Priya D Vashishta

List of Publications by Year in Descending Order

222 papers	5,566 citations	44 h-index	66 g-index
237 ext. papers	6,353 ext. citations	5.5 avg, IF	5.46 L-index

#	Paper	IF	Citations
222	Flexible polyolefin dielectric by strategic design of organic modules for harsh condition electrification. *Energy and Environmental Science*, **2022**, 15, 1307-1314	35.4	5
221	Exploring far-from-equilibrium ultrafast polarization control in ferroelectric oxides with excited-state neural network quantum molecular dynamics.. *Science Advances*, **2022**, 8, eabk2625	14.3	1
220	Review of strategies toward the development of alloy two-dimensional (2D) transition metal dichalcogenides.. *IScience*, **2021**, 24, 103532	6.1	3
219	Domain-specific compilers for dynamic simulations of quantum materials on quantum computers. *Quantum Science and Technology*, **2021**, 6, 014007	5.5	2
218	Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations. *Journal of Chemical Information and Modeling*, **2021**, 61, 2175-2186	6.1	8
217	Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics. *Physical Review Letters*, **2021**, 126, 216403	7.4	6
216	Neural Network Quantum Molecular Dynamics, Intermediate Range Order in GeSe, and Neutron Scattering Experiments. *Journal of Physical Chemistry Letters*, **2021**, 12, 6020-6028	6.4	2
215	PND: Physics-informed neural-network software for molecular dynamics applications. *SoftwareX*, **2021**, 15, 100789	2.7	1
214	Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials. *Npj Computational Materials*, **2021**, 7,	10.9	4
213	Carrier-specific dynamics in 2H-MoTe observed by femtosecond soft x-ray absorption spectroscopy using an x-ray free-electron laser. *Structural Dynamics*, **2021**, 8, 014501	3.2	5
212	Sulfurization of MoO in the Chemical Vapor Deposition Synthesis of MoS Enhanced by an HS/H Mixture. *Journal of Physical Chemistry Letters*, **2021**, 12, 1997-2003	6.4	3
211	Mechanical behavior of ultralight nickel metamaterial. *Applied Physics Letters*, **2021**, 118, 081902	3.4	1
210	Unveiling oxidation mechanism of bulk ZrS2. *MRS Advances*, **2021**, 6, 303-306	0.7	0
209	Autonomous reinforcement learning agent for stretchable kirigami design of 2D materials. *Npj Computational Materials*, **2021**, 7,	10.9	2
208	Lattice thermal transport in two-dimensional alloys and fractal heterostructures. *Scientific Reports*, **2021**, 11, 1656	4.9	2
207	Reactive molecular dynamics simulations and machine learning. *Journal of Physics: Conference Series*, **2020**, 1461, 012182	0.3	2
206	Towards simulation of the dynamics of materials on quantum computers. *Physical Review B*, **2020**, 101,	3.3	7

205	Memristive Device Characteristics Engineering by Controlling the Crystallinity of Switching Layer Materials. *ACS Applied Electronic Materials*, **2020**, 2, 1529-1537	4	3
204	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. *Langmuir*, **2020**, 36, 7658-7668	4	8
203	Frequency-dependent dielectric constant prediction of polymers using machine learning. *Npj Computational Materials*, **2020**, 6,	10.9	35
202	Evolutionary multi-objective optimization and Pareto-frontal uncertainty quantification of interatomic forcefields for thermal conductivity simulations. *Computer Physics Communications*, **2020**, 254, 107337	4.2	4
201	Enhancing combustion performance of nano-Al/PVDF composites with PVDF. *Combustion and Flame*, **2020**, 219, 467-477	5.3	17
200	Direct Atomic Simulations of Facet Formation and Equilibrium Shapes of SiC Nanoparticles. *Crystal Growth and Design*, **2020**, 20, 2147-2152	3.5	1
199	Synergistically Chemical and Thermal Coupling between Graphene Oxide and Graphene Fluoride for Enhancing Aluminum Combustion. *ACS Applied Materials & Interfaces*, **2020**, 12, 7451-7458	9.5	22
198	RXMD: A scalable reactive molecular dynamics simulator for optimized time-to-solution. *SoftwareX*, **2020**, 11, 100389	2.7	7
197	Quantum Dynamics at Scale **2020**,		1
196	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	6.4	6
195	Field-Induced Carrier Localization Transition in Dielectric Polymers. *Journal of Physical Chemistry Letters*, **2020**, 11, 352-358	6.4	4
194	Tellurene Photodetector with High Gain and Wide Bandwidth. *ACS Nano*, **2020**, 14, 303-310	16.7	55
193	Boltzmann machine modeling of layered MoS2 synthesis on a quantum annealer. *Computational Materials Science*, **2020**, 173, 109429	3.2	2
192	Neural Network Molecular Dynamics at Scale **2020**,		2
191	Differences in Sb2Te3 growth by pulsed laser and sputter deposition. *Acta Materialia*, **2020**, 200, 811-820	8.4	4
190	Photoexcitation Induced Ultrafast Nonthermal Amorphization in SbTe. *Journal of Physical Chemistry Letters*, **2020**, 11, 10242-10249	6.4	5
189	Growth Kinetics and Atomistic Mechanisms of Native Oxidation of ZrSSe and MoS Crystals. *Nano Letters*, **2020**, 20, 8592-8599	11.5	6
188	Simultaneous Observation of Carrier-Specific Redistribution and Coherent Lattice Dynamics in 2H-MoTe with Femtosecond Core-Level Spectroscopy. *ACS Nano*, **2020**, 14, 15829-15840	16.7	15

187	Optically Induced Three-Stage Picosecond Amorphization in Low-Temperature SrTiO. *Journal of Physical Chemistry Letters*, **2020**, 11, 9605-9612	6.4	2
186	Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality. *SoftwareX*, **2019**, 9, 112-116	2.7	5
185	Effects of chemical defects on anisotropic dielectric response of polyethylene. *AIP Advances*, **2019**, 9, 045022	1.5	5
184	Nanoindentation on Monolayer MoS Kirigami. *ACS Omega*, **2019**, 4, 9952-9956	3.9	4
183	Defect Healing in Layered Materials: A Machine Learning-Assisted Characterization of MoS Crystal Phases. *Journal of Physical Chemistry Letters*, **2019**, 10, 2739-2744	6.4	11
182	Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering. *Nature Photonics*, **2019**, 13, 425-430	33.9	19
181	Thermal conductivity of MoS2 monolayers from molecular dynamics simulations. *AIP Advances*, **2019**, 9, 035042	1.5	13
180	Rapid and reversible lithiation of doped biogenous iron oxide nanoparticles. *Scientific Reports*, **2019** , 9, 1828	4.9	2
179	Structural phase transitions in a MoWSe2 monolayer: Molecular dynamics simulations and variational autoencoder analysis. *Physical Review B*, **2019**, 100,	3.3	4
178	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. *SoftwareX*, **2019**, 10, 100307	2.7	21
177	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. *Nano Letters*, **2019**, 19, 6078-6086	11.5	27
176	Two-Dimensional Lateral Epitaxy of 2H (MoSe)-1T′ (ReSe) Phases. *Nano Letters*, **2019**, 19, 6338-6345	11.5	18
175	Optical Control of Non-Equilibrium Phonon Dynamics. *Nano Letters*, **2019**, 19, 4981-4989	11.5	18
174	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. *Journal of Physical Chemistry Letters*, **2019**, 10, 3937-3943	6.4	6
173	Hydrogen Bond Preserving Stress Release Mechanism Is Key to the Resilience of Aramid Fibers. *Journal of Physical Chemistry B*, **2019**, 123, 9719-9723	3.4	2
172	Guidelines for creating artificial neural network empirical interatomic potential from first-principles molecular dynamics data under specific conditions and its application to AgSe. *Journal of Chemical Physics*, **2019**, 151, 124303	3.9	12
171	Electrostrictive Cavitation in Water Induced by a SnO Nanoparticle. *ACS Omega*, **2019**, 4, 22274-22279	3.9	1
170	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. *Physical Review B*, **2019**, 100,	3.3	7

169	Neural Network Analysis of Dynamic Fracture in a Layered Material. *MRS Advances*, **2019**, 4, 1109-1117	0.7	2
168	Polytypism in ultrathin tellurium. *2D Materials*, **2019**, 6, 015013	5.9	48
167	Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis. *Computing in Science and Engineering*, **2019**, 21, 64-75	1.5	3
166	Structural Phase Transformation in Strained Monolayer MoWSe Alloy. *ACS Nano*, **2018**, 12, 3468-3476	16.7	38
165	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	3.8	29
164	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. *Journal of Applied Physics*, **2018**, 123, 145902	2.5	19
163	A Reactive Molecular Dynamics Study of Atomistic Mechanisms During Synthesis of MoS2 Layers by Chemical Vapor Deposition. *MRS Advances*, **2018**, 3, 307-311	0.7	3
162	Semiconductor-metal structural phase transformation in MoTe monolayers by electronic excitation. *Nanoscale*, **2018**, 10, 2742-2747	7.7	25
161	Plane shock loading on mono- and nano-crystalline silicon carbide. *Applied Physics Letters*, **2018**, 112, 111909	3.4	15
160	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. *MRS Advances*, **2018**, 3, 397-402	0.7	4
159	Multiobjective genetic training and uncertainty quantification of reactive force fields. *Npj Computational Materials*, **2018**, 4,	10.9	19
158	Faceting, Grain Growth, and Crack Healing in Alumina. *ACS Nano*, **2018**, 12, 9005-9010	16.7	10
157	Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in MoSe Monolayer. *Nano Letters*, **2018**, 18, 4653-4658	11.5	14
156	Molecular Simulation of MoS Exfoliation. *Scientific Reports*, **2018**, 8, 16761	4.9	9
155	Active learning for accelerated design of layered materials. *Npj Computational Materials*, **2018**, 4,	10.9	71
154	Photo-induced lattice contraction in layered materials. *Journal of Physics Condensed Matter*, **2018**, 30, 32LT02	1.8	3
153	Role of H Transfer in the Gas-Phase Sulfidation Process of MoO: A Quantum Molecular Dynamics Study. *Journal of Physical Chemistry Letters*, **2018**, 9, 6517-6523	6.4	6
152	Free energy of hydration and heat capacity of calcium dipicolinate in Bacillus spore cores. *Applied Physics Letters*, **2018**, 113, 113702	3.4	1

151	Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites. *ACS Nano*, **2018**, 12, 11366-11375	16.7	51
150	Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. *Chemistry of Materials*, **2018**, 30, 7262-7268	9.6	23
149	Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals. *Applied Physics Letters*, **2018**, 112, 211604	3.4	6
148	Multistage reaction pathways in detonating RDX **2017**,		4
147	Picosecond amorphization of SiO stishovite under tension. *Science Advances*, **2017**, 3, e1602339	14.3	11
146	Re Doping in 2D Transition Metal Dichalcogenides as a New Route to Tailor Structural Phases and Induced Magnetism. *Advanced Materials*, **2017**, 29, 1703754	24	130
145	Multiple Reaction Pathways in Shocked 2,4,6-Triamino-1,3,5-trinitrobenzene Crystal. *Journal of Physical Chemistry C*, **2017**, 121, 16029-16034	3.8	14
144	Reactivity of Sulfur Molecules on MoO (010) Surface. *Journal of Physical Chemistry Letters*, **2017**, 8, 6206-6210	6.4	8
143	Gel phase in hydrated calcium dipicolinate. *Applied Physics Letters*, **2017**, 111, 213701	3.4	3
142	Ultrafast non-radiative dynamics of atomically thin MoSe. *Nature Communications*, **2017**, 8, 1745	17.4	35
141	Computational Synthesis of MoS Layers by Reactive Molecular Dynamics Simulations: Initial Sulfidation of MoO Surfaces. *Nano Letters*, **2017**, 17, 4866-4872	11.5	45
140	Analysis of killing of growing cells and dormant and germinated spores of Bacillus species by black silicon nanopillars. *Scientific Reports*, **2017**, 7, 17768	4.9	15
139	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	0.7	2
138	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. *Scientific Reports*, **2016**, 6, 24109	4.9	14
137	Crystalline anisotropy of shock-induced phenomena: Omni-directional multiscale shock technique. *Applied Physics Letters*, **2016**, 108, 071901	3.4	10
136	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	3.9	11
135	The nature of free-carrier transport in organometal halide perovskites. *Scientific Reports*, **2016**, 6, 19599	4.9	35
134	An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. *Computer Physics Communications*, **2015**, 192, 91-96	4.2	20

133	Reactive Molecular Dynamics Simulations, Data Analytics and Visualization. *Materials Research Society Symposia Proceedings*, **2015**, 1756, 1		
132	A crossover in anisotropic nanomechanochemistry of van der Waals crystals. *Applied Physics Letters*, **2015**, 107, 231903	3.4	9
131	Reactive Molecular Dynamics Study of Oxidation of Aggregated Aluminum Nanoparticles. *Materials Research Society Symposia Proceedings*, **2015**, 1758, 1		1
130	Multistage reaction pathways in detonating high explosives. *Applied Physics Letters*, **2014**, 105, 204103	3.4	21
129	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand **2014**,		4
128	Small interfering ribonucleic acid induces liquid-to-ripple phase transformation in a phospholipid membrane. *Applied Physics Letters*, **2014**, 105, 113702	3.4	5
127	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. *Journal of Chemical Physics*, **2014**, 140, 18A529	3.9	50
126	Universal stretched exponential relaxation in nanoconfined water. *Applied Physics Letters*, **2014**, 105, 161907	3.4	14
125	Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study. *Applied Physics Letters*, **2014**, 104, 141904	3.4	14
124	Bonding and structure of ceramic-ceramic interfaces. *Physical Review Letters*, **2013**, 111, 066103	7.4	13
123	Analysis of scalable data-privatization threading algorithms for hybrid MPI/OpenMP parallelization of molecular dynamics. *Journal of Supercomputing*, **2013**, 66, 406-430	2.5	13
122	Cholesterol translocation in a phospholipid membrane. *Biophysical Journal*, **2013**, 104, 2429-36	2.9	60
121	Collective oxidation behavior of aluminum nanoparticle aggregate. *Applied Physics Letters*, **2013**, 102, 221904	3.4	9
120	Large nonadiabatic quantum molecular dynamics simulations on parallel computers. *Computer Physics Communications*, **2013**, 184, 1-8	4.2	32
119	Nanobubble collapse on a silica surface in water: billion-atom reactive molecular dynamics simulations. *Physical Review Letters*, **2013**, 111, 184503	7.4	49
118	Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. *Journal of Applied Physics*, **2013**, 114, 134312	2.5	36
117	Oxidation Dynamics of a Chain of Aluminum Nanoparticles. *Materials Research Society Symposia Proceedings*, **2013**, 1521, 1		
116	Oxidation Dynamics of Aluminum Nanorods. *Materials Research Society Symposia Proceedings*, **2013**, 1521, 1		

115	Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. *Journal of Supercomputing*, **2012**, 62, 946-966	2.5	10
114	Supercrystals of DNA-Functionalized Gold Nanoparticles: A Million-Atom Molecular Dynamics Simulation Study. *Journal of Physical Chemistry C*, **2012**, 116, 19579-19585	3.8	20
113	Ion dynamics at porous alumina surfaces. *Applied Physics Letters*, **2012**, 101, 063106	3.4	4
112	Heat-Initiated Oxidation of an Aluminum Nanoparticle. *Materials Research Society Symposia Proceedings*, **2012**, 1405,		5
111	Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. *AIP Advances*, **2011**, 1, 042149	1.5	10
110	Exploiting hierarchical parallelisms for molecular dynamics simulation on multicore clusters. *Journal of Supercomputing*, **2011**, 57, 20-33	2.5	6
109	Sulfur-impurity induced amorphization of nickel. *Journal of Applied Physics*, **2011**, 110, 063501	2.5	2
108	Poration of lipid bilayers by shock-induced nanobubble collapse. *Applied Physics Letters*, **2011**, 98, 023701	3.4	35
107	Atomistic mechanisms of rapid energy transport in light-harvesting molecules. *Applied Physics Letters*, **2011**, 98, 113302	3.4	10
106	Defect migration and recombination in nanoindentation of silica glass. *Applied Physics Letters*, **2011**, 99, 111906	3.4	30
105	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, 033514	2.5	50
104	Molecular dynamics simulations of rapid hydrogen production from water using aluminum clusters as catalyzers. *Physical Review Letters*, **2010**, 104, 126102	7.4	78
103	Embrittlement of metal by solute segregation-induced amorphization. *Physical Review Letters*, **2010**, 104, 155502	7.4	58
102	Nanoductility induced brittle fracture in shocked high performance ceramics. *Applied Physics Letters* , **2010**, 97, 111903	3.4	23
101	Enhanced reactivity of nanoenergetic materials: A first-principles molecular dynamics study based on divide-and-conquer density functional theory. *Applied Physics Letters*, **2009**, 95, 043114	3.4	32
100	Response to Comment on Nanoindentation hardness anisotropy of alumina crystal: a molecular-dynamics study [Appl. Phys. Lett. 94, 146101 (2009)]. *Applied Physics Letters*, **2009**, 94, 146102	3.4	2
99	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. *Journal of Applied Physics*, **2008**, 103, 083504	2.5	104
98	Deformation mechanisms and damage in alumina under hypervelocity impact loading. *Journal of Applied Physics*, **2008**, 103, 083508	2.5	36

97	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. *International Journal of High Performance Computing Applications*, **2008**, 22, 113-128	1.8	41
96	Molecular dynamics nanoindentation simulation of an energetic material. *Applied Physics Letters*, **2008**, 93, 171908	3.4	11
95	Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. *Physical Review B*, **2008**, 77,	3.3	58
94	Electronic processes in fast thermite chemical reactions: a first-principles molecular dynamics study. *Physical Review E*, **2008**, 77, 066103	2.4	64
93	Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. *Applied Physics Letters*, **2008**, 92, 161904	3.4	20
92	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. *Computer Physics Communications*, **2008**, 178, 73-87	4.2	63
91	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	4.2	5
90	Parallel history matching and associated forecast at the center for interactive smart oilfield technologies. *Journal of Supercomputing*, **2007**, 41, 109-117	2.5	1
89	Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials. *Journal of Propulsion and Power*, **2007**, 23, 688-692	1.8	13
88	Interaction of voids and nanoductility in silica glass. *Physical Review Letters*, **2007**, 99, 155506	7.4	51
87	Dynamic transition in the structure of an energetic crystal during chemical reactions at shock front prior to detonation. *Physical Review Letters*, **2007**, 99, 148303	7.4	113
86	A divide-and-conquer/cellular-decomposition framework for million-to-billion atom simulations of chemical reactions. *Computational Materials Science*, **2007**, 38, 642-652	3.2	82
85	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	2.5	208
84	Grid applications---Sustainable adaptive grid supercomputing **2006**,		3
83	A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. *MRS Bulletin*, **2006**, 31, 410-418	3.2	38
82	**2006**,		10
81	Multimillion atom simulations of dynamics of oxidation of an aluminum nanoparticle and nanoindentation on ceramics. *Journal of Physical Chemistry B*, **2006**, 110, 3727-33	3.4	58
80	A crossover in the mechanical response of nanocrystalline ceramics. *Science*, **2005**, 309, 911-4	33.3	185

79	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	4.2	57
78	Dynamics of Consolidation and Crack Growth in Nanocluster-Assembled Amorphous Silicon Nitride. *Journal of the American Ceramic Society*, **2005**, 81, 433-436	3.8	20
77	Brittle dynamic fracture of crystalline cubic silicon carbide (3C-SiC) via molecular dynamics simulation. *Journal of Applied Physics*, **2005**, 98, 103524	2.5	79
76	Atomistic mechanisms of amorphization during nanoindentation of SiC: A molecular dynamics study. *Physical Review B*, **2005**, 71,	3.3	50
75	Oxidation of aluminum nanoclusters. *Physical Review B*, **2005**, 71,	3.3	78
74	Atomistic processes during nanoindentation of amorphous silicon carbide. *Applied Physics Letters*, **2005**, 86, 021915	3.4	28
73	Coupling atomistic and continuum length scales in heteroepitaxial systems: Multiscale molecular-dynamics/finite-element simulations of strain relaxation in Si□i3N4 nanopixels. *Physical Review B*, **2005**, 72,	3.3	6
72	Effect of geometry on stress relaxation in InAs□aAs rectangular nanomesas: Multimillion-atom molecular dynamics simulations. *Journal of Applied Physics*, **2005**, 98, 114313	2.5	2
71	Dynamics of wing cracks and nanoscale damage in glass. *Physical Review Letters*, **2005**, 95, 135501	7.4	33
70	Strategic Application of Asia-Pacific GRID for Ultrascale Materials Simulations. *Journal of the Society of Mechanical Engineers*, **2005**, 108, 815-817	0	
69	VIRTUALIZATION-AWARE APPLICATION FRAMEWORK FOR HIERARCHICAL MULTISCALE SIMULATIONS ON A GRID. *Lecture Notes Series, Institute for Mathematical Sciences*, **2005**, 229-243	0.1	
68	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	2.5	42
67	Atomistic mechanisms for wurtzite-to-rocksalt structural transformation in cadmium selenide under pressure. *Physical Review B*, **2004**, 70,	3.3	70
66	Large-scale molecular dynamics simulations of alkanethiol self-assembled monolayers. *Journal of Chemical Physics*, **2004**, 121, 4323-30	3.9	63
65	Nanoindentation-induced amorphization in silicon carbide. *Applied Physics Letters*, **2004**, 85, 378-380	3.4	67
64	Electric field induced switching of poly(ethylene glycol) terminated self-assembled monolayers: a parallel molecular dynamics simulation. *Journal of Chemical Physics*, **2004**, 121, 5427-33	3.9	22
63	Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. *Physical Review B*, **2004**, 70,	3.3	59
62	Immersive and Interactive Exploration of Billion-Atom Systems. *Presence: Teleoperators and Virtual Environments*, **2003**, 12, 85-95	2.9	22

61	Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers. *Journal of Nanoparticle Research*, **2003**, 5, 119-135	2.3	18
60	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. *International Journal of Fracture*, **2003**, 121, 71-79	2.3	21
59	Scalable and portable implementation of the fast multipole method on parallel computers. *Computer Physics Communications*, **2003**, 153, 445-461	4.2	44
58	Nanoindentation of silicon nitride: A multimillion-atom molecular dynamics study. *Applied Physics Letters*, **2003**, 82, 118-120	3.4	66
57	Molecular dynamics study of structural, mechanical, and vibrational properties of crystalline and amorphous Ga1−InxAs alloys. *Journal of Applied Physics*, **2003**, 94, 3840-3848	2.5	27
56	Structural, mechanical, and vibrational properties of Ga1−InxAs alloys: A molecular dynamics study. *Applied Physics Letters*, **2003**, 82, 1057-1059	3.4	24
55	InAs/GaAs square nanomesas: Multimillion-atom molecular dynamics simulations on parallel computers. *Journal of Applied Physics*, **2003**, 94, 6762-6773	2.5	12
54	Scalable Atomistic Simulation Algorithms for Materials Research. *Scientific Programming*, **2002**, 10, 263-270	1.4	18
53	Pressure-induced structural transformation in GaAs: A molecular-dynamics study. *Physical Review B*, **2002**, 65,	3.3	24
52	Multimillion atom simulation of materials on parallel computers nanopixel, interfacial fracture, nanoindentation, and oxidation. *Applied Surface Science*, **2001**, 182, 258-264	6.7	19
51	Hybrid finite-element/molecular-dynamics/electronic-density-functional approach to materials simulations on parallel computers. *Computer Physics Communications*, **2001**, 138, 143-154	4.2	123
50	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	4.2	106
49	Structural transformation, amorphization, and fracture in nanowires: A multimillion-atom molecular dynamics study. *Applied Physics Letters*, **2001**, 78, 3328-3330	3.4	32
48	Dynamic Fracture Mechanisms in Nanostructured and Amorphous Silica Glasses Million-Atom Molecular Dynamics Simulations. *Materials Research Society Symposia Proceedings*, **2001**, 703, 1		9
47	Million-atom molecular dynamics simulation of flat InAs overlayers with self-limiting thickness on GaAs square nanomesas. *Applied Physics Letters*, **2001**, 78, 3717-3719	3.4	11
46	Coupling length scales for multiscale atomistics-continuum simulations: atomistically induced stress distributions in Si/Si3N4 nanopixels. *Physical Review Letters*, **2001**, 87, 086104	7.4	66
45	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	3.4	17
44	Coupling of Length Scales: Hybrid Molecular Dynamics and Finite Element Approach for Multiscale Nanodevice Simulations. *Materials Research Society Symposia Proceedings*, **2000**, 653, 1		

43	Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. *Journal of Applied Physics*, **2000**, 87, 7708-7711	2.5	30
42	Amorphization and anisotropic fracture dynamics during nanoindentation of silicon nitride: A multimillion atom molecular dynamics study. *Applied Physics Letters*, **2000**, 77, 4332-4334	3.4	44
41	Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers. *Progress of Theoretical Physics Supplement*, **2000**, 138, 175-190		10
40	Molecular dynamics simulation of structural transformation in silicon carbide under pressure. *Physical Review Letters*, **2000**, 84, 3338-41	7.4	158
39	Sintering, structure, and mechanical properties of nanophase SiC: A molecular-dynamics and neutron scattering study. *Applied Physics Letters*, **2000**, 77, 1132-1134	3.4	37
38	Dynamics of Oxidation of Aluminum Nanoclusters using Variable Charge Molecular-Dynamics Simulations on Parallel Computers. *Physical Review Letters*, **1999**, 82, 4866-4869	7.4	267
37	Variable-charge interatomic potentials for molecular-dynamics simulations of TiO2. *Journal of Applied Physics*, **1999**, 86, 3036-3041	2.5	60
36	Multimillion-Atom Simulations of Atomic-Level Surface Stresses and Pressure Distribution on InAs/GaAs Mesas. *Materials Research Society Symposia Proceedings*, **1999**, 584, 269		1
35	Molecular Dynamics Simulations of Nanoindentation of Silicon Nitride. *Materials Research Society Symposia Proceedings*, **1998**, 539, 119		2
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