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	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
2	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
3	Structure of rings in vitreousSiO2. Physical Review B, 1993, 47, 3053-3062.	1.1	216
4	A Crossover in the Mechanical Response of Nanocrystalline Ceramics. Science, 2005, 309, 911-914.	6.0	209
5	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
6	Molecular Dynamics Simulation of Structural Transformation in Silicon Carbide under Pressure. Physical Review Letters, 2000, 84, 3338-3341.	2.9	183
7	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. Journal of Applied Physics, 2008, 103, .	1.1	139
8	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
9	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
10	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
11	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	3.5	107
12	Phonons in graphitic tubules: A tightâ€binding molecular dynamics study. Journal of Chemical Physics, 1995, 103, 6697-6705.	1.2	104
13	Tellurene Photodetector with High Gain and Wide Bandwidth. ACS Nano, 2020, 14, 303-310.	7.3	101
14	Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites. ACS Nano, 2018, 12, 11366-11375.	7.3	99
15	Brittle dynamic fracture of crystalline cubic silicon carbide (3C-SiC) via molecular dynamics simulation. Journal of Applied Physics, 2005, 98, 103524.	1.1	98
16	Structural transformation, intermediate-range order, and dynamical behavior ofSiO2glass at high pressures. Physical Review Letters, 1993, 71, 3146-3149.	2.9	95
17	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
18	Oxidation of aluminum nanoclusters. Physical Review B, 2005, 71, .	1.1	88

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19	Molecular Dynamics Simulations of Rapid Hydrogen Production from Water Using Aluminum Clusters as Catalyzers. Physical Review Letters, 2010, 104, 126102.	2.9	88
20	Nanoindentation-induced amorphization in silicon carbide. Applied Physics Letters, 2004, 85, 378-380.	1.5	78
21	Coupling Length Scales for Multiscale Atomistics-Continuum Simulations: Atomistically Induced Stress Distributions inSi/Si3N4Nanopixels. Physical Review Letters, 2001, 87, 086104.	2.9	77
22	Electronic processes in fast thermite chemical reactions: A first-principles molecular dynamics study. Physical Review E, 2008, 77, 066103.	0.8	76
23	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. Computer Physics Communications, 2008, 178, 73-87.	3.0	75
24	Frequency-dependent dielectric constant prediction of polymers using machine learning. Npj Computational Materials, 2020, 6, .	3.5	75
25	Atomistic mechanisms for wurtzite-to-rocksalt structural transformation in cadmium selenide under pressure. Physical Review B, 2004, 70, .	1.1	74
26	Nanoindentation of silicon nitride: A multimillion-atom molecular dynamics study. Applied Physics Letters, 2003, 82, 118-120.	1.5	73
27	Large-scale molecular dynamics simulations of alkanethiol self-assembled monolayers. Journal of Chemical Physics, 2004, 121, 4323-4330.	1.2	68
28	Polytypism in ultrathin tellurium. 2D Materials, 2019, 6, 015013.	2.0	68
29	Multiresolution molecular dynamics algorithm for realistic materials modeling on parallel computers. Computer Physics Communications, 1994, 83, 197-214.	3.0	67
30	Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. Physical Review B, 2004, 70, .	1.1	65
31	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
32	Variable-charge interatomic potentials for molecular-dynamics simulations of TiO2. Journal of Applied Physics, 1999, 86, 3036-3041.	1.1	64
33	Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. Physical Review B, 2008, 77, .	1.1	63
34	Cholesterol Translocation in a Phospholipid Membrane. Biophysical Journal, 2013, 104, 2429-2436.	0.2	63
35	Atomistic mechanisms of amorphization during nanoindentation of SiC: A molecular dynamics study. Physical Review B, 2005, 71, .	1.1	62
36	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

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37	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
38	Growth of Pore Interfaces and Roughness of Fracture Surfaces in Porous Silica: Million Particle Molecular-Dynamics Simulations. Physical Review Letters, 1994, 73, 2336-2339.	2.9	60
39	Interaction of Voids and Nanoductility in Silica Glass. Physical Review Letters, 2007, 99, 155506.	2.9	60
40	Embrittlement of Metal by Solute Segregation-Induced Amorphization. Physical Review Letters, 2010, 104, 155502.	2.9	60
41	Computational Synthesis of MoS₂ Layers by Reactive Molecular Dynamics Simulations: Initial Sulfidation of MoO₃ Surfaces. Nano Letters, 2017, 17, 4866-4872.	4.5	60
42	Nanobubble Collapse on a Silica Surface in Water: Billion-Atom Reactive Molecular Dynamics Simulations. Physical Review Letters, 2013, 111, 184503.	2.9	59
43	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 18A529.	1.2	57
44	Structural Phase Transformation in Strained Monolayer MoWSe₂ Alloy. ACS Nano, 2018, 12, 3468-3476.	7.3	57
45	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
46	Flexible polyolefin dielectric by strategic design of organic modules for harsh condition electrification. Energy and Environmental Science, 2022, 15, 1307-1314.	15.6	56
47	Enhancing combustion performance of nano-Al/PVDF composites with Î²-PVDF. Combustion and Flame, 2020, 219, 467-477.	2.8	55
48	Ultrafast non-radiative dynamics of atomically thin MoSe2. Nature Communications, 2017, 8, 1745.	5.8	52
49	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
50	Scalable and portable implementation of the fast multipole method on parallel computers. Computer Physics Communications, 2003, 153, 445-461.	3.0	49
51	A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. MRS Bulletin, 2006, 31, 410-418.	1.7	49
52	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
53	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. International Journal of High Performance Computing Applications, 2008, 22, 113-128.	2.4	47
54	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

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55	Deformation mechanisms and damage in Î±-alumina under hypervelocity impact loading. Journal of Applied Physics, 2008, 103, .	1.1	43
56	Poration of lipid bilayers by shock-induced nanobubble collapse. Applied Physics Letters, 2011, 98, .	1.5	43
57	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. Nano Letters, 2019, 19, 6078-6086.	4.5	43
58	Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. Journal of Applied Physics, 2013, 114, 134312.	1.1	42
59	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
60	Structural transformation, amorphization, and fracture in nanowires: A multimillion-atom molecular dynamics study. Applied Physics Letters, 2001, 78, 3328-3330.	1.5	38
61	The nature of free-carrier transport in organometal halide perovskites. Scientific Reports, 2016, 6, 19599.	1.6	38
62	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
63	Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. Chemistry of Materials, 2018, 30, 7262-7268.	3.2	37
64	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
65	Defect migration and recombination in nanoindentation of silica glass. Applied Physics Letters, 2011, 99, .	1.5	36
66	Dynamics of Wing Cracks and Nanoscale Damage in Glass. Physical Review Letters, 2005, 95, 135501.	2.9	35
67	Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. Journal of Applied Physics, 2000, 87, 7708-7711.	1.1	34
68	Semiconductorâ€“metal structural phase transformation in MoTe₂ monolayers by electronic excitation. Nanoscale, 2018, 10, 2742-2747.	2.8	34
69	Large nonadiabatic quantum molecular dynamics simulations on parallel computers. Computer Physics Communications, 2013, 184, 1-8.	3.0	33
70	Atomistic processes during nanoindentation of amorphous silicon carbide. Applied Physics Letters, 2005, 86, 021915.	1.5	32
71	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. SoftwareX, 2019, 10, 100307.	1.2	32
72	Two-Dimensional Lateral Epitaxy of 2H (MoSe₂)â€“1Tâ€² (ReSe₂) Phases. Nano Letters, 2019, 19, 6338-6345.	4.5	30

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73	Pressure-induced structural transformation in GaAs:â€ƒA molecular-dynamics study. Physical Review B, 2002, 65, .	1.1	29
74	Immersive and Interactive Exploration of Billion-Atom Systems. Presence: Teleoperators and Virtual Environments, 2003, 12, 85-95.	0.3	29
75	Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. Applied Physics Letters, 2008, 92, .	1.5	29
76	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
77	Nanoductility induced brittle fracture in shocked high performance ceramics. Applied Physics Letters, 2010, 97, .	1.5	28
78	Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering. Nature Photonics, 2019, 13, 425-430.	15.6	28
79	Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations. Journal of Chemical Information and Modeling, 2021, 61, 2175-2186.	2.5	28
80	Scalable Atomistic Simulation Algorithms for Materials Research. Scientific Programming, 2002, 10, 263-270.	0.5	27
81	Structural, mechanical, and vibrational properties of Ga1â^'xInxAs alloys: A molecular dynamics study. Applied Physics Letters, 2003, 82, 1057-1059.	1.5	27
82	Optical Control of Non-Equilibrium Phonon Dynamics. Nano Letters, 2019, 19, 4981-4989.	4.5	27
83	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. Langmuir, 2020, 36, 7658-7668.	1.6	26
84	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. International Journal of Fracture, 2003, 121, 71-79.	1.1	25
85	Multistage reaction pathways in detonating high explosives. Applied Physics Letters, 2014, 105, .	1.5	25
86	Multiobjective genetic training and uncertainty quantification of reactive force fields. Npj Computational Materials, 2018, 4, .	3.5	25
87	Phonon dispersion and density of states of solid C60. Applied Physics Letters, 1993, 63, 3152-3154.	1.5	24
88	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
89	An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. Computer Physics Communications, 2015, 192, 91-96.	3.0	24
90	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. Journal of Applied Physics, 2018, 123, .	1.1	24

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91	Towards simulation of the dynamics of materials on quantum computers. Physical Review B, 2020, 101, .	1.1	23
92	Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers. Journal of Nanoparticle Research, 2003, 5, 119-135.	0.8	22
93	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
94	Plane shock loading on mono- and nano-crystalline silicon carbide. Applied Physics Letters, 2018, 112, .	1.5	22
95	Thermal conductivity of MoS2 monolayers from molecular dynamics simulations. AIP Advances, 2019, 9, .	0.6	22
96	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
97	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
98	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
99	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
100	Critical lateral size for stress domain formation in InAs/GaAs square nanomesas: A multimillion-atom molecular dynamics study. Applied Physics Letters, 2001, 79, 4577-4579.	1.5	19
101	Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. Journal of Supercomputing, 2012, 62, 946-966.	2.4	19
102	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
103	Molecular Simulation of MoS2 Exfoliation. Scientific Reports, 2018, 8, 16761.	1.6	19
104	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
105	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
106	Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	18
107	Molecular dynamics nanoindentation simulation of an energetic material. Applied Physics Letters, 2008, 93, 171908.	1.5	17
108	Universal stretched exponential relaxation in nanoconfined water. Applied Physics Letters, 2014, 105, .	1.5	17

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109	Picosecond amorphization of SiO ₂ stishovite under tension. Science Advances, 2017, 3, e1602339.	4.7	17
110	Bonding and Structure of Ceramic-Ceramic Interfaces. Physical Review Letters, 2013, 111, 066103.	2.9	16
111	Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in MoSe₂ Monolayer. Nano Letters, 2018, 18, 4653-4658.	4.5	16
112	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
113	Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics. Physical Review Letters, 2021, 126, 216403.	2.9	16
114	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
115	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. Scientific Reports, 2016, 6, 24109.	1.6	15
116	RXMD: A scalable reactive molecular dynamics simulator for optimized time-to-solution. SoftwareX, 2020, 11, 100389.	1.2	15
117	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
118	Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials. Journal of Propulsion and Power, 2007, 23, 688-692.	1.3	14
119	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
120	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
121	Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials. Npj Computational Materials, 2021, 7, .	3.5	14
122	InAs/GaAs square nanomesas: Multimillion-atom molecular dynamics simulations on parallel computers. Journal of Applied Physics, 2003, 94, 6762-6773.	1.1	13
123	Grid applications---Sustainable adaptive grid supercomputing. , 2006, , .		13
124	Crystalline anisotropy of shock-induced phenomena: Omni-directional multiscale shock technique. Applied Physics Letters, 2016, 108, .	1.5	13
125	Faceting, Grain Growth, and Crack Healing in Alumina. ACS Nano, 2018, 12, 9005-9010.	7.3	13
126	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

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127	Autonomous reinforcement learning agent for stretchable kirigami design of 2D materials. Npj Computational Materials, 2021, 7, .	3.5	13
128	Photoexcitation Induced Ultrafast Nonthermal Amorphization in Sb₂Te₃. Journal of Physical Chemistry Letters, 2020, 11, 10242-10249.	2.1	12
129	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
130	Sustainable Adaptive Grid Supercomputing: Multiscale Simulation of Semiconductor Processing across the Pacific. , 2006, , .		11
131	Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. AIP Advances, 2011, 1, .	0.6	11
132	Collective oxidation behavior of aluminum nanoparticle aggregate. Applied Physics Letters, 2013, 102, 221904.	1.5	11
133	A crossover in anisotropic nanomechanochemistry of van der Waals crystals. Applied Physics Letters, 2015, 107, .	1.5	11
134	Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality. SoftwareX, 2019, 9, 112-116.	1.2	11
135	Review of strategies toward the development of alloy two-dimensional (2D) transition metal dichalcogenides. IScience, 2021, 24, 103532.	1.9	11
136	Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers. Progress of Theoretical Physics Supplement, 2000, 138, 175-190.	0.2	10
137	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
138	Exploiting hierarchical parallelisms for molecular dynamics simulation on multicore clusters. Journal of Supercomputing, 2011, 57, 20-33.	2.4	10
139	Atomistic mechanisms of rapid energy transport in light-harvesting molecules. Applied Physics Letters, 2011, 98, 113302.	1.5	10
140	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
141	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
142	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, .	1.1	10
143	Boltzmann machine modeling of layered MoS2 synthesis on a quantum annealer. Computational Materials Science, 2020, 173, 109429.	1.4	10
144	Differences in Sb2Te3 growth by pulsed laser and sputter deposition. Acta Materialia, 2020, 200, 811-820.	3.8	10

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145	Phononâ€induced electron localization and magneticâ€field effects in a double quantum dot. Applied Physics Letters, 1993, 62, 3470-3472.	1.5	9
146	Reactivity of Sulfur Molecules on MoO₃ (010) Surface. Journal of Physical Chemistry Letters, 2017, 8, 6206-6210.	2.1	9
147	Effects of chemical defects on anisotropic dielectric response of polyethylene. AIP Advances, 2019, 9, .	0.6	9
148	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
149	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand. , 2014, , .		8
150	Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals. Applied Physics Letters, 2018, 112, .	1.5	8
151	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. Journal of Physical Chemistry Letters, 2019, 10, 3937-3943.	2.1	8
152	Nanoindentation on Monolayer MoS₂ Kirigami. ACS Omega, 2019, 4, 9952-9956.	1.6	8
153	Lattice thermal transport in two-dimensional alloys and fractal heterostructures. Scientific Reports, 2021, 11, 1656.	1.6	8
154	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
155	Nonlinear electron dynamics in a resonant tunneling diode: Langevinâ€quantumâ€dynamics simulations on a massively parallel computer. Applied Physics Letters, 1994, 64, 2569-2571.	1.5	7
156	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
157	Memristive Device Characteristics Engineering by Controlling the Crystallinity of Switching Layer Materials. ACS Applied Electronic Materials, 2020, 2, 1529-1537.	2.0	7
158	Direct Atomic Simulations of Facet Formation and Equilibrium Shapes of SiC Nanoparticles. Crystal Growth and Design, 2020, 20, 2147-2152.	1.4	7
159	Distribution of Rings and Intermediate Range Correlations in Silica Glass Under Pressure-A Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 1995, 408, 333.	0.1	6
160	Heat-Initiated Oxidation of an Aluminum Nanoparticle. Materials Research Society Symposia Proceedings, 2012, 1405, .	0.1	6
161	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
162	Field-Induced Carrier Localization Transition in Dielectric Polymers. Journal of Physical Chemistry Letters, 2020, 11, 352-358.	2.1	6

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163	PND: Physics-informed neural-network software for molecular dynamics applications. SoftwareX, 2021, 15, 100789.	1.2	6
164	Effect of pressure on intermolecular and intramolecular phonons in solid C60. Journal of Chemical Physics, 1993, 99, 10001-10010.	1.2	5
165	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
166	Ion dynamics at porous alumina surfaces. Applied Physics Letters, 2012, 101, 063106.	1.5	5
167	Small interfering ribonucleic acid induces liquid-to-ripple phase transformation in a phospholipid membrane. Applied Physics Letters, 2014, 105, 113702.	1.5	5
168	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.5	5
169	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. Computing in Science and Engineering, 2019, 21, 64-75.	1.2	5
170	Domain-specific compilers for dynamic simulations of quantum materials on quantum computers. Quantum Science and Technology, 2021, 6, 014007.	2.6	5
171	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
172	Multistage reaction pathways in detonating RDX. AIP Conference Proceedings, 2017, , .	0.3	4
173	Gel phase in hydrated calcium dipicolinate. Applied Physics Letters, 2017, 111, .	1.5	4
174	Photo-induced lattice contraction in layered materials. Journal of Physics Condensed Matter, 2018, 30, 32LT02.	0.7	4
175	Rapid and reversible lithiation of doped biogenous iron oxide nanoparticles. Scientific Reports, 2019, 9, 1828.	1.6	4
176	Neural Network Analysis of Dynamic Fracture in a Layered Material. MRS Advances, 2019, 4, 1109-1117.	0.5	4
177	Optically Induced Three-Stage Picosecond Amorphization in Low-Temperature SrTiO₃. Journal of Physical Chemistry Letters, 2020, 11, 9605-9612.	2.1	4
178	Reactive molecular dynamics simulations and machine learning. Journal of Physics: Conference Series, 2020, 1461, 012182.	0.3	4
179	Parallel Algorithms for Molecular-Dynamics Simulations of Coulombic Systems. Materials Research Society Symposia Proceedings, 1992, 291, 267.	0.1	3
180	Large Scale Molecular Dynamics Study of Amorphous Carbon and Graphite on Parallel Machines. Materials Research Society Symposia Proceedings, 1995, 408, 113.	0.1	3

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181	Molecular Dynamics Study Of Si/Si₃N₄ Interface. Materials Research Society Symposia Proceedings, 1996, 446, 157.	0.1	3
182	Oxidation Dynamics of Nanophase Aluminum Clusters: A Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 1997, 481, 625.	0.1	3
183	Large-scale atomistic simulations of nanoindentation and crack propagation under compression. , 2004, , .		3
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