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	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
2	Modeling environment-dependent atomic-level properties in complex-concentrated alloys. Journal of Chemical Physics, 2022, 156, 114102.	1.2	4
3	Sim2Ls: FAIR simulation workflows and data. PLoS ONE, 2022, 17, e0264492.	1.1	4
4	Uncovering the role of nanoscale precipitates on martensitic transformation and superelasticity. Acta Materialia, 2022, 229, 117790.	3.8	8
5	Active learning and molecular dynamics simulations to find high melting temperature alloys. Computational Materials Science, 2022, 209, 111386.	1.4	8
6	Systematic Builder for Allâ€Atom Simulations of Plastically Bonded Explosives. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	8
7	Deviatoric stress driven transient melting below the glass transition temperature in shocked polymers. Journal of Applied Physics, 2022, 132, .	1.1	3
8	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
9	Expanding Materials Selection Via Transfer Learning for High-Temperature Oxide Selection. Jom, 2021, 73, 103-115.	0.9	5
10	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
11	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
12	Role of strain and composition on the piezoelectric and dielectric response of AlxGa1âˆ’xN: Implications for power electronics device reliability. Journal of Applied Physics, 2021, 129, 075701.	1.1	1
13	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
14	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
15	Computational study of first-row transition metals in monodoped 4H-SiC. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 055008.	0.8	2
16	Multiferroic ground states in free standing perovskite-based nanodots: a density functional theory study. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 055002.	0.8	1
17	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
18	Hybrid Polymer-Garnet Materials for All-Solid-State Energy Storage Devices. ACS Omega, 2021, 6, 15551-15558.	1.6	7

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19	Parsimonious neural networks learn interpretable physical laws. Scientific Reports, 2021, 11, 12761.	1.6	14
20	Chemistry Under Shock Conditions. Annual Review of Materials Research, 2021, 51, 101-130.	4.3	25
21	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
22	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
23	Fourier-like Thermal Relaxation of Nanoscale Explosive Hot Spots. Journal of Physical Chemistry C, 2021, 125, 20570-20582.	1.5	18
24	Automated approach to discover coherent precipitates in multi-component shape memory alloys. Computational Materials Science, 2021, 197, 110651.	1.4	1
25	Neural network reactive force field for C, H, N, and O systems. Npj Computational Materials, 2021, 7, .	3.5	39
26	Martensitic transformation in superlattices of two non-transforming metals. Journal of Applied Physics, 2021, 130, 165105.	1.1	1
27	Complexion dictated thermal resistance with interface density in reactive metal multilayers. Physical Review B, 2020, 101, .	1.1	8
28	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
29	The nucleonic thermal conductivity of â€œpastasâ€•in neutron star matter. Nuclear Physics A, 2020, 1002, 122004.	0.6	7
30	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
31	Opportunities and challenges of 2D materials in back-end-of-line interconnect scaling. Journal of Applied Physics, 2020, 128, .	1.1	36
32	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
33	Novel Mode of Noncrystallographic Branching in the Initial Stages of Polymer Fibril Growth. Physical Review Letters, 2020, 125, 247801.	2.9	4
34	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
35	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
36	Roadmap on multiscale materials modeling. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 043001.	0.8	100

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37	Tuning martensitic transformations via coherent second phases in nanolaminates using free energy landscape engineering. Journal of Applied Physics, 2020, 127, .	1.1	5
38	Tunability of martensitic transformation in Mg-Sc shape memory alloys: A DFT study. Acta Materialia, 2020, 189, 1-9.	3.8	14
39	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
40	Uncharacteristic second order martensitic transformation in metals via epitaxial stress fields. Journal of Applied Physics, 2020, 127, 045107.	1.1	4
41	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
42	Online simulation powered learning modules for materials science. MRS Advances, 2019, 4, 2727-2742.	0.5	1
43	Preface for focus issue on uncertainty quantification in materials modeling. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 080301.	0.8	1
44	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
45	Phonon thermal transport in encapsulated copper hybrids. Journal of Applied Physics, 2019, 125, 045106.	1.1	3
46	Mechanically induced amorphization of small molecule organic crystals. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 074005.	0.8	7
47	Prediction of low energy phase transition in metal doped MoTe2 from first principle calculations. Journal of Applied Physics, 2019, 125, .	1.1	5
48	Online Tools for Uncertainty Quantification in nanoHUB. Jom, 2019, 71, 2635-2645.	0.9	1
49	Investigation of structural ordering in network forming ionic liquids: A molecular dynamics study. Journal of Chemical Physics, 2019, 150, 144904.	1.2	0
50	Prediction of PEKK properties related to crystallization by molecular dynamics simulations with a united-atom model. Polymer, 2019, 174, 25-32.	1.8	23
51	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
52	Shock-Induced Chemistry: Molecular Dynamics and Coarse Grain Modeling. Challenges and Advances in Computational Chemistry and Physics, 2019, , 187-208.	0.6	4
53	Reactive Molecular Dynamics Simulations to Investigate the Shock Response of Liquid Nitromethane. Journal of Physical Chemistry C, 2019, 123, 2613-2626.	1.5	31
54	Cohesive energy density and solubility parameter evolution during the curing of thermoset. Polymer, 2018, 135, 162-170.	1.8	50

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55	Using Ions to Control Transport in Two-Dimensional Materials for Ion-Controlled Electronics. , 2018, , .		0
56	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
57	Role of Molecular Disorder on the Reactivity of RDX. Journal of Physical Chemistry C, 2018, 122, 27032-27043.	1.5	27
58	Crystalline and pseudo-crystalline phases of polyacrylonitrile from molecular dynamics: Implications for carbon fiber precursors. Polymer, 2018, 155, 13-26.	1.8	17
59	Tunability of martensitic behavior through coherent nanoprecipitates and other nanostructures. Acta Materialia, 2018, 154, 295-302.	3.8	6
60	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
61	Coarse-grained molecular dynamics modeling of reaction-induced phase separation. Polymer, 2018, 149, 30-38.	1.8	9
62	Role of electronic thermal transport in amorphous metal recrystallization: A molecular dynamics study. Journal of Chemical Physics, 2018, 149, 064502.	1.2	2
63	Error correction in multi-fidelity molecular dynamics simulations using functional uncertainty quantification. Journal of Computational Physics, 2017, 334, 207-220.	1.9	23
64	First-principles study of elastic mechanical responses to applied deformation of metal-organic frameworks. Journal of Chemical Physics, 2017, 146, .	1.2	17
65	Modeling resistive switching materials and devices across scales. Journal of Electroceramics, 2017, 39, 39-60.	0.8	19
66	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
67	Harnessing mechanical instabilities at the nanoscale to achieve ultra-low stiffness metals. Nature Communications, 2017, 8, 1137.	5.8	11
68	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
69	Novel doping alternatives for single-layer transition metal dichalcogenides. Journal of Applied Physics, 2017, 122, .	1.1	61
70	Molecular modeling of the microstructure evolution during carbon fiber processing. Journal of Chemical Physics, 2017, 147, 224705.	1.2	21
71	Interactions between copper and transition metal dichalcogenides: A density functional theory study. Physical Review Materials, 2017, 1, .	0.9	7
72	Structural and electronic properties of copper-doped chalcogenide glasses. Physical Review Materials, 2017, 1, .	0.9	8

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73	The dynamics of copper intercalated molybdenum ditelluride. Journal of Chemical Physics, 2016, 145, 194702.	1.2	8
74	Role of energy distribution in contacts on thermal transport in Si: A molecular dynamics study. Journal of Applied Physics, 2016, 120, .	1.1	17
75	Atomistic simulations of electrochemical metallization cells: mechanisms of ultra-fast resistance switching in nanoscale devices. Nanoscale, 2016, 8, 14037-14047.	2.8	22
76	Shockwave Energy Dissipation in Metalâ€“Organic Framework MOF-5. Journal of Physical Chemistry C, 2016, 120, 12463-12471.	1.5	31
77	Free volume evolution in the process of epoxy curing and its effect on mechanical properties. Polymer, 2016, 97, 456-464.	1.8	38
78	Nonequilibrium Reaction Kinetics in Molecular Solids. Journal of Physical Chemistry C, 2016, 120, 542-552.	1.5	12
79	Exothermic Self-Sustained Waves with Amorphous Nickel. Journal of Physical Chemistry C, 2016, 120, 5827-5838.	1.5	23
80	Shock Loading of Granular Ni/Al Composites. Part 2: Shock-Induced Chemistry. Journal of Physical Chemistry C, 2016, 120, 6804-6813.	1.5	35
81	Separation of aleatory and epistemic uncertainty in probabilistic model validation. Reliability Engineering and System Safety, 2016, 147, 49-59.	5.1	56
82	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
83	Voltage equilibration for reactive atomistic simulations of electrochemical processes. Journal of Chemical Physics, 2015, 143, 054109.	1.2	46
84	Nanohub as a Platform for Implementing ICME Simulations in Research and Education. , 2015, , 269-276.		0
85	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
86	Mesoscale simulations of shockwave energy dissipation via chemical reactions. Journal of Chemical Physics, 2015, 142, 084108.	1.2	14
87	PUQ: A code for non-intrusive uncertainty propagation in computer simulations. Computer Physics Communications, 2015, 194, 97-107.	3.0	27
88	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
89	Molecular dynamics simulations of the reaction mechanism in Ni/Al reactive intermetallics. Acta Materialia, 2015, 96, 1-9.	3.8	33
90	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

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91	Model form uncertainty versus intrinsic atomic variability in amorphous silicon oxides and nitrides. Computational Materials Science, 2015, 109, 124-128.	1.4	1
92	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
93	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
94	Atomic origin of ultrafast resistance switching in nanoscale electrometallization cells. Nature Materials, 2015, 14, 440-446.	13.3	172
95	nanoHUB.org: A Gateway to Undergraduate Simulation-Based Research in Materials Science and Related Fields. Materials Research Society Symposia Proceedings, 2015, 1762, 7.	0.1	0
96	Optimal Ge/SiGe nanofin geometries for hole mobility enhancement: Technology limit from atomic simulations. Journal of Applied Physics, 2015, 117, .	1.1	1
97	Stability and migration of small copper clusters in amorphous dielectrics. Journal of Applied Physics, 2015, 117, .	1.1	24
98	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
99	Mechanisms of Plastic Deformation of Metalâ€“Organic Framework-5. Journal of Physical Chemistry C, 2015, 119, 25845-25852.	1.5	36
100	Molecular scale simulations on thermoset polymers: A review. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 103-122.	2.4	179
101	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
102	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
103	Mesodynamics with implicit degrees of freedom. Journal of Chemical Physics, 2014, 141, 064107.	1.2	18
104	Material property prediction of thermoset polymers by molecular dynamics simulations. Acta Mechanica, 2014, 225, 1187-1196.	1.1	58
105	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
106	Engineering Curvature in Graphene Ribbons Using Ultrathin Polymer Films. Nano Letters, 2014, 14, 7085-7089.	4.5	10
107	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
108	Shock Loading of Granular Ni/Al Composites. Part 1: Mechanics of Loading. Journal of Physical Chemistry C, 2014, 118, 26377-26386.	1.5	47

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109	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
110	Uncertainty Quantification in Materials Modeling. Jom, 2014, 66, 1342-1344.	0.9	9
111	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
112	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
113	Phonon thermal transport outside of local equilibrium in nanowires via molecular dynamics. Journal of Chemical Physics, 2013, 138, 124704.	1.2	5
114	Thermal transport in SiGe superlattice thin films and nanowires: Effects of specimen and periodic lengths. Physical Review B, 2013, 87, .	1.1	47
115	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
116	Role of atomic variability in dielectric charging: A first-principles-based multiscale modeling study. Physical Review B, 2013, 88, .	1.1	12
117	Molecular dynamics simulations of PMMA slabs: role of annealing conditions. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 065010.	0.8	4
118	Molecular dynamics simulations on cyclic deformation of an epoxy thermoset. Polymer, 2013, 54, 881-890.	1.8	30
119	Multiphysics Simulation of RF-MEMS With Quantified Uncertainties. , 2013, , .		0
120	Limit for thermal transport reduction in Si nanowires with nanoengineered corrugations. Applied Physics Letters, 2013, 103, .	1.5	9
121	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
122	nanoHUB-U: A science gateway ventures into structured online education. , 2013, , .		1
123	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
124	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
125	Amorphous Ni/Al nanoscale laminates as high-energy intermolecular reactive composites. Physical Review B, 2012, 85, .	1.1	16
126	Energy-based yield criterion for PMMA from large-scale molecular dynamics simulations. Physical Review B, 2012, 85, .	1.1	38

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127	Role of nanostructure on reaction and transport in Ni/Al intermolecular reactive composites. Physical Review B, 2012, 86, .	1.1	33
128	Size-dependent hardness of nanoscale metallic contacts from molecular dynamics simulations. Physical Review B, 2012, 86, .	1.1	4
129	Estimating the In-Plane Young's Modulus of Polycrystalline Films in MEMS. Journal of Microelectromechanical Systems, 2012, 21, 840-849.	1.7	19
130	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
131	Tailored Reactivity of Ni+Al Nanocomposites: Microstructural Correlations. Journal of Physical Chemistry C, 2012, 116, 21027-21038.	1.5	97
132	Atomistic simulations on multilayer graphene reinforced epoxy composites. Composites Part A: Applied Science and Manufacturing, 2012, 43, 1293-1300.	3.8	116
133	Molecular dynamics simulations and experimental studies of the thermomechanical response of an epoxy thermoset polymer. Polymer, 2012, 53, 4222-4230.	1.8	131
134	Size effects in NiTi from density functional theory calculations. Physical Review B, 2012, 85, .	1.1	22
135	Defect level distributions and atomic relaxations induced by charge trapping in amorphous silica. Applied Physics Letters, 2012, 100, .	1.5	30
136	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
137	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
138	Effect of Thickness on the Thermo-Mechanical Response of Free-Standing Thermoset Nanofilms from Molecular Dynamics. Macromolecules, 2011, 44, 9448-9454.	2.2	36
139	Uncertainty propagation in a multiscale model of nanocrystalline plasticity. Reliability Engineering and System Safety, 2011, 96, 1161-1170.	5.1	39
140	Molecular dynamics predictions of thermal and mechanical properties of thermoset polymer EPON862/DETDA. Polymer, 2011, 52, 2920-2928.	1.8	244
141	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
142	Strain engineering via amorphization and recrystallization in Si/Ge heterostructures. Physical Review B, 2011, 84, .	1.1	4
143	Effect of core energy on mobility in a continuum dislocation model. Physical Review B, 2011, 83, .	1.1	30
144	Molecular dynamics characterization of the contact between clean metallic surfaces with nanoscale asperities. Physical Review B, 2011, 83, .	1.1	6

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145	Cyber-Enabled Simulations in Nanoscale Science and Engineering. Computing in Science and Engineering, 2010, 12, 12-17.	1.2	30
146	Molecular Dynamics Simulations of Strain Engineering and Thermal Transport in Nanostructured Materials. Computing in Science and Engineering, 2010, 12, 36-42.	1.2	0
147	Molecular simulations of crosslinking process of thermosetting polymers. Polymer, 2010, 51, 6058-6070.	1.8	222
148	Phase stability and transformations in NiTi from density functional theory calculations. Acta Materialia, 2010, 58, 745-752.	3.8	53
149	Nanoscale Metal-Metal Contact Physics from Molecular Dynamics: The Strongest Contact Size. Physical Review Letters, 2010, 104, 215504.	2.9	14
150	Complex martensitic nanostructure in Zr nanowires: A molecular dynamics study. Physical Review B, 2010, 81, .	1.1	9
151	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
152	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
153	Strain relaxation in Si/Ge/Si nanoscale bars from molecular dynamics simulations. Journal of Applied Physics, 2009, 106, 034304.	1.1	15
154	Structures and energetics of silicon nanotubes from molecular dynamics and density functional theory. Physical Review B, 2008, 78, .	1.1	32
155	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
156	Reply to â€œComment on â€˜Melting dynamics of superheated argon: Nucleation and growthâ€™â€•[J. Chem. Phys. 126, 034505 (2007)]. Journal of Chemical Physics, 2007, 126, 187102.	1.2	0
157	Heteroepitaxial integration of metallic nanowires: transition from coherent to defective interfaces via molecular dynamics. Nanotechnology, 2007, 18, 345705.	1.3	10
158	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>â^•</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
159	Phonon thermal conductivity in nanolaminated composite metals via molecular dynamics. Journal of Chemical Physics, 2007, 127, 184702.	1.2	45
160	Melting dynamics of superheated argon: Nucleation and growth. Journal of Chemical Physics, 2007, 126, 034505.	1.2	21
161	Atomic-level view of inelastic deformation in a shock loaded molecular crystal. Physical Review B, 2007, 76, .	1.1	88
162	Molecular dynamics simulation of dynamical response of perfect and porousNiâ^•Alnanolaminates under shock loading. Physical Review B, 2007, 76, .	1.1	39

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163	Molecular Dynamics Simulation of Ultrafast Laser Ablation of Fused Silica. , 2006, , 517.		0
164	Reactive Force Fields Based on Quantum Mechanics for Applications to Materials at Extreme Conditions. AIP Conference Proceedings, 2006, , .	0.3	10
165	Molecular Dynamics Simulations of Shock-Induced Chemical, Mechanical, and Thermal Processes in Ni/Al Nanolaminates. AIP Conference Proceedings, 2006, , .	0.3	1
166	Atomistic simulations of shock-induced alloying reactions in Niâˆ•Al nanolaminates. Journal of Chemical Physics, 2006, 125, 164707.	1.2	83
167	Interplay of Shock-induced Melting and Alloying in Nanostructured Multilayer Films. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	1
168	Non-Equilibrium Molecular Dynamics Studies of Shock and Detonation Processes in Energetic Materials. , 2005, , 269-296.		2
169	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
170	Large electrostrictive strain at gigahertz frequencies in a polymer nanoactuator: Computational device design. Applied Physics Letters, 2005, 86, 083103.	1.5	14
171	Energy Exchange between Mesoparticles and Their Internal Degrees of Freedom. Physical Review Letters, 2005, 94, 014301.	2.9	55
172	Vibrational density of states and Lindemann melting law. Journal of Chemical Physics, 2005, 122, 194709.	1.2	52
173	Thermal decomposition of RDX from reactive molecular dynamics. Journal of Chemical Physics, 2005, 122, 054502.	1.2	366
174	First principles force field for metallic tantalum. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S445-S459.	0.8	34
175	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
176	Normal modes and frequencies from covariances in molecular dynamics or Monte Carlo simulations. Journal of Chemical Physics, 2004, 120, 1-4.	1.2	73
177	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
178	Nonequilibrium melting and crystallization of a model Lennard-Jones system. Journal of Chemical Physics, 2004, 120, 11640-11649.	1.2	163
179	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
180	Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX. Physical Review Letters, 2003, 91, 098301.	2.9	495

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