Priya Vashishta

List of Publications by Year
in descending order

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208	7,831	34493	73587
papers	citations	54 h-index	79 g-index

208	208	208	6856
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	EZFF: Python library for multi-objective parameterization and uncertainty quantification of interatomic forcefields for molecular dynamics. SoftwareX, 2021, 13, 100663.	1.2	6
2	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
3	PND: Physics-informed neural-network software for molecular dynamics applications. SoftwareX, 2021, 15, 100789.	1.2	6
4	Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials. Npj Computational Materials, 2021, 7, .	3.5	14
5	Lattice thermal transport in two-dimensional alloys and fractal heterostructures. Scientific Reports, 2021, 11, 1656.	1.6	8
6	Review of strategies toward the development of alloy two-dimensional (2D) transition metal dichalcogenides. IScience, 2021, 24, 103532.	1.9	11
7	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
8	Reactive molecular dynamics simulations and machine learning. Journal of Physics: Conference Series, 2020, 1461, 012182.	0.3	4
9	Towards simulation of the dynamics of materials on quantum computers. Physical Review B, 2020, 101, .	1.1	23
10	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. Langmuir, 2020, 36, 7658-7668.	1.6	26
11	Direct Atomic Simulations of Facet Formation and Equilibrium Shapes of SiC Nanoparticles. Crystal Growth and Design, 2020, 20, 2147-2152.	1.4	7
12	RXMD: A scalable reactive molecular dynamics simulator for optimized time-to-solution. SoftwareX, 2020, 11, 100389.	1.2	15
13	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
14	Quantum Dynamics at Scale. , 2020, , .		1
15	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
16	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. SoftwareX, 2019, 10, 100307.	1.2	32
17	Two-Dimensional Lateral Epitaxy of 2H (MoSe₂)â€“1Tâ€² (ReSe₂) Phases. Nano Letters, 2019, 19, 6338-6345.	4.5	30
18	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

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19	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, .	1.1	10
20	Neural Network Analysis of Dynamic Fracture in a Layered Material. MRS Advances, 2019, 4, 1109-1117.	0.5	4
21	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. Computing in Science and Engineering, 2019, 21, 64-75.	1.2	5
22	Structural Phase Transformation in Strained Monolayer MoWSe₂ Alloy. ACS Nano, 2018, 12, 3468-3476.	7.3	57
23	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. Journal of Applied Physics, 2018, 123, .	1.1	24
24	Acceleration of Dynamic n-Tuple Computations in Many-Body Molecular Dynamics. , 2018, , .		0
25	Atomistic Study of Wet-heat Resistance of Calcium Dipicolinate in the Core of Spores. MRS Advances, 2018, 3, 1457-1462.	0.5	0
26	Semiconductorâ€“metal structural phase transformation in MoTe₂ monolayers by electronic excitation. Nanoscale, 2018, 10, 2742-2747.	2.8	34
27	Photo-induced Contraction of Layered Materials. MRS Advances, 2018, 3, 333-338.	0.5	0
28	Plane shock loading on mono- and nano-crystalline silicon carbide. Applied Physics Letters, 2018, 112, .	1.5	22
29	Shift-Collapse Acceleration of Generalized Polarizable Reactive Molecular Dynamics for Machine Learning-Assisted Computational Synthesis of Layered Materials. , 2018, , .		6
30	Photo-induced lattice contraction in layered materials. Journal of Physics Condensed Matter, 2018, 30, 32LT02.	0.7	4
31	Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. Chemistry of Materials, 2018, 30, 7262-7268.	3.2	37
32	Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals. Applied Physics Letters, 2018, 112, .	1.5	8
33	Multiobjective genetic training and uncertainty quantification of reactive force fields. Npj Computational Materials, 2018, 4, .	3.5	25
34	Faceting, Grain Growth, and Crack Healing in Alumina. ACS Nano, 2018, 12, 9005-9010.	7.3	13
35	Multistage reaction pathways in detonating RDX. AIP Conference Proceedings, 2017, , .	0.3	4
36	Picosecond amorphization of SiO ₂ stishovite under tension. Science Advances, 2017, 3, e1602339.	4.7	17

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37	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
38	Gel phase in hydrated calcium dipicolinate. Applied Physics Letters, 2017, 111, .	1.5	4
39	A derivation and scalable implementation of the synchronous parallel kinetic Monte Carlo method for simulating long-time dynamics. Computer Physics Communications, 2017, 219, 246-254.	3.0	4
40	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
41	Quantum Molecular Dynamics Validation of Nanocarbon Synthesis by High-Temperature Oxidation of Nanoparticles. MRS Advances, 2016, 1, 1811-1816.	0.5	0
42	Anisotropic mechanoresponse of energetic crystallites: a quantum molecular dynamics study of nano-collision. Nanoscale, 2016, 8, 9714-9720.	2.8	2
43	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. Scientific Reports, 2016, 6, 24109.	1.6	15
44	Reactive Molecular Dynamics Simulations, Data Analytics and Visualization. Materials Research Society Symposia Proceedings, 2015, 1756, 1.	0.1	0
45	An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. Computer Physics Communications, 2015, 192, 91-96.	3.0	24
46	Large-Scale Computing for Molecular Dynamics Simulation. , 2015, , 765-770.		0
47	Multistage reaction pathways in detonating high explosives. Applied Physics Letters, 2014, 105, .	1.5	25
48	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand. , 2014, , .		8
49	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 18A529.	1.2	57
50	Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	18
51	Rapid hydrogen production from water using aluminum nanoclusters: A quantum molecular dynamics simulation study. Solid State Ionics, 2014, 262, 908-910.	1.3	4
52	Hydrogen-on-Demand Using Metallic Alloy Nanoparticles in Water. Nano Letters, 2014, 14, 4090-4096.	4.5	33
53	Divide-Conquer-Recombine. , 2014, , .		3
54	Bonding and Structure of Ceramic-Ceramic Interfaces. Physical Review Letters, 2013, 111, 066103.	2.9	16

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55	Shock loading on AlN ceramics: A large scale molecular dynamics study. International Journal of Plasticity, 2013, 51, 122-131.	4.1	47
56	Scalability study of molecular dynamics simulation on Godson-T many-core architecture. Journal of Parallel and Distributed Computing, 2013, 73, 1469-1482.	2.7	3
57	Large nonadiabatic quantum molecular dynamics simulations on parallel computers. Computer Physics Communications, 2013, 184, 1-8.	3.0	33
58	A scalable parallel algorithm for dynamic range-limited n -tuple computation in many-body molecular dynamics simulation. , 2013, , .		5
59	Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. Journal of Applied Physics, 2013, 114, 134312.	1.1	42
60	Oxidation Dynamics of a Chain of Aluminum Nanoparticles. Materials Research Society Symposia Proceedings, 2013, 1521, 1.	0.1	0
61	Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. Journal of Supercomputing, 2012, 62, 946-966.	2.4	19
62	Ion dynamics at porous alumina surfaces. Applied Physics Letters, 2012, 101, 063106.	1.5	5
63	Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. AIP Advances, 2011, 1, .	0.6	11
64	Performance analysis and optimization of molecular dynamics simulation onGodson-Tmany-core processor. , 2011, , .		1
65	Sulfur-impurity induced amorphization of nickel. Journal of Applied Physics, 2011, 110, .	1.1	2
66	Poration of lipid bilayers by shock-induced nanobubble collapse. Applied Physics Letters, 2011, 98, .	1.5	43
67	Reaction of aluminum clusters with water. Journal of Chemical Physics, 2011, 134, 244702.	1.2	41
68	Atomistic mechanisms of rapid energy transport in light-harvesting molecules. Applied Physics Letters, 2011, 98, 113302.	1.5	10
69	Defect migration and recombination in nanoindentation of silica glass. Applied Physics Letters, 2011, 99, .	1.5	36
70	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
71	Molecular Dynamics Simulations of Rapid Hydrogen Production from Water Using Aluminum Clusters as Catalyzers. Physical Review Letters, 2010, 104, 126102.	2.9	88
72	Embrittlement of Metal by Solute Segregation-Induced Amorphization. Physical Review Letters, 2010, 104, 155502.	2.9	60

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73	Nanoductility induced brittle fracture in shocked high performance ceramics. Applied Physics Letters, 2010, 97, .	1.5	28
74	Density functional study of 1,3,5-trinitro-1,3,5-triazine molecular crystal with van der Waals interactions. Journal of Chemical Physics, 2010, 132, 094106.	1.2	44
75	Void Deformation and Breakup in Shearing Silica Glass. Physical Review Letters, 2009, 103, 035501.	2.9	13
76	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
77	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
78	Interaction and coalescence of nanovoids and dynamic fracture in silica glass: multimillion-to-billion atom molecular dynamics simulations. Journal Physics D: Applied Physics, 2009, 42, 214011.	1.3	29
79	A Multilevel Parallelization Framework for High-Order Stencil Computations. Lecture Notes in Computer Science, 2009, , 642-653.	1.0	34
80	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
81	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. Computer Physics Communications, 2008, 178, 73-87.	3.0	75
82	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. Journal of Applied Physics, 2008, 103, .	1.1	139
83	Deformation mechanisms and damage in Î±-alumina under hypervelocity impact loading. Journal of Applied Physics, 2008, 103, .	1.1	43
84	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. International Journal of High Performance Computing Applications, 2008, 22, 113-128.	2.4	47
85	Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. Physical Review B, 2008, 77, .	1.1	63
86	Electronic processes in fast thermite chemical reactions: A first-principles molecular dynamics study. Physical Review E, 2008, 77, 066103.	0.8	76
87	Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. Applied Physics Letters, 2008, 92, .	1.5	29
88	Parallel Lattice Boltzmann Flow Simulation on Emerging Multi-core Platforms. Lecture Notes in Computer Science, 2008, , 763-777.	1.0	15
89	Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials. Journal of Propulsion and Power, 2007, 23, 688-692.	1.3	14
90	Hypervelocity impact induced deformation modes in Î±-alumina. Applied Physics Letters, 2007, 91, 071906.	1.5	26

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91	A molecular dynamics study of nanoindentation of amorphous silicon carbide. Journal of Applied Physics, 2007, 102, 023509.	1.1	38
92	Interaction of Voids and Nanoductility in Silica Glass. Physical Review Letters, 2007, 99, 155506.	2.9	60
93	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
94	Reactive nanojets: Nanostructure-enhanced chemical reactions in a defected energetic crystal. Applied Physics Letters, 2007, 91, .	1.5	66
95	Nanoscale Thermal Property of Amorphous SiC: A Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 2007, 1022, 1.	0.1	2
96	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
97	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
98	Multimillion-atom nanoindentation simulation of crystalline silicon carbide: Orientation dependence and anisotropic pileup. Journal of Applied Physics, 2007, 102, .	1.1	62
99	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
100	Pressure-induced structural transformations in cadmium selenide nanorods. Applied Physics Letters, 2006, 89, 093101.	1.5	20
101	A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. MRS Bulletin, 2006, 31, 410-418.	1.7	49
102	Sustainable Adaptive Grid Supercomputing: Multiscale Simulation of Semiconductor Processing across the Pacific. , 2006, , .		11
103	Shock-Induced Structural Phase Transition, Plasticity, and Brittle Cracks in Aluminum Nitride Ceramic. Physical Review Letters, 2006, 96, 065502.	2.9	64
104	Collision-free spatial hash functions for structural analysis of billion-vertex chemical bond networks. Computer Physics Communications, 2006, 175, 339-347.	3.0	15
105	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
106	Grid applications---Sustainable adaptive grid supercomputing. , 2006, , .		13
107	Embedded divide-and-conquer algorithm on hierarchical real-space grids: parallel molecular dynamics simulation based on linear-scaling density functional theory. Computer Physics Communications, 2005, 167, 151-164.	3.0	65
108	Brittle dynamic fracture of crystalline cubic silicon carbide (3C-SiC) via molecular dynamics simulation. Journal of Applied Physics, 2005, 98, 103524.	1.1	98

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109	Atomistic mechanisms of amorphization during nanoindentation of SiC: A molecular dynamics study. Physical Review B, 2005, 71, .	1.1	62
110	Oxidation of aluminum nanoclusters. Physical Review B, 2005, 71, .	1.1	88
111	Atomistic processes during nanoindentation of amorphous silicon carbide. Applied Physics Letters, 2005, 86, 021915.	1.5	32
112	Coupling atomistic and continuum length scales in heteroepitaxial systems: Multiscale molecular-dynamics/finite-element simulations of strain relaxation inSiâˆ•Si3N4nanopixels. Physical Review B, 2005, 72, .	1.1	7
113	A Crossover in the Mechanical Response of Nanocrystalline Ceramics. Science, 2005, 309, 911-914.	6.0	209
114	Multimillion Atom Molecular-Dynamics Simulations of Nanostructured Materials and Processes on Parallel Computers. , 2005, , 875-928.		1
115	Multimillion Atom Molecular-Dynamics Simulations of Nanostructured Materials and Processes on Parallel Computers. , 2005, , 875-928.		0
116	Environmental effects of H2O on fracture initiation in silicon: A hybrid electronic-density-functional/molecular-dynamics study. Journal of Applied Physics, 2004, 95, 5316-5323.	1.1	45
117	Atomistic mechanisms for wurtzite-to-rocksalt structural transformation in cadmium selenide under pressure. Physical Review B, 2004, 70, .	1.1	74
118	Large-scale molecular dynamics simulations of alkanethiol self-assembled monolayers. Journal of Chemical Physics, 2004, 121, 4323-4330.	1.2	68
119	Nanoindentation-induced amorphization in silicon carbide. Applied Physics Letters, 2004, 85, 378-380.	1.5	78
120	Multiple Grains in Nanocrystals: Effect of Initial Shape and Size on Transformed Structures Under Pressure. Physical Review Letters, 2004, 93, 203401.	2.9	26
121	Scalable and portable visualization of large atomistic datasets. Computer Physics Communications, 2004, 163, 53-64.	3.0	8
122	Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. Physical Review B, 2004, 70, .	1.1	65
123	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. International Journal of Fracture, 2003, 121, 71-79.	1.1	25
124	Scalable and portable implementation of the fast multipole method on parallel computers. Computer Physics Communications, 2003, 153, 445-461.	3.0	49
125	Nanoindentation of silicon nitride: A multimillion-atom molecular dynamics study. Applied Physics Letters, 2003, 82, 118-120.	1.5	73
126	Molecular dynamics study of structural, mechanical, and vibrational properties of crystalline and amorphous Ga1âˆ’xInxAs alloys. Journal of Applied Physics, 2003, 94, 3840-3848.	1.1	28

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127	Structural, mechanical, and vibrational properties of Ga1â^'xInxAs alloys: A molecular dynamics study. Applied Physics Letters, 2003, 82, 1057-1059.	1.5	27
128	InAs/GaAs square nanomesas: Multimillion-atom molecular dynamics simulations on parallel computers. Journal of Applied Physics, 2003, 94, 6762-6773.	1.1	13
129	Immersive and Interactive Exploration of Billion-Atom Systems. Presence: Teleoperators and Virtual Environments, 2003, 12, 85-95.	0.3	29
130	Scalable multiresolution algorithms for classical and quantum molecular dynamics simulations of nanosystems. Handbook of Numerical Analysis, 2003, , 639-666.	0.9	0
131	Mechanisms of Stress Corrosion Cracking in Si: A Hybrid Quantum-Mechanical/Molecular-Dynamics Simulation. Materials Research Society Symposia Proceedings, 2002, 750, 1.	0.1	0
132	Atomistic Aspects of Crack Propagation in Brittle Materials: Multimillion Atom Molecular Dynamics Simulations. Annual Review of Materials Research, 2002, 32, 377-400.	4.3	177
133	Scalable Atomistic Simulation Algorithms for Materials Research. Scientific Programming, 2002, 10, 263-270.	0.5	27
134	Hybrid quantum mechanical/molecular dynamics simulation on parallel computers: density functional theory on real-space multigrids. Computer Physics Communications, 2002, 149, 30-38.	3.0	56
135	Applications: Physical and Electronic Materials. , 2002, , 83-106.		0
136	Large-scale molecular dynamics simulations of materials on parallel computers. AIP Conference Proceedings, 2001, , .	0.3	0
137	Multimillion atom simulation of materials on parallel computers â€" nanopixel, interfacial fracture, nanoindentation, and oxidation. Applied Surface Science, 2001, 182, 258-264.	3.1	21
138	Hybrid finite-element/molecular-dynamics/electronic-density-functional approach to materials simulations on parallel computers. Computer Physics Communications, 2001, 138, 143-154.	3.0	136
139	Linear-scaling density-functional-theory calculations of electronic structure based on real-space grids: design, analysis, and scalability test of parallel algorithms. Computer Physics Communications, 2001, 140, 303-314.	3.0	126
140	Scalable atomistic simulation algorithms for materials research. , 2001, , .		14
141	Dynamic Fracture Mechanisms in Nanostructured and Amorphous Silica Glasses Million-Atom Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2001, 703, 1.	0.1	10
142	Grain Boundaries in Gallium Arsenide Nanocrystals Under Pressure: A Parallel Molecular-Dynamics Study. Physical Review Letters, 2001, 86, 55-58.	2.9	60
143	Initial Stages of Sintering of TiO2 Nanoparticles: Variable-Charge Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2000, 634, 761.	0.1	0
144	Hybrid Electronic-density-functional/molecular-dynamics Simulation on Parallel Computers: Oxidation of Si Surface. Materials Research Society Symposia Proceedings, 2000, 653, .	0.1	0

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145	Scalable I/O of large-scale molecular dynamics simulations: A data-compression algorithm. Computer Physics Communications, 2000, 131, 78-85.	3.0	40
146	A scalable molecular-dynamics algorithm suite for materials simulations: design-space diagram on 1024 Cray T3E processors. Future Generation Computer Systems, 2000, 17, 279-291.	4.9	33
147	Multiresolution algorithms for massively parallel molecular dynamics simulations of nanostructured materials. Computer Physics Communications, 2000, 128, 245-259.	3.0	21
148	Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. Journal of Applied Physics, 2000, 87, 7708-7711.	1.1	34
149	Stress Domains inSi(111)/aâ^'Si3N4Nanopixel: Ten-Million-Atom Molecular Dynamics Simulations on Parallel Computers. Physical Review Letters, 2000, 84, 318-321.	2.9	33
150	Amorphization and anisotropic fracture dynamics during nanoindentation of silicon nitride: A multimillion atom molecular dynamics study. Applied Physics Letters, 2000, 77, 4332-4334.	1.5	56
151	Role of atomic charge transfer on sintering of TiO2 nanoparticles: Variable-charge molecular dynamics. Journal of Applied Physics, 2000, 88, 6011-6015.	1.1	37
152	Incipient phase separation in Ag/Ge/Se glasses: clustering of Ag atoms. Journal of Non-Crystalline Solids, 2000, 262, 135-142.	1.5	26
153	Molecular Dynamics Simulation of Structural Transformation in Silicon Carbide under Pressure. Physical Review Letters, 2000, 84, 3338-3341.	2.9	183
154	Dislocation Emission at the Silicon/Silicon Nitride Interface: A Million Atom Molecular Dynamics Simulation on Parallel Computers. Physical Review Letters, 2000, 84, 322-325.	2.9	32
155	Sintering, structure, and mechanical properties of nanophase SiC: A molecular-dynamics and neutron scattering study. Applied Physics Letters, 2000, 77, 1132-1134.	1.5	47
156	Hybrid Electronic-density-functional/molecular-dynamics Simulation on Parallel Computers: Oxidation of Si Surface. Materials Research Society Symposia Proceedings, 2000, 653, 1.	0.1	0
157	Structural Correlations and Mechanical Behavior in Nanophase Silica Glasses. Physical Review Letters, 1999, 82, 4018-4021.	2.9	70
158	Parallel Molecular Dynamics Simulations of High Temperature Ceramics. Journal of the European Ceramic Society, 1999, 19, 2257-2264.	2.8	5
159	Structural correlations at Si/Si3N4 interface and atomic stresses in Si/Si3N4 nanopixel-10 million-atom molecular dynamics simulation on parallel computers. Journal of the European Ceramic Society, 1999, 19, 2265-2272.	2.8	6
160	Dynamics of Oxidation of Aluminum Nanoclusters using Variable Charge Molecular-Dynamics Simulations on Parallel Computers. Physical Review Letters, 1999, 82, 4866-4869.	2.9	313
161	Variable-charge interatomic potentials for molecular-dynamics simulations of TiO2. Journal of Applied Physics, 1999, 86, 3036-3041.	1.1	64
162	Intercluster Interaction of TiO2 Nanoclusters Using Variable-Charge Interatomic Potentials. Materials Research Society Symposia Proceedings, 1999, 581, 667.	0.1	1

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163	Multimillion-atom molecular dynamics simulation of atomic level stresses in Si(111)/Si3N4(0001) nanopixels. Applied Physics Letters, 1998, 72, 1969-1971.	1.5	37
164	N-body problems: Atomistic simulation of nanostructured materials. IEEE Computational Science and Engineering, 1998, 5, 68-78.	0.6	7
165	Molecular Dynamics Simulations of Nanoindentation of Silicon Nitride. Materials Research Society Symposia Proceedings, 1998, 539, 119.	0.1	2
166	Dynamics of Consolidation and Crack Growth in Nanoclusterâ€Assembled Amorphous Silicon Nitride. Journal of the American Ceramic Society, 1998, 81, 433-436.	1.9	22
167	Structure and mechanical failure in nanophase silicon nitride. Advances in Metal and Semiconductor Clusters, 1998, , 263-298.	1.5	4
168	Morphology of Pores and Interfaces and Mechanical Behavior of Nanocluster-Assembled Silicon Nitride Ceramic. Physical Review Letters, 1997, 78, 689-692.	2.9	67
169	Crack Front Propagation and Fracture in a Graphite Sheet: A Molecular-Dynamics Study on Parallel Computers. Physical Review Letters, 1997, 78, 2148-2151.	2.9	126
170	Role of Ultrafine Microstructures in Dynamic Fracture in Nanophase Silicon Nitride. Physical Review Letters, 1997, 78, 2144-2147.	2.9	79
171	Oxidation Dynamics of Nanophase Aluminum Clusters: A Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 1997, 481, 625.	0.1	3
172	Direct atomistic simulation of quartz crystal oscillators: Bulk properties and nanoscale devices. Physical Review B, 1997, 56, 611-618.	1.1	118
173	Molecular Dynamics Methods and Large-Scale Simulations of Amorphous Materials. , 1997, , 151-213.		26
174	Molecular Dynamics Study Of Si/Si₃N₄ Interface. Materials Research Society Symposia Proceedings, 1996, 446, 157.	0.1	3
175	Fracture in Silicon Nitride and Alumina thin Films: a Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 1996, 446, 163.	0.1	0
176	Molecular Dynamics Simulations of Fracture in Amorphous Silica. Materials Research Society Symposia Proceedings, 1996, 455, 267.	0.1	1
177	Fracture of Nanophase Ceramics: A Molecular-Dynamics Study. Materials Research Society Symposia Proceedings, 1996, 457, 187.	0.1	0
178	Structure, Mechanical Properties, and Dynamic Fracture in Nanophase Silicon Nitride via Parallel Molecular Dynamics. Materials Research Society Symposia Proceedings, 1996, 457, 205.	0.1	0
179	Crack propagation and fracture in ceramic filmsâ€"million atom molecular dynamics simulations on parallel computers. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 56-71.	1.7	29
180	Amorphization and Fracture in Silicon Diselenide Nanowires: A Molecular Dynamics Study. Physical Review Letters, 1996, 77, 2241-2244.	2.9	32

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181	Crack propagation and fracture in ceramic filmsâ€"million atom molecular dynamics simulations on parallel computers. , 1996, , 56-71.		0
182	Large Scale Molecular Dynamics Study of Amorphous Carbon and Graphite on Parallel Machines. Materials Research Society Symposia Proceedings, 1995, 408, 113.	0.1	3
183	Early Stages of Sintering of Si3N4 Nanoclusters Via Parallel Molecular Dynamics. Materials Research Society Symposia Proceedings, 1995, 408, 181.	0.1	0
184	Dynamics and Morphology of Cracks in Silicon Nitride Films: A Molecular Dynamics Study on Parallel Computers. Materials Research Society Symposia Proceedings, 1995, 408, 205.	0.1	0
185	Molecular Dynamics Simulations of SiSe2 Nanowires. Materials Research Society Symposia Proceedings, 1995, 408, 489.	0.1	1
186	Sintering of Amorphous Si3N4 Nanoclusters: A Molecular Dynamics Study of Stress Analysis. Materials Research Society Symposia Proceedings, 1995, 408, 573.	0.1	1
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