Priya D Vashishta

List of Publications by Year
in descending order

234	7,188	43973	74018
papers	citations	48 h-index	75 g-index

237	237	237	6731
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Flexible polyolefin dielectric by strategic design of organic modules for harsh condition electrification. Energy and Environmental Science, 2022, 15, 1307-1314.	15.6	56
2	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
3	Improving the Rotational Freedom of Polyetherimide: Enhancement of the Dielectric Properties of a Commodity High-Temperature Polymer Using a Structural Defect. Chemistry of Materials, 2022, 34, 6553-6558.	3.2	22
4	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
5	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
6	Mechanical behavior of ultralight nickel metamaterial. Applied Physics Letters, 2021, 118, .	1.5	2
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	Lattice thermal transport in two-dimensional alloys and fractal heterostructures. Scientific Reports, 2021, 11, 1656.	1.6	8
16	Domain-specific compilers for dynamic simulations of quantum materials on quantum computers. Quantum Science and Technology, 2021, 6, 014007.	2.6	5
17	Review of strategies toward the development of alloy two-dimensional (2D) transition metal dichalcogenides. IScience, 2021, 24, 103532.	1.9	11
18	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

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19	Field-Induced Carrier Localization Transition in Dielectric Polymers. Journal of Physical Chemistry Letters, 2020, 11, 352-358.	2.1	6
20	Tellurene Photodetector with High Gain and Wide Bandwidth. ACS Nano, 2020, 14, 303-310.	7.3	101
21	Boltzmann machine modeling of layered MoS2 synthesis on a quantum annealer. Computational Materials Science, 2020, 173, 109429.	1.4	10
22	Neural Network Molecular Dynamics at Scale. , 2020, , .		2
23	Differences in Sb2Te3 growth by pulsed laser and sputter deposition. Acta Materialia, 2020, 200, 811-820.	3.8	10
24	Photoexcitation Induced Ultrafast Nonthermal Amorphization in Sb₂Te₃. Journal of Physical Chemistry Letters, 2020, 11, 10242-10249.	2.1	12
25	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
26	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
27	Optically Induced Three-Stage Picosecond Amorphization in Low-Temperature SrTiO₃. Journal of Physical Chemistry Letters, 2020, 11, 9605-9612.	2.1	4
28	Reactive molecular dynamics simulations and machine learning. Journal of Physics: Conference Series, 2020, 1461, 012182.	0.3	4
29	Towards simulation of the dynamics of materials on quantum computers. Physical Review B, 2020, 101, .	1.1	23
30	Memristive Device Characteristics Engineering by Controlling the Crystallinity of Switching Layer Materials. ACS Applied Electronic Materials, 2020, 2, 1529-1537.	2.0	7
31	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. Langmuir, 2020, 36, 7658-7668.	1.6	26
32	Frequency-dependent dielectric constant prediction of polymers using machine learning. Npj Computational Materials, 2020, 6, .	3.5	75
33	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
34	Enhancing combustion performance of nano-Al/PVDF composites with Î²-PVDF. Combustion and Flame, 2020, 219, 467-477.	2.8	55
35	Direct Atomic Simulations of Facet Formation and Equilibrium Shapes of SiC Nanoparticles. Crystal Growth and Design, 2020, 20, 2147-2152.	1.4	7
36	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

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37	RXMD: A scalable reactive molecular dynamics simulator for optimized time-to-solution. SoftwareX, 2020, 11, 100389.	1.2	15
38	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
39	Quantum Dynamics at Scale. , 2020, , .		1
40	Fast deformation of shocked quartz and implications for planar deformation features observed in shocked quartz. AIP Conference Proceedings, 2020, , .	0.3	0
41	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
42	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. SoftwareX, 2019, 10, 100307.	1.2	32
43	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. Nano Letters, 2019, 19, 6078-6086.	4.5	43
44	Two-Dimensional Lateral Epitaxy of 2H (MoSe₂)â€“1Tâ€² (ReSe₂) Phases. Nano Letters, 2019, 19, 6338-6345.	4.5	30
45	Optical Control of Non-Equilibrium Phonon Dynamics. Nano Letters, 2019, 19, 4981-4989.	4.5	27
46	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. Journal of Physical Chemistry Letters, 2019, 10, 3937-3943.	2.1	8
47	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
48	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
49	Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality. SoftwareX, 2019, 9, 112-116.	1.2	11
50	Effects of chemical defects on anisotropic dielectric response of polyethylene. AIP Advances, 2019, 9, .	0.6	9
51	Nanoindentation on Monolayer MoS₂ Kirigami. ACS Omega, 2019, 4, 9952-9956.	1.6	8
52	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
53	Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering. Nature Photonics, 2019, 13, 425-430.	15.6	28
54	Thermal conductivity of MoS2 monolayers from molecular dynamics simulations. AIP Advances, 2019, 9, .	0.6	22

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55	Rapid and reversible lithiation of doped biogenous iron oxide nanoparticles. Scientific Reports, 2019, 9, 1828.	1.6	4
56	Electrostrictive Cavitation in Water Induced by a SnO₂ Nanoparticle. ACS Omega, 2019, 4, 22274-22279.	1.6	3
57	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, .	1.1	10
58	Neural Network Analysis of Dynamic Fracture in a Layered Material. MRS Advances, 2019, 4, 1109-1117.	0.5	4
59	Polytypism in ultrathin tellurium. 2D Materials, 2019, 6, 015013.	2.0	68
60	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. Computing in Science and Engineering, 2019, 21, 64-75.	1.2	5
61	Structural Phase Transformation in Strained Monolayer MoWSe₂ Alloy. ACS Nano, 2018, 12, 3468-3476.	7.3	57
62	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
63	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. Journal of Applied Physics, 2018, 123, .	1.1	24
64	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
65	Semiconductorâ€“metal structural phase transformation in MoTe₂ monolayers by electronic excitation. Nanoscale, 2018, 10, 2742-2747.	2.8	34
66	Plane shock loading on mono- and nano-crystalline silicon carbide. Applied Physics Letters, 2018, 112, .	1.5	22
67	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.5	5
68	Molecular Simulation of MoS2 Exfoliation. Scientific Reports, 2018, 8, 16761.	1.6	19
69	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	3.5	107
70	Photo-induced lattice contraction in layered materials. Journal of Physics Condensed Matter, 2018, 30, 32LT02.	0.7	4
71	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
72	Free energy of hydration and heat capacity of calcium dipicolinate inBacillusspore cores. Applied Physics Letters, 2018, 113, 113702.	1.5	1

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73	Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites. ACS Nano, 2018, 12, 11366-11375.	7.3	99
74	Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. Chemistry of Materials, 2018, 30, 7262-7268.	3.2	37
75	Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals. Applied Physics Letters, 2018, 112, .	1.5	8
76	Multiobjective genetic training and uncertainty quantification of reactive force fields. Npj Computational Materials, 2018, 4, .	3.5	25
77	Faceting, Grain Growth, and Crack Healing in Alumina. ACS Nano, 2018, 12, 9005-9010.	7.3	13
78	Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in MoSe₂ Monolayer. Nano Letters, 2018, 18, 4653-4658.	4.5	16
79	Multistage reaction pathways in detonating RDX. AIP Conference Proceedings, 2017, , .	0.3	4
80	Picosecond amorphization of SiO ₂ stishovite under tension. Science Advances, 2017, 3, e1602339.	4.7	17
81	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
82	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
83	Reactivity of Sulfur Molecules on MoO₃ (010) Surface. Journal of Physical Chemistry Letters, 2017, 8, 6206-6210.	2.1	9
84	Gel phase in hydrated calcium dipicolinate. Applied Physics Letters, 2017, 111, .	1.5	4
85	Ultrafast non-radiative dynamics of atomically thin MoSe2. Nature Communications, 2017, 8, 1745.	5.8	52
86	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
87	Computational Synthesis of MoS₂ Layers by Reactive Molecular Dynamics Simulations: Initial Sulfidation of MoO₃ Surfaces. Nano Letters, 2017, 17, 4866-4872.	4.5	60
88	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
89	Order-Invariant Real Number Summation: Circumventing Accuracy Loss for Multimillion Summands on Multiple Parallel Architectures. , 2016, , .		1
90	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

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91	The nature of free-carrier transport in organometal halide perovskites. Scientific Reports, 2016, 6, 19599.	1.6	38
92	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
93	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. Scientific Reports, 2016, 6, 24109.	1.6	15
94	Crystalline anisotropy of shock-induced phenomena: Omni-directional multiscale shock technique. Applied Physics Letters, 2016, 108, .	1.5	13
95	Reactive Molecular Dynamics Simulations, Data Analytics and Visualization. Materials Research Society Symposia Proceedings, 2015, 1756, 1.	0.1	0
96	A crossover in anisotropic nanomechanochemistry of van der Waals crystals. Applied Physics Letters, 2015, 107, .	1.5	11
97	Reactive Molecular Dynamics Study of Oxidation of Aggregated Aluminum Nanoparticles. Materials Research Society Symposia Proceedings, 2015, 1758, 1.	0.1	1
98	An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. Computer Physics Communications, 2015, 192, 91-96.	3.0	24
99	Large-Scale Computing for Molecular Dynamics Simulation. , 2015, , 765-770.		0
100	Multistage reaction pathways in detonating high explosives. Applied Physics Letters, 2014, 105, .	1.5	25
101	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand. , 2014, , .		8
102	Small interfering ribonucleic acid induces liquid-to-ripple phase transformation in a phospholipid membrane. Applied Physics Letters, 2014, 105, 113702.	1.5	5
103	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 18A529.	1.2	57
104	Universal stretched exponential relaxation in nanoconfined water. Applied Physics Letters, 2014, 105, .	1.5	17
105	Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	18
106	Bonding and Structure of Ceramic-Ceramic Interfaces. Physical Review Letters, 2013, 111, 066103.	2.9	16
107	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
108	Cholesterol Translocation in a Phospholipid Membrane. Biophysical Journal, 2013, 104, 2429-2436.	0.2	63

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109	Collective oxidation behavior of aluminum nanoparticle aggregate. Applied Physics Letters, 2013, 102, 221904.	1.5	11
110	Large nonadiabatic quantum molecular dynamics simulations on parallel computers. Computer Physics Communications, 2013, 184, 1-8.	3.0	33
111	Nanobubble Collapse on a Silica Surface in Water: Billion-Atom Reactive Molecular Dynamics Simulations. Physical Review Letters, 2013, 111, 184503.	2.9	59
112	Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. Journal of Applied Physics, 2013, 114, 134312.	1.1	42
113	Oxidation Dynamics of a Chain of Aluminum Nanoparticles. Materials Research Society Symposia Proceedings, 2013, 1521, 1.	0.1	0
114	Oxidation Dynamics of Aluminum Nanorods. Materials Research Society Symposia Proceedings, 2013, 1521, 1.	0.1	0
115	Heat-Initiated Oxidation of an Aluminum Nanoparticle. Materials Research Society Symposia Proceedings, 2012, 1405, .	0.1	6
116	Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. Journal of Supercomputing, 2012, 62, 946-966.	2.4	19
117	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
118	Ion dynamics at porous alumina surfaces. Applied Physics Letters, 2012, 101, 063106.	1.5	5
119	Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. AIP Advances, 2011, 1, .	0.6	11
120	Exploiting hierarchical parallelisms for molecular dynamics simulation on multicore clusters. Journal of Supercomputing, 2011, 57, 20-33.	2.4	10
121	Sulfur-impurity induced amorphization of nickel. Journal of Applied Physics, 2011, 110, .	1.1	2
122	Poration of lipid bilayers by shock-induced nanobubble collapse. Applied Physics Letters, 2011, 98, .	1.5	43
123	Atomistic mechanisms of rapid energy transport in light-harvesting molecules. Applied Physics Letters, 2011, 98, 113302.	1.5	10
124	Defect migration and recombination in nanoindentation of silica glass. Applied Physics Letters, 2011, 99, .	1.5	36
125	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
126	Molecular Dynamics Simulations of Rapid Hydrogen Production from Water Using Aluminum Clusters as Catalyzers. Physical Review Letters, 2010, 104, 126102.	2.9	88

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127	Embrittlement of Metal by Solute Segregation-Induced Amorphization. Physical Review Letters, 2010, 104, 155502.	2.9	60
128	Nanoductility induced brittle fracture in shocked high performance ceramics. Applied Physics Letters, 2010, 97, .	1.5	28
129	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
130	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
131	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. Computer Physics Communications, 2008, 178, 73-87.	3.0	75
132	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. Journal of Applied Physics, 2008, 103, .	1.1	139
133	Deformation mechanisms and damage in Î±-alumina under hypervelocity impact loading. Journal of Applied Physics, 2008, 103, .	1.1	43
134	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. International Journal of High Performance Computing Applications, 2008, 22, 113-128.	2.4	47
135	Molecular dynamics nanoindentation simulation of an energetic material. Applied Physics Letters, 2008, 93, 171908.	1.5	17
136	Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. Physical Review B, 2008, 77, .	1.1	63
137	Electronic processes in fast thermite chemical reactions: A first-principles molecular dynamics study. Physical Review E, 2008, 77, 066103.	0.8	76
138	Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. Applied Physics Letters, 2008, 92, .	1.5	29
139	Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials. Journal of Propulsion and Power, 2007, 23, 688-692.	1.3	14
140	Interaction of Voids and Nanoductility in Silica Glass. Physical Review Letters, 2007, 99, 155506.	2.9	60
141	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
142	Intelligent Optimization of Parallel and Distributed Applications. , 2007, , .		1
143	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
144	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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145	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
146	Parallel history matching and associated forecast atÂtheÂcenter for interactive smart oilfield technologies. Journal of Supercomputing, 2007, 41, 109-117.	2.4	1
147	A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. MRS Bulletin, 2006, 31, 410-418.	1.7	49
148	Sustainable Adaptive Grid Supercomputing: Multiscale Simulation of Semiconductor Processing across the Pacific. , 2006, , .		11
149	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
150	Grid applications---Sustainable adaptive grid supercomputing. , 2006, , .		13
151	MULTIMILLION ATOM SIMULATIONS AND VISUALIZATION OF HYPERVELOCITY IMPACT DAMAGE AND OXIDATION. , 2006, , .		0
152	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
153	Brittle dynamic fracture of crystalline cubic silicon carbide (3C-SiC) via molecular dynamics simulation. Journal of Applied Physics, 2005, 98, 103524.	1.1	98
154	Atomistic mechanisms of amorphization during nanoindentation of SiC: A molecular dynamics study. Physical Review B, 2005, 71, .	1.1	62
155	Oxidation of aluminum nanoclusters. Physical Review B, 2005, 71, .	1.1	88
156	Atomistic processes during nanoindentation of amorphous silicon carbide. Applied Physics Letters, 2005, 86, 021915.	1.5	32
157	Coupling atomistic and continuum length scales in heteroepitaxial systems: Multiscale molecular-dynamics/finite-element simulations of strain relaxation inSiâ^•Si3N4nanopixels. Physical Review B, 2005, 72, .	1.1	7
158	Effect of geometry on stress relaxation in InAsâ^•GaAs rectangular nanomesas: Multimillion-atom molecular dynamics simulations. Journal of Applied Physics, 2005, 98, 114313.	1.1	2
159	Dynamics of Wing Cracks and Nanoscale Damage in Glass. Physical Review Letters, 2005, 95, 135501.	2.9	35
160	A Crossover in the Mechanical Response of Nanocrystalline Ceramics. Science, 2005, 309, 911-914.	6.0	209
161	Strategic Application of Asia-Pacific GRID for Ultrascale Materials Simulations. Journal of the Society of Mechanical Engineers, 2005, 108, 815-817.	0.0	0
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163	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
164	Atomistic mechanisms for wurtzite-to-rocksalt structural transformation in cadmium selenide under pressure. Physical Review B, 2004, 70, .	1.1	74
165	Large-scale molecular dynamics simulations of alkanethiol self-assembled monolayers. Journal of Chemical Physics, 2004, 121, 4323-4330.	1.2	68
166	Nanoindentation-induced amorphization in silicon carbide. Applied Physics Letters, 2004, 85, 378-380.	1.5	78
167	Electric field induced switching of poly(ethylene glycol) terminated self-assembled monolayers: A parallel molecular dynamics simulation. Journal of Chemical Physics, 2004, 121, 5427-5433.	1.2	24
168	Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. Physical Review B, 2004, 70, .	1.1	65
169	Large-scale atomistic simulations of nanoindentation and crack propagation under compression. , 2004, , .		3
170	Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers. Journal of Nanoparticle Research, 2003, 5, 119-135.	0.8	22
171	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. International Journal of Fracture, 2003, 121, 71-79.	1.1	25
172	Scalable and portable implementation of the fast multipole method on parallel computers. Computer Physics Communications, 2003, 153, 445-461.	3.0	49
173	Nanoindentation of silicon nitride: A multimillion-atom molecular dynamics study. Applied Physics Letters, 2003, 82, 118-120.	1.5	73
174	Molecular dynamics study of structural, mechanical, and vibrational properties of crystalline and amorphous Ga1â^'xInxAs alloys. Journal of Applied Physics, 2003, 94, 3840-3848.	1.1	28
175	Structural, mechanical, and vibrational properties of Ga1â^'xInxAs alloys: A molecular dynamics study. Applied Physics Letters, 2003, 82, 1057-1059.	1.5	27
176	InAs/GaAs square nanomesas: Multimillion-atom molecular dynamics simulations on parallel computers. Journal of Applied Physics, 2003, 94, 6762-6773.	1.1	13
177	Immersive and Interactive Exploration of Billion-Atom Systems. Presence: Teleoperators and Virtual Environments, 2003, 12, 85-95.	0.3	29
178	Pressure-induced structural transformation in GaAs:â€ƒA molecular-dynamics study. Physical Review B, 2002, 65, .	1.1	29
179	Scalable Atomistic Simulation Algorithms for Materials Research. Scientific Programming, 2002, 10, 263-270.	0.5	27
180	Large-scale molecular dynamics simulations of materials on parallel computers. AIP Conference Proceedings, 2001, , .	0.3	0

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182	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
183	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
184	Structural transformation, amorphization, and fracture in nanowires: A multimillion-atom molecular dynamics study. Applied Physics Letters, 2001, 78, 3328-3330.	1.5	38
185	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
186	Million-atom molecular dynamics simulation of flat InAs overlayers with self-limiting thickness on GaAs square nanomesas. Applied Physics Letters, 2001, 78, 3717-3719.	1.5	14
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