
135	Engineering Curvature in Graphene Ribbons Using Ultrathin Polymer Films. Nano Letters, 2014, 14, 7085-7089.	4.5	10
136	Complex martensitic nanostructure in Zr nanowires: A molecular dynamics study. Physical Review B, 2010, 81, .	1.1	9
137	Limit for thermal transport reduction in Si nanowires with nanoengineered corrugations. Applied Physics Letters, 2013, 103, .	1.5	9
138	Uncertainty Quantification in Materials Modeling. Jom, 2014, 66, 1342-1344.	0.9	9
139	Coarse-grained molecular dynamics modeling of reaction-induced phase separation. Polymer, 2018, 149, 30-38.	1.8	9
140	Effects of an atomistic modeling approach on predicted mechanical properties of glassy polymers via molecular dynamics. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 025006.	0.8	9
141	Molecular Dynamics Characterization of the Response of Ni/Al Nanolaminates Under Dynamic Loading. Journal of Propulsion and Power, 2007, 23, 693-697.	1.3	8
142	The dynamics of copper intercalated molybdenum ditelluride. Journal of Chemical Physics, 2016, 145, 194702.	1.2	8
143	Complexion dictated thermal resistance with interface density in reactive metal multilayers. Physical Review B, 2020, 101, .	1.1	8
144	Structural and electronic properties of copper-doped chalcogenide glasses. Physical Review Materials, 2017, 1, .	0.9	8

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145	Uncovering the role of nanoscale precipitates on martensitic transformation and superelasticity. Acta Materialia, 2022, 229, 117790.	3.8	8
146	Active learning and molecular dynamics simulations to find high melting temperature alloys. Computational Materials Science, 2022, 209, 111386.	1.4	8
147	Systematic Builder for Allâ€Atom Simulations of Plastically Bonded Explosives. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	8
148	Kinks in the a/2ã€ˆ111ã€‰ screw dislocation in Ta. Journal of Computer-Aided Materials Design, 2001, 8, 117-125.	0.7	7
149	Mechanical response of nanocrystalline platinum via molecular dynamics: size effects in bulk versus thin-film samples. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 065012.	0.8	7
150	The use of strain to tailor electronic thermoelectric transport properties: A first principles study of 2H-phase CuAlO₂. Journal of Applied Physics, 2019, 125, 082531.	1.1	7
151	Mechanically induced amorphization of small molecule organic crystals. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 074005.	0.8	7
152	The nucleonic thermal conductivity of â€œpastasâ€•in neutron star matter. Nuclear Physics A, 2020, 1002, 122004.	0.6	7
153	Hybrid Polymer-Garnet Materials for All-Solid-State Energy Storage Devices. ACS Omega, 2021, 6, 15551-15558.	1.6	7
154	Interactions between copper and transition metal dichalcogenides: A density functional theory study. Physical Review Materials, 2017, 1, .	0.9	7
155	Crack propagation in a Tantalum nano-slab. Journal of Computer-Aided Materials Design, 2001, 8, 151-159.	0.7	6
156	Molecular dynamics characterization of the contact between clean metallic surfaces with nanoscale asperities. Physical Review B, 2011, 83, .	1.1	6
157	Tunability of martensitic behavior through coherent nanoprecipitates and other nanostructures. Acta Materialia, 2018, 154, 295-302.	3.8	6
158	Role of surface orientation on atomic layer deposited Al2O3/GaAs interface structure and Fermi level pinning: A density functional theory study. Applied Physics Letters, 2011, 99, 093508.	1.5	5
159	Phonon thermal transport outside of local equilibrium in nanowires via molecular dynamics. Journal of Chemical Physics, 2013, 138, 124704.	1.2	5
160	Prediction of low energy phase transition in metal doped MoTe2 from first principle calculations. Journal of Applied Physics, 2019, 125, .	1.1	5
161	Tuning martensitic transformations via coherent second phases in nanolaminates using free energy landscape engineering. Journal of Applied Physics, 2020, 127, .	1.1	5
162	Expanding Materials Selection Via Transfer Learning for High-Temperature Oxide Selection. Jom, 2021, 73, 103-115.	0.9	5

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163	Shock-induced hotspot formation in amorphous and crystalline 1,3,5,7-tetranitro-1,3,5,7-tetrazoctane (HMX): A molecular dynamics comparative study. Journal of Applied Physics, 2021, 130, .	1.1	5
164	Strain engineering via amorphization and recrystallization in Si/Ge heterostructures. Physical Review B, 2011, 84, .	1.1	4
165	Size-dependent hardness of nanoscale metallic contacts from molecular dynamics simulations. Physical Review B, 2012, 86, .	1.1	4
166	Molecular dynamics simulations of PMMA slabs: role of annealing conditions. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 065010.	0.8	4
167	Enhanced Learning of Mechanical Behavior of Materials via Combined Experiments and nanoHUB Simulations: Learning Modules for Sophomore MSE Students. Materials Research Society Symposia Proceedings, 2015, 1762, 31.	0.1	4
168	Shock-Induced Chemistry: Molecular Dynamics and Coarse Grain Modeling. Challenges and Advances in Computational Chemistry and Physics, 2019, , 187-208.	0.6	4
169	Universality in Spatio-Temporal High-Mobility Domains Across the Glass Transition from Bulk Polymers to Single Chains. Macromolecules, 2020, 53, 9375-9385.	2.2	4
170	Novel Mode of Noncrystallographic Branching in the Initial Stages of Polymer Fibril Growth. Physical Review Letters, 2020, 125, 247801.	2.9	4
171	Uncharacteristic second order martensitic transformation in metals via epitaxial stress fields. Journal of Applied Physics, 2020, 127, 045107.	1.1	4
172	Modeling environment-dependent atomic-level properties in complex-concentrated alloys. Journal of Chemical Physics, 2022, 156, 114102.	1.2	4
173	Sim2Ls: FAIR simulation workflows and data. PLoS ONE, 2022, 17, e0264492.	1.1	4
174	Role of direct electron-phonon coupling across metal-semiconductor interfaces in thermal transport via molecular dynamics. Journal of Chemical Physics, 2015, 143, 034703.	1.2	3
175	Phonon thermal transport in encapsulated copper hybrids. Journal of Applied Physics, 2019, 125, 045106.	1.1	3
176	Functional uncertainty quantification for isobaric molecular dynamics simulations and defect formation energies. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 044002.	0.8	3
177	Deviatoric stress driven transient melting below the glass transition temperature in shocked polymers. Journal of Applied Physics, 2022, 132, .	1.1	3
178	Statistical thermodynamics of cluster phase transitions. Physica A: Statistical Mechanics and Its Applications, 1998, 257, 526-529.	1.2	2
179	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. Materials Research Society Symposia Proceedings, 2000, 644, 231.	0.1	2
180	Non-Equilibrium Molecular Dynamics Studies of Shock and Detonation Processes in Energetic Materials. , 2005, , 269-296.		2

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181	Effect of surface roughness and size of beam on squeeze-film dampingâ€"Molecular dynamics simulation study. Journal of Applied Physics, 2015, 118, 204304.	1.1	2
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