Aiichiro Nakano

List of Publications by Year
in descending order

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261	7,665	43973	71532
papers	citations	48 h-index	76 g-index

266	266	266	7137
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring far-from-equilibrium ultrafast polarization control in ferroelectric oxides with excited-state neural network quantum molecular dynamics. Science Advances, 2022, 8, eabk2625.	4.7	8
2	Carrier-specific dynamics in 2H-MoTe2 observed by femtosecond soft x-ray absorption spectroscopy using an x-ray free-electron laser. Structural Dynamics, 2021, 8, 014501.	0.9	14
3	EZFF: Python library for multi-objective parameterization and uncertainty quantification of interatomic forcefields for molecular dynamics. SoftwareX, 2021, 13, 100663.	1.2	6
4	Sulfurization of MoO₃ in the Chemical Vapor Deposition Synthesis of MoS₂ Enhanced by an H₂S/H₂ Mixture. Journal of Physical Chemistry Letters, 2021, 12, 1997-2003.	2.1	13
5	Mechanical behavior of ultralight nickel metamaterial. Applied Physics Letters, 2021, 118, .	1.5	2
6	Molecular Dynamics Simulations of Dielectric Breakdown of Lunar Regolith: Implications for Water Ice Formation on Lunar Surface. Geophysical Research Letters, 2021, 48, e2020GL091681.	1.5	7
7	Unveiling oxidation mechanism of bulk ZrS2. MRS Advances, 2021, 6, 303-306.	0.5	3
8	Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations. Journal of Chemical Information and Modeling, 2021, 61, 2175-2186.	2.5	28
9	Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics. Physical Review Letters, 2021, 126, 216403.	2.9	16
10	Neural Network Quantum Molecular Dynamics, Intermediate Range Order in GeSe₂, and Neutron Scattering Experiments. Journal of Physical Chemistry Letters, 2021, 12, 6020-6028.	2.1	2
11	Ex-NNQMD: Extreme-Scale Neural Network Quantum Molecular Dynamics. , 2021, , .		1
12	PND: Physics-informed neural-network software for molecular dynamics applications. SoftwareX, 2021, 15, 100789.	1.2	6
13	Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials. Npj Computational Materials, 2021, 7, .	3.5	14
14	Autonomous reinforcement learning agent for stretchable kirigami design of 2D materials. Npj Computational Materials, 2021, 7, .	3.5	13
15	Graph signal recovery using restricted Boltzmann machines. Expert Systems With Applications, 2021, 185, 115635.	4.4	4
16	Lattice thermal transport in two-dimensional alloys and fractal heterostructures. Scientific Reports, 2021, 11, 1656.	1.6	8
17	Domain-specific compilers for dynamic simulations of quantum materials on quantum computers. Quantum Science and Technology, 2021, 6, 014007.	2.6	5
18	Review of strategies toward the development of alloy two-dimensional (2D) transition metal dichalcogenides. IScience, 2021, 24, 103532.	1.9	11

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19	Deep Well Trapping of Hot Carriers in a Hexagonal Boron Nitride Coating of Polymer Dielectrics. ACS Applied Materials & Interfaces, 2021, 13, 60393-60400.	4.0	5
20	Dielectric Polymer Genome: Integrating Valence-Aware Polarizable Reactive Force Fields and Machine Learning. Transactions on Computational Science and Computational Intelligence, 2021, , 51-64.	0.3	2
21	sDMD: An open source program for discontinuous molecular dynamics simulation of protein folding and aggregation. Computer Physics Communications, 2020, 247, 106873.	3.0	6
22	Field-Induced Carrier Localization Transition in Dielectric Polymers. Journal of Physical Chemistry Letters, 2020, 11, 352-358.	2.1	6
23	Tellurene Photodetector with High Gain and Wide Bandwidth. ACS Nano, 2020, 14, 303-310.	7.3	101
24	Boltzmann machine modeling of layered MoS2 synthesis on a quantum annealer. Computational Materials Science, 2020, 173, 109429.	1.4	10
25	Neural Network Molecular Dynamics at Scale. , 2020, , .		2
26	Differences in Sb2Te3 growth by pulsed laser and sputter deposition. Acta Materialia, 2020, 200, 811-820.	3.8	10
27	Photoexcitation Induced Ultrafast Nonthermal Amorphization in Sb₂Te₃. Journal of Physical Chemistry Letters, 2020, 11, 10242-10249.	2.1	12
28	Growth Kinetics and Atomistic Mechanisms of Native Oxidation of ZrS_xSe_{2â€“x} and MoS₂ Crystals. Nano Letters, 2020, 20, 8592-8599.	4.5	16
29	Simultaneous Observation of Carrier-Specific Redistribution and Coherent Lattice Dynamics in 2H-MoTe₂ with Femtosecond Core-Level Spectroscopy. ACS Nano, 2020, 14, 15829-15840.	7.3	38
30	Optically Induced Three-Stage Picosecond Amorphization in Low-Temperature SrTiO₃. Journal of Physical Chemistry Letters, 2020, 11, 9605-9612.	2.1	4
31	Reactive molecular dynamics simulations and machine learning. Journal of Physics: Conference Series, 2020, 1461, 012182.	0.3	4
32	Towards simulation of the dynamics of materials on quantum computers. Physical Review B, 2020, 101, .	1.1	23
33	Memristive Device Characteristics Engineering by Controlling the Crystallinity of Switching Layer Materials. ACS Applied Electronic Materials, 2020, 2, 1529-1537.	2.0	7
34	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. Langmuir, 2020, 36, 7658-7668.	1.6	26
35	Evolutionary multi-objective optimization and Pareto-frontal uncertainty quantification of interatomic forcefields for thermal conductivity simulations. Computer Physics Communications, 2020, 254, 107337.	3.0	9
36	Enhancing combustion performance of nano-Al/PVDF composites with Î²-PVDF. Combustion and Flame, 2020, 219, 467-477.	2.8	55

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37	Direct Atomic Simulations of Facet Formation and Equilibrium Shapes of SiC Nanoparticles. Crystal Growth and Design, 2020, 20, 2147-2152.	1.4	7
38	Synergistically Chemical and Thermal Coupling between Graphene Oxide and Graphene Fluoride for Enhancing Aluminum Combustion. ACS Applied Materials & Interfaces, 2020, 12, 7451-7458.	4.0	52
39	RXMD: A scalable reactive molecular dynamics simulator for optimized time-to-solution. SoftwareX, 2020, 11, 100389.	1.2	15
40	Application of First-Principles-Based Artificial Neural Network Potentials to Multiscale-Shock Dynamics Simulations on Solid Materials. Journal of Physical Chemistry Letters, 2020, 11, 4536-4541.	2.1	12
41	Quantum Dynamics at Scale. , 2020, , .		1
42	Fast deformation of shocked quartz and implications for planar deformation features observed in shocked quartz. AIP Conference Proceedings, 2020, , .	0.3	0
43	Structural phase transitions in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">MoWSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> monolayer: Molecular dynamics simulations and variational autoencoder analysis. Physical Review B, 2019, 100, .	1.1	10
44	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. SoftwareX, 2019, 10, 100307.	1.2	32
45	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. Nano Letters, 2019, 19, 6078-6086.	4.5	43
46	Two-Dimensional Lateral Epitaxy of 2H (MoSe₂)â€“1Tâ€² (ReSe₂) Phases. Nano Letters, 2019, 19, 6338-6345.	4.5	30
47	Optical Control of Non-Equilibrium Phonon Dynamics. Nano Letters, 2019, 19, 4981-4989.	4.5	27
48	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. Journal of Physical Chemistry Letters, 2019, 10, 3937-3943.	2.1	8
49	Hydrogen Bond Preserving Stress Release Mechanism Is Key to the Resilience of Aramid Fibers. Journal of Physical Chemistry B, 2019, 123, 9719-9723.	1.2	6
50	Guidelines for creating artificial neural network empirical interatomic potential from first-principles molecular dynamics data under specific conditions and its application to Î±-Ag2Se. Journal of Chemical Physics, 2019, 151, 124303.	1.2	19
51	Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality. SoftwareX, 2019, 9, 112-116.	1.2	11
52	Effects of chemical defects on anisotropic dielectric response of polyethylene. AIP Advances, 2019, 9, .	0.6	9
53	Nanoindentation on Monolayer MoS₂ Kirigami. ACS Omega, 2019, 4, 9952-9956.	1.6	8
54	Defect Healing in Layered Materials: A Machine Learning-Assisted Characterization of MoS₂ Crystal Phases. Journal of Physical Chemistry Letters, 2019, 10, 2739-2744.	2.1	19

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55	Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering. Nature Photonics, 2019, 13, 425-430.	15.6	28
56	Adaptive Kinetic Architecture and Collective Behavior: A Dynamic Analysis for Emergency Evacuation. Buildings, 2019, 9, 44.	1.4	4
57	Thermal conductivity of MoS2 monolayers from molecular dynamics simulations. AIP Advances, 2019, 9, .	0.6	22
58	Rapid and reversible lithiation of doped biogenous iron oxide nanoparticles. Scientific Reports, 2019, 9, 1828.	1.6	4
59	Electrostrictive Cavitation in Water Induced by a SnO₂ Nanoparticle. ACS Omega, 2019, 4, 22274-22279.	1.6	3
60	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, .	1.1	10
61	Neural Network Analysis of Dynamic Fracture in a Layered Material. MRS Advances, 2019, 4, 1109-1117.	0.5	4
62	Ab initio molecular dynamics study of prebiotic production processes of organic compounds at meteorite impacts on ocean. Journal of Computational Chemistry, 2019, 40, 349-359.	1.5	5
63	Polytypism in ultrathin tellurium. 2D Materials, 2019, 6, 015013.	2.0	68
64	Shift/collapse on neighbor list (SC-NBL): Fast evaluation of dynamic many-body potentials in molecular dynamics simulations. Computer Physics Communications, 2019, 235, 88-94.	3.0	4
65	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. Computing in Science and Engineering, 2019, 21, 64-75.	1.2	5
66	Structural Phase Transformation in Strained Monolayer MoWSe₂ Alloy. ACS Nano, 2018, 12, 3468-3476.	7.3	57
67	Chemical Vapor Deposition Synthesis of MoS₂ Layers from the Direct Sulfidation of MoO₃ Surfaces Using Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 7494-7503.	1.5	41
68	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. Journal of Applied Physics, 2018, 123, .	1.1	24
69	Acceleration of Dynamic n-Tuple Computations in Many-Body Molecular Dynamics. , 2018, , .		0
70	A Reactive Molecular Dynamics Study of Atomistic Mechanisms During Synthesis of MoS2 Layers by Chemical Vapor Deposition. MRS Advances, 2018, 3, 307-311.	0.5	3
71	Semiconductorâ€“metal structural phase transformation in MoTe₂ monolayers by electronic excitation. Nanoscale, 2018, 10, 2742-2747.	2.8	34
72	Photo-induced Contraction of Layered Materials. MRS Advances, 2018, 3, 333-338.	0.5	0

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73	Plane shock loading on mono- and nano-crystalline silicon carbide. Applied Physics Letters, 2018, 112, .	1.5	22
74	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.5	5
75	Shift-Collapse Acceleration of Generalized Polarizable Reactive Molecular Dynamics for Machine Learning-Assisted Computational Synthesis of Layered Materials. , 2018, , .		6
76	Molecular Simulation of MoS2 Exfoliation. Scientific Reports, 2018, 8, 16761.	1.6	19
77	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	3.5	107
78	Photo-induced lattice contraction in layered materials. Journal of Physics Condensed Matter, 2018, 30, 32LT02.	0.7	4
79	Role of H Transfer in the Gas-Phase Sulfidation Process of MoO₃: A Quantum Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2018, 9, 6517-6523.	2.1	10
80	Free energy of hydration and heat capacity of calcium dipicolinate inBacillusspore cores. Applied Physics Letters, 2018, 113, 113702.	1.5	1
81	Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites. ACS Nano, 2018, 12, 11366-11375.	7.3	99
82	Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. Chemistry of Materials, 2018, 30, 7262-7268.	3.2	37
83	Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals. Applied Physics Letters, 2018, 112, .	1.5	8
84	Multiobjective genetic training and uncertainty quantification of reactive force fields. Npj Computational Materials, 2018, 4, .	3.5	25
85	Faceting, Grain Growth, and Crack Healing in Alumina. ACS Nano, 2018, 12, 9005-9010.	7.3	13
86	Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in MoSe₂ Monolayer. Nano Letters, 2018, 18, 4653-4658.	4.5	16
87	Multistage reaction pathways in detonating RDX. AIP Conference Proceedings, 2017, , .	0.3	4
88	Picosecond amorphization of SiO ₂ stishovite under tension. Science Advances, 2017, 3, e1602339.	4.7	17
89	Directional melting of alumina via polarized microwave heating. Applied Physics Letters, 2017, 110, .	1.5	2
90	Re Doping in 2D Transition Metal Dichalcogenides as a New Route to Tailor Structural Phases and Induced Magnetism. Advanced Materials, 2017, 29, 1703754.	11.1	191

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91	Multiple Reaction Pathways in Shocked 2,4,6-Triamino-1,3,5-trinitrobenzene Crystal. Journal of Physical Chemistry C, 2017, 121, 16029-16034.	1.5	19
92	Reactivity of Sulfur Molecules on MoO₃ (010) Surface. Journal of Physical Chemistry Letters, 2017, 8, 6206-6210.	2.1	9
93	Gel phase in hydrated calcium dipicolinate. Applied Physics Letters, 2017, 111, .	1.5	4
94	Ultrafast non-radiative dynamics of atomically thin MoSe2. Nature Communications, 2017, 8, 1745.	5.8	52
95	2D Materials: Re Doping in 2D Transition Metal Dichalcogenides as a New Route to Tailor Structural Phases and Induced Magnetism (Adv. Mater. 43/2017). Advanced Materials, 2017, 29, .	11.1	1
96	Computational Synthesis of MoS₂ Layers by Reactive Molecular Dynamics Simulations: Initial Sulfidation of MoO₃ Surfaces. Nano Letters, 2017, 17, 4866-4872.	4.5	60
97	Massively parallel inverse rendering using Multi-objective Particle Swarm Optimization. Journal of Visualization, 2017, 20, 195-204.	1.1	2
98	Analysis of killing of growing cells and dormant and germinated spores of Bacillus species by black silicon nanopillars. Scientific Reports, 2017, 7, 17768.	1.6	20
99	Order-Invariant Real Number Summation: Circumventing Accuracy Loss for Multimillion Summands on Multiple Parallel Architectures. , 2016, , .		1
100	Rotation mechanism of methylammonium molecules in organometal halide perovskite in cubic phase: An ab initio molecular dynamics study. Journal of Chemical Physics, 2016, 145, 224503.	1.2	14
101	Quantum Molecular Dynamics Validation of Nanocarbon Synthesis by High-Temperature Oxidation of Nanoparticles. MRS Advances, 2016, 1, 1811-1816.	0.5	0
102	Meteorite Impact-Induced Rapid NH3 Production on Early Earth: Ab Initio Molecular Dynamics Simulation. Scientific Reports, 2016, 6, 38953.	1.6	14
103	The nature of free-carrier transport in organometal halide perovskites. Scientific Reports, 2016, 6, 19599.	1.6	38
104	Anisotropic mechanoresponse of energetic crystallites: a quantum molecular dynamics study of nano-collision. Nanoscale, 2016, 8, 9714-9720.	2.8	2
105	Shock-Induced Decomposition of 1, 3, 5-triamino-2, 4, 6-trinitrobenzene: A Reactive-Force-Field Molecular Dynamics Study. MRS Advances, 2016, 1, 1247-1253.	0.5	3
106	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. Scientific Reports, 2016, 6, 24109.	1.6	15
107	Doping effect on photoabsorption and charge-separation dynamics in light-harvesting organic molecule. AIP Advances, 2016, 6, 015305.	0.6	4
108	Crystalline anisotropy of shock-induced phenomena: Omni-directional multiscale shock technique. Applied Physics Letters, 2016, 108, .	1.5	13

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109	Decaheme Cytochrome MtrF Adsorption and Electron Transfer on Gold Surface. Journal of Physical Chemistry Letters, 2016, 7, 929-936.	2.1	19
110	Facile Five-Step Heteroepitaxial Growth of GaAs Nanowires on Silicon Substrates and the Twin Formation Mechanism. ACS Nano, 2016, 10, 2424-2435.	7.3	19
111	Reactive Molecular Dynamics Simulations, Data Analytics and Visualization. Materials Research Society Symposia Proceedings, 2015, 1756, 1.	0.1	0
112	A crossover in anisotropic nanomechanochemistry of van der Waals crystals. Applied Physics Letters, 2015, 107, .	1.5	11
113	Enhanced charge recombination due to surfaces and twin defects in GaAs nanostructures. Journal of Applied Physics, 2015, 117, 054307.	1.1	16
114	Reactive Molecular Dynamics Study of Oxidation of Aggregated Aluminum Nanoparticles. Materials Research Society Symposia Proceedings, 2015, 1758, 1.	0.1	1
115	Quantum Molecular Dynamics in the Post-Petaflops Era. Computer, 2015, 48, 33-41.	1.2	12
116	GPU-based inverse rendering with multi-objective particle swarm optimization. , 2015, , .		1
117	An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. Computer Physics Communications, 2015, 192, 91-96.	3.0	24
118	Large-Scale Computing for Molecular Dynamics Simulation. , 2015, , 765-770.		0
119	Kinetic Monte Carlo Simulations and Molecular Conductance Measurements of the Bacterial Decaheme Cytochrome MtrF. ChemElectroChem, 2014, 1, 1932-1939.	1.7	34
120	Multistage reaction pathways in detonating high explosives. Applied Physics Letters, 2014, 105, .	1.5	25
121	Twin superlattice-induced large surface recombination velocity in GaAs nanostructures. Applied Physics Letters, 2014, 105, 231602.	1.5	1
122	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand. , 2014, , .		8
123	Small interfering ribonucleic acid induces liquid-to-ripple phase transformation in a phospholipid membrane. Applied Physics Letters, 2014, 105, 113702.	1.5	5
124	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 18A529.	1.2	57
125	Universal stretched exponential relaxation in nanoconfined water. Applied Physics Letters, 2014, 105, .	1.5	17
126	Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	18

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127	Hydrogen-on-Demand Using Metallic Alloy Nanoparticles in Water. Nano Letters, 2014, 14, 4090-4096.	4.5	33
128	Divide-Conquer-Recombine. , 2014, , .		3
129	Bonding and Structure of Ceramic-Ceramic Interfaces. Physical Review Letters, 2013, 111, 066103.	2.9	16
130	Critical size for the generation of misfit dislocations and their effects on electronic properties in GaAs nanosheets on Si substrate. Journal of Applied Physics, 2013, 114, 074316.	1.1	3
131	Analysis of scalable data-privatization threading algorithms for hybrid MPI/OpenMP parallelization of molecular dynamics. Journal of Supercomputing, 2013, 66, 406-430.	2.4	15
132	Effects of twins on the electronic properties of GaAs. Applied Physics Letters, 2013, 103, 022105.	1.5	42
133	Collective oxidation behavior of aluminum nanoparticle aggregate. Applied Physics Letters, 2013, 102, 221904.	1.5	11
134	Large nonadiabatic quantum molecular dynamics simulations on parallel computers. Computer Physics Communications, 2013, 184, 1-8.	3.0	33
135	A scalable parallel algorithm for dynamic range-limited n -tuple computation in many-body molecular dynamics simulation. , 2013, , .		5
136	Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. Journal of Applied Physics, 2013, 114, 134312.	1.1	42
137	Oxidation Dynamics of a Chain of Aluminum Nanoparticles. Materials Research Society Symposia Proceedings, 2013, 1521, 1.	0.1	0
138	Nanoscopic mechanisms of singlet fission in amorphous molecular solid. Applied Physics Letters, 2013, 102, .	1.5	33
139	Interfacial design for reducing charge recombination in photovoltaics. Applied Physics Letters, 2013, 102, .	1.5	4
140	Oxidation Dynamics of Aluminum Nanorods. Materials Research Society Symposia Proceedings, 2013, 1521, 1.	0.1	0
141	Heat-Initiated Oxidation of an Aluminum Nanoparticle. Materials Research Society Symposia Proceedings, 2012, 1405, .	0.1	6
142	Core/shell structural transformation and brittle-to-ductile transition in nanowires. Applied Physics Letters, 2012, 100, .	1.5	12
143	Molecular control of photoexcited charge transfer and recombination at a quaterthiophene/zinc oxide interface. Applied Physics Letters, 2012, 100, .	1.5	29
144	Effect of substrate strain on critical dimensions of highly lattice mismatched defect-free nanorods. Journal of Applied Physics, 2012, 111, 054907.	1.1	7

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145	A core/shell mechanism for stacking-fault generation in GaAs nanowires. Applied Physics Letters, 2012, 100, 163103.	1.5	13
146	Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. Journal of Supercomputing, 2012, 62, 946-966.	2.4	19
147	Supercrystals of DNA-Functionalized Gold Nanoparticles: A Million-Atom Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2012, 116, 19579-19585.	1.5	20
148	Enhanced charge transfer by phenyl groups at a rubrene/C60 interface. Journal of Chemical Physics, 2012, 136, 184705.	1.2	10
149	Ion dynamics at porous alumina surfaces. Applied Physics Letters, 2012, 101, 063106.	1.5	5
150	Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. AIP Advances, 2011, 1, .	0.6	11
151	Exploiting hierarchical parallelisms for molecular dynamics simulation on multicore clusters. Journal of Supercomputing, 2011, 57, 20-33.	2.4	10
152	Sulfur-impurity induced amorphization of nickel. Journal of Applied Physics, 2011, 110, .	1.1	2
153	Poration of lipid bilayers by shock-induced nanobubble collapse. Applied Physics Letters, 2011, 98, .	1.5	43
154	Atomistic mechanisms of rapid energy transport in light-harvesting molecules. Applied Physics Letters, 2011, 98, 113302.	1.5	10
155	Defect migration and recombination in nanoindentation of silica glass. Applied Physics Letters, 2011, 99, .	1.5	36
156	Interaction potential for aluminum nitride: A molecular dynamics study of mechanical and thermal properties of crystalline and amorphous aluminum nitride. Journal of Applied Physics, 2011, 109, .	1.1	62
157	Molecular Dynamics Simulations of Rapid Hydrogen Production from Water Using Aluminum Clusters as Catalyzers. Physical Review Letters, 2010, 104, 126102.	2.9	88
158	Embrittlement of Metal by Solute Segregation-Induced Amorphization. Physical Review Letters, 2010, 104, 155502.	2.9	60
159	Nanoductility induced brittle fracture in shocked high performance ceramics. Applied Physics Letters, 2010, 97, .	1.5	28
160	Effects of oxide-shell structures on the dynamics of oxidation of Al nanoparticles. Applied Physics Letters, 2010, 96, 181906.	1.5	23
161	Enhanced reactivity of nanoenergetic materials: A first-principles molecular dynamics study based on divide-and-conquer density functional theory. Applied Physics Letters, 2009, 95, .	1.5	36
162	Response to â€œComment on â€˜Nanoindentation hardness anisotropy of alumina crystal: a molecular-dynamics studyâ€™â€•[Appl. Phys. Lett. 94, 146101 (2009)]. Applied Physics Letters, 2009, 94, 146102.	1.5	3

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163	Fast reaction mechanism of a core(Al)-shell (Al2O3) nanoparticle in oxygen. Applied Physics Letters, 2009, 95, .	1.5	37
164	Atomistic damage mechanisms during hypervelocity projectile impact on AlN: A large-scale parallel molecular dynamics simulation study. Journal of the Mechanics and Physics of Solids, 2008, 56, 1955-1988.	2.3	50
165	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. Computer Physics Communications, 2008, 178, 73-87.	3.0	75
166	A spaceâ€“time-ensemble parallel nudged elastic band algorithm for molecular kinetics simulation. Computer Physics Communications, 2008, 178, 280-289.	3.0	110
167	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. Journal of Applied Physics, 2008, 103, .	1.1	139
168	Deformation mechanisms and damage in Î±-alumina under hypervelocity impact loading. Journal of Applied Physics, 2008, 103, .	1.1	43
169	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. International Journal of High Performance Computing Applications, 2008, 22, 113-128.	2.4	47
170	Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. Physical Review B, 2008, 77, .	1.1	63
171	Electronic processes in fast thermite chemical reactions: A first-principles molecular dynamics study. Physical Review E, 2008, 77, 066103.	0.8	76
172	Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. Applied Physics Letters, 2008, 92, .	1.5	29
173	Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials. Journal of Propulsion and Power, 2007, 23, 688-692.	1.3	14
174	1,3,5-trinitro-1,3,5-triazine decomposition and chemisorption on Al(111) surface: First-principles molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234702.	1.2	34
175	Hypervelocity impact induced deformation modes in Î±-alumina. Applied Physics Letters, 2007, 91, 071906.	1.5	26
176	Interaction of Voids and Nanoductility in Silica Glass. Physical Review Letters, 2007, 99, 155506.	2.9	60
177	Dynamic Transition in the Structure of an Energetic Crystal during Chemical Reactions at Shock Front Prior to Detonation. Physical Review Letters, 2007, 99, 148303.	2.9	129
178	Reactive nanojets: Nanostructure-enhanced chemical reactions in a defected energetic crystal. Applied Physics Letters, 2007, 91, .	1.5	66
179	A divide-and-conquer/cellular-decomposition framework for million-to-billion atom simulations of chemical reactions. Computational Materials Science, 2007, 38, 642-652.	1.4	94
180	Interaction potential for silicon carbide: A molecular dynamics study of elastic constants and vibrational density of states for crystalline and amorphous silicon carbide. Journal of Applied Physics, 2007, 101, 103515.	1.1	283

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181	Multimillion-atom nanoindentation simulation of crystalline silicon carbide: Orientation dependence and anisotropic pileup. Journal of Applied Physics, 2007, 102, .	1.1	62
182	Fracture initiation mechanisms in Î±-alumina under hypervelocity impact. Applied Physics Letters, 2007, 91, 121911.	1.5	20
183	Multimillion atom simulations of dynamics of wing cracks and nanoscale damage in glass, and hypervelocity impact damage in ceramics. Computer Physics Communications, 2007, 177, 202-205.	3.0	5
184	Parallel history matching and associated forecast atÂtheÂcenter for interactive smart oilfield technologies. Journal of Supercomputing, 2007, 41, 109-117.	2.4	1
185	Pathfinder: A parallel search algorithm for concerted atomistic events. Computer Physics Communications, 2007, 176, 292-299.	3.0	7
186	Pressure-induced structural transformations in cadmium selenide nanorods. Applied Physics Letters, 2006, 89, 093101.	1.5	20
187	A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. MRS Bulletin, 2006, 31, 410-418.	1.7	49
188	Sustainable Adaptive Grid Supercomputing: Multiscale Simulation of Semiconductor Processing across the Pacific. , 2006, , .		11
189	Multimillion Atom Simulations of Dynamics of Oxidation of an Aluminum Nanoparticle and Nanoindentation on Ceramicsâ€. Journal of Physical Chemistry B, 2006, 110, 3727-3733.	1.2	61
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