Priya D Vashishta

List of Publications by Citations

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	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
221	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
220	Structure of rings in vitreous SiO2. *Physical Review B*, **1993**, 47, 3053-3062	3.3	198
219	A crossover in the mechanical response of nanocrystalline ceramics. *Science*, **2005**, 309, 911-4	33.3	185
218	Molecular dynamics simulation of structural transformation in silicon carbide under pressure. *Physical Review Letters*, **2000**, 84, 3338-41	7.4	158
217	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
216	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
215	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
214	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
213	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. *Journal of Applied Physics*, **2008**, 103, 083504	2.5	104
212	Phonons in graphitic tubules: A tight-binding molecular dynamics study. *Journal of Chemical Physics*, **1995**, 103, 6697-6705	3.9	97
211	Structural transformation, intermediate-range order, and dynamical behavior of SiO2 glass at high pressures. *Physical Review Letters*, **1993**, 71, 3146-3149	7.4	90
210	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
209	Brittle dynamic fracture of crystalline cubic silicon carbide (3C-SiC) via molecular dynamics simulation. *Journal of Applied Physics*, **2005**, 98, 103524	2.5	79
208	Molecular dynamics simulations of rapid hydrogen production from water using aluminum clusters as catalyzers. *Physical Review Letters*, **2010**, 104, 126102	7.4	78
207	Oxidation of aluminum nanoclusters. *Physical Review B*, **2005**, 71,	3.3	78
206	Active learning for accelerated design of layered materials. *Npj Computational Materials*, **2018**, 4,	10.9	71

205	Atomistic mechanisms for wurtzite-to-rocksalt structural transformation in cadmium selenide under pressure. *Physical Review B*, **2004**, 70,	3.3	70
204	Nanoindentation-induced amorphization in silicon carbide. *Applied Physics Letters*, **2004**, 85, 378-380	3.4	67
203	Nanoindentation of silicon nitride: A multimillion-atom molecular dynamics study. *Applied Physics Letters*, **2003**, 82, 118-120	3.4	66
202	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
201	Electronic processes in fast thermite chemical reactions: a first-principles molecular dynamics study. *Physical Review E*, **2008**, 77, 066103	2.4	64
200	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. *Computer Physics Communications*, **2008**, 178, 73-87	4.2	63
199	Large-scale molecular dynamics simulations of alkanethiol self-assembled monolayers. *Journal of Chemical Physics*, **2004**, 121, 4323-30	3.9	63
198	Cholesterol translocation in a phospholipid membrane. *Biophysical Journal*, **2013**, 104, 2429-36	2.9	60
197	Variable-charge interatomic potentials for molecular-dynamics simulations of TiO2. *Journal of Applied Physics*, **1999**, 86, 3036-3041	2.5	60
196	Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. *Physical Review B*, **2004**, 70,	3.3	59
195	Embrittlement of metal by solute segregation-induced amorphization. *Physical Review Letters*, **2010**, 104, 155502	7.4	58
194	Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. *Physical Review B*, **2008**, 77,	3.3	58
193	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
192	Multiresolution molecular dynamics algorithm for realistic materials modeling on parallel computers. *Computer Physics Communications*, **1994**, 83, 197-214	4.2	58
191	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
190	Growth of pore interfaces and roughness of fracture surfaces in porous silica: Million particle molecular-dynamics simulations. *Physical Review Letters*, **1994**, 73, 2336-2339	7.4	56
189	Tellurene Photodetector with High Gain and Wide Bandwidth. *ACS Nano*, **2020**, 14, 303-310	16.7	55
188	Interaction of voids and nanoductility in silica glass. *Physical Review Letters*, **2007**, 99, 155506	7.4	51

187	Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites. *ACS Nano*, **2018**, 12, 11366-11375	16.7	51
186	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. *Journal of Chemical Physics*, **2014**, 140, 18A529	3.9	50
185	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
184	Atomistic mechanisms of amorphization during nanoindentation of SiC: A molecular dynamics study. *Physical Review B*, **2005**, 71,	3.3	50
183	Nanobubble collapse on a silica surface in water: billion-atom reactive molecular dynamics simulations. *Physical Review Letters*, **2013**, 111, 184503	7.4	49
182	Polytypism in ultrathin tellurium. *2D Materials*, **2019**, 6, 015013	5.9	48
181	Computational Synthesis of MoS Layers by Reactive Molecular Dynamics Simulations: Initial Sulfidation of MoO Surfaces. *Nano Letters*, **2017**, 17, 4866-4872	11.5	45
180	Scalable and portable implementation of the fast multipole method on parallel computers. *Computer Physics Communications*, **2003**, 153, 445-461	4.2	44
179	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
178	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
177	De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. *International Journal of High Performance Computing Applications*, **2008**, 22, 113-128	1.8	41
176	Structural Phase Transformation in Strained Monolayer MoWSe Alloy. *ACS Nano*, **2018**, 12, 3468-3476	16.7	38
175	A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. *MRS Bulletin*, **2006**, 31, 410-418	3.2	38
174	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
173	Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. *Journal of Applied Physics*, **2013**, 114, 134312	2.5	36
172	Deformation mechanisms and damage in □alumina under hypervelocity impact loading. *Journal of Applied Physics*, **2008**, 103, 083508	2.5	36
171	Frequency-dependent dielectric constant prediction of polymers using machine learning. *Npj Computational Materials*, **2020**, 6,	10.9	35
170	Ultrafast non-radiative dynamics of atomically thin MoSe. *Nature Communications*, **2017**, 8, 1745	17.4	35

169	Poration of lipid bilayers by shock-induced nanobubble collapse. *Applied Physics Letters*, **2011**, 98, 023701	3.4	35
168	The nature of free-carrier transport in organometal halide perovskites. *Scientific Reports*, **2016**, 6, 19599	4.9	35
167	Dynamics of wing cracks and nanoscale damage in glass. *Physical Review Letters*, **2005**, 95, 135501	7.4	33
166	Large nonadiabatic quantum molecular dynamics simulations on parallel computers. *Computer Physics Communications*, **2013**, 184, 1-8	4.2	32
165	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
164	Structural transformation, amorphization, and fracture in nanowires: A multimillion-atom molecular dynamics study. *Applied Physics Letters*, **2001**, 78, 3328-3330	3.4	32
163	Defect migration and recombination in nanoindentation of silica glass. *Applied Physics Letters*, **2011**, 99, 111906	3.4	30
162	Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. *Journal of Applied Physics*, **2000**, 87, 7708-7711	2.5	30
161	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
160	Atomistic processes during nanoindentation of amorphous silicon carbide. *Applied Physics Letters*, **2005**, 86, 021915	3.4	28
159	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. *Nano Letters*, **2019**, 19, 6078-6086	11.5	27
158	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
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156	Structural, mechanical, and vibrational properties of Ga1□InxAs alloys: A molecular dynamics study. *Applied Physics Letters*, **2003**, 82, 1057-1059	3.4	24
155	Pressure-induced structural transformation in GaAs: A molecular-dynamics study. *Physical Review B*, **2002**, 65,	3.3	24
154	Nanoductility induced brittle fracture in shocked high performance ceramics. *Applied Physics Letters* , **2010**, 97, 111903	3.4	23
153	Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. *Chemistry of Materials*, **2018**, 30, 7262-7268	9.6	23
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151	Immersive and Interactive Exploration of Billion-Atom Systems. *Presence: Teleoperators and Virtual Environments*, **2003**, 12, 85-95	2.9	22
150	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
149	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. *SoftwareX*, **2019**, 10, 100307	2.7	21
148	Multistage reaction pathways in detonating high explosives. *Applied Physics Letters*, **2014**, 105, 204103	3.4	21
147	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. *International Journal of Fracture*, **2003**, 121, 71-79	2.3	21
146	Phonon dispersion and density of states of solid C60. *Applied Physics Letters*, **1993**, 63, 3152-3154	3.4	21
145	An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. *Computer Physics Communications*, **2015**, 192, 91-96	4.2	20
144	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
143	Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. *Applied Physics Letters*, **2008**, 92, 161904	3.4	20
142	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
141	Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering. *Nature Photonics*, **2019**, 13, 425-430	33.9	19
140	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. *Journal of Applied Physics*, **2018**, 123, 145902	2.5	19
139	Multiobjective genetic training and uncertainty quantification of reactive force fields. *Npj Computational Materials*, **2018**, 4,	10.9	19
138	Multimillion atom simulation of materials on parallel computers nanopixel, interfacial fracture, nanoindentation, and oxidation. *Applied Surface Science*, **2001**, 182, 258-264	6.7	19
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136	Optical Control of Non-Equilibrium Phonon Dynamics. *Nano Letters*, **2019**, 19, 4981-4989	11.5	18
135	Scalable Atomistic Simulation Algorithms for Materials Research. *Scientific Programming*, **2002**, 10, 263-270	1.4	18
134	Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers. *Journal of Nanoparticle Research*, **2003**, 5, 119-135	2.3	18

133	Enhancing combustion performance of nano-Al/PVDF composites with PVDF. *Combustion and Flame*, **2020**, 219, 467-477	5.3	17
132	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
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128	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. *Scientific Reports*, **2016**, 6, 24109	4.9	14
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126	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
125	Universal stretched exponential relaxation in nanoconfined water. *Applied Physics Letters*, **2014**, 105, 161907	3.4	14
124	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
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111	Faceting, Grain Growth, and Crack Healing in Alumina. *ACS Nano*, **2018**, 12, 9005-9010	16.7	10
110	Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. *Journal of Supercomputing*, **2012**, 62, 946-966	2.5	10
109	Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. *AIP Advances*, **2011**, 1, 042149	1.5	10
108	Atomistic mechanisms of rapid energy transport in light-harvesting molecules. *Applied Physics Letters*, **2011**, 98, 113302	3.4	10
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105	A crossover in anisotropic nanomechanochemistry of van der Waals crystals. *Applied Physics Letters*, **2015**, 107, 231903	3.4	9
104	Collective oxidation behavior of aluminum nanoparticle aggregate. *Applied Physics Letters*, **2013**, 102, 221904	3.4	9
103	Dynamic Fracture Mechanisms in Nanostructured and Amorphous Silica Glasses Million-Atom Molecular Dynamics Simulations. *Materials Research Society Symposia Proceedings*, **2001**, 703, 1		9
102	Phonon-induced electron localization and magnetic-field effects in a double quantum dot. *Applied Physics Letters*, **1993**, 62, 3470-3472	3.4	9
101	Molecular Simulation of MoS Exfoliation. *Scientific Reports*, **2018**, 8, 16761	4.9	9
100	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. *Langmuir*, **2020**, 36, 7658-7668	4	8
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98	Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations. *Journal of Chemical Information and Modeling*, **2021**, 61, 2175-2186	6.1	8

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86	Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality. *SoftwareX*, **2019**, 9, 112-116	2.7	5
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83	Heat-Initiated Oxidation of an Aluminum Nanoparticle. *Materials Research Society Symposia Proceedings*, **2012**, 1405,		5
82	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
81	Nonlinear electron dynamics in a resonant tunneling diode: Langevin-quantum-dynamics simulations on a massively parallel computer. *Applied Physics Letters*, **1994**, 64, 2569-2571	3.4	5
80	Photoexcitation Induced Ultrafast Nonthermal Amorphization in SbTe. *Journal of Physical Chemistry Letters*, **2020**, 11, 10242-10249	6.4	5

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72	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand **2014**,		4
71	Ion dynamics at porous alumina surfaces. *Applied Physics Letters*, **2012**, 101, 063106	3.4	4
70	Distribution of Rings and Intermediate Range Correlations in Silica Glass Under Pressure - A Molecular Dynamics Study. *Materials Research Society Symposia Proceedings*, **1995**, 408, 333		4
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64	A Reactive Molecular Dynamics Study of Atomistic Mechanisms During Synthesis of MoS2 Layers by Chemical Vapor Deposition. *MRS Advances*, **2018**, 3, 307-311	0.7	3
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61	Molecular Dynamics Study Of Si/Si3N4 Interface. *Materials Research Society Symposia Proceedings*, **1996**, 446, 157		3
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49	Sulfur-impurity induced amorphization of nickel. *Journal of Applied Physics*, **2011**, 110, 063501	2.5	2
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47	Effect of geometry on stress relaxation in InAs GaAs rectangular nanomesas: Multimillion-atom molecular dynamics simulations. *Journal of Applied Physics*, **2005**, 98, 114313	2.5	2
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