# Aiichiro Nakano

List of Publications by Year
in descending order



| 261 | 7,665 | 43973 | 71532 |
|---|---|---|---|
| papers | citations | 48 h-index | 76 g-index |

| 266 | 266 | 266 | 7137 |
|---|---|---|---|
| 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 | Atomistic Aspects of Crack Propagation in Brittle Materials: Multimillion Atom Molecular Dynamics Simulations. Annual Review of Materials Research, 2002, 32, 377-400. | 4.3 | 177 |
| 8 | Parallel multilevel preconditioned conjugate-gradient approach to variable-charge molecular dynamics. Computer Physics Communications, 1997, 104, 59-69. | 3.0 | 171 |
| 9 | Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. Journal of Applied Physics, 2008, 103, . | 1.1 | 139 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | A spaceâ€“time-ensemble parallel nudged elastic band algorithm for molecular kinetics simulation. Computer Physics Communications, 2008, 178, 280-289. | 3.0 | 110 |
| 14 | Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, . | 3.5 | 107 |
| 15 | Tellurene Photodetector with High Gain and Wide Bandwidth. ACS Nano, 2020, 14, 303-310. | 7.3 | 101 |
| 16 | Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites. ACS Nano, 2018, 12, 11366-11375. | 7.3 | 99 |
| 17 | Brittle dynamic fracture of crystalline cubic silicon carbide (3C-SiC) via molecular dynamics simulation. Journal of Applied Physics, 2005, 98, 103524. | 1.1 | 98 |
| 18 | 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 |

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| 19 | Oxidation of aluminum nanoclusters. Physical Review B, 2005, 71, . | 1.1 | 88 |
| 20 | Molecular Dynamics Simulations of Rapid Hydrogen Production from Water Using Aluminum Clusters as Catalyzers. Physical Review Letters, 2010, 104, 126102. | 2.9 | 88 |
| 21 | Nanoindentation-induced amorphization in silicon carbide. Applied Physics Letters, 2004, 85, 378-380. | 1.5 | 78 |
| 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 | Atomistic mechanisms for wurtzite-to-rocksalt structural transformation in cadmium selenide under pressure. Physical Review B, 2004, 70, . | 1.1 | 74 |
| 25 | Large-scale molecular dynamics simulations of alkanethiol self-assembled monolayers. Journal of Chemical Physics, 2004, 121, 4323-4330. | 1.2 | 68 |
| 26 | Polytypism in ultrathin tellurium. 2D Materials, 2019, 6, 015013. | 2.0 | 68 |
| 27 | Multiresolution molecular dynamics algorithm for realistic materials modeling on parallel computers. Computer Physics Communications, 1994, 83, 197-214. | 3.0 | 67 |
| 28 | Reactive nanojets: Nanostructure-enhanced chemical reactions in a defected energetic crystal. Applied Physics Letters, 2007, 91, . | 1.5 | 66 |
| 29 | Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. Physical Review B, 2004, 70, . | 1.1 | 65 |
| 30 | 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 |
| 31 | Variable-charge interatomic potentials for molecular-dynamics simulations of TiO2. Journal of Applied Physics, 1999, 86, 3036-3041. | 1.1 | 64 |
| 32 | Divide-and-conquer density functional theory on hierarchical real-space grids: Parallel implementation and applications. Physical Review B, 2008, 77, . | 1.1 | 63 |
| 33 | Atomistic mechanisms of amorphization during nanoindentation of SiC: A molecular dynamics study. Physical Review B, 2005, 71, . | 1.1 | 62 |
| 34 | Multimillion-atom nanoindentation simulation of crystalline silicon carbide: Orientation dependence and anisotropic pileup. Journal of Applied Physics, 2007, 102, . | 1.1 | 62 |
| 35 | 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 |
| 36 | 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 |

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| 37 | 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 |
| 38 | Interaction of Voids and Nanoductility in Silica Glass. Physical Review Letters, 2007, 99, 155506. | 2.9 | 60 |
| 39 | Embrittlement of Metal by Solute Segregation-Induced Amorphization. Physical Review Letters, 2010, 104, 155502. | 2.9 | 60 |
| 40 | Computational Synthesis of MoS<sub>2</sub> Layers by Reactive Molecular Dynamics Simulations: Initial Sulfidation of MoO<sub>3</sub> Surfaces. Nano Letters, 2017, 17, 4866-4872. | 4.5 | 60 |
| 41 | A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 18A529. | 1.2 | 57 |
| 42 | Structural Phase Transformation in Strained Monolayer MoWSe<sub>2</sub> Alloy. ACS Nano, 2018, 12, 3468-3476. | 7.3 | 57 |
| 43 | Hybrid quantum mechanical/molecular dynamics simulation on parallel computers: density functional theory on real-space multigrids. Computer Physics Communications, 2002, 149, 30-38. | 3.0 | 56 |
| 44 | Enhancing combustion performance of nano-Al/PVDF composites with Î²-PVDF. Combustion and Flame, 2020, 219, 467-477. | 2.8 | 55 |
| 45 | Ultrafast non-radiative dynamics of atomically thin MoSe2. Nature Communications, 2017, 8, 1745. | 5.8 | 52 |
| 46 | 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 |
| 47 | Atomistic damage mechanisms during hypervelocity projectile impact on AlN: A large-scale parallel molecular dynamics simulation study. Journal of the Mechanics and Physics of Solids, 2008, 56, 1955-1988. | 2.3 | 50 |
| 48 | Scalable and portable implementation of the fast multipole method on parallel computers. Computer Physics Communications, 2003, 153, 445-461. | 3.0 | 49 |
| 49 | A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultrahigh-Temperature Ceramics. MRS Bulletin, 2006, 31, 410-418. | 1.7 | 49 |
| 50 | De Novo Ultrascale Atomistic Simulations On High-End Parallel Supercomputers. International Journal of High Performance Computing Applications, 2008, 22, 113-128. | 2.4 | 47 |
| 51 | 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 |
| 52 | Deformation mechanisms and damage in Î±-alumina under hypervelocity impact loading. Journal of Applied Physics, 2008, 103, . | 1.1 | 43 |
| 53 | Poration of lipid bilayers by shock-induced nanobubble collapse. Applied Physics Letters, 2011, 98, . | 1.5 | 43 |
| 54 | Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. Nano Letters, 2019, 19, 6078-6086. | 4.5 | 43 |

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| 55 | Effects of twins on the electronic properties of GaAs. Applied Physics Letters, 2013, 103, 022105. | 1.5 | 42 |
| 56 | Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations. Journal of Applied Physics, 2013, 114, 134312. | 1.1 | 42 |
| 57 | Chemical Vapor Deposition Synthesis of MoS<sub>2</sub> Layers from the Direct Sulfidation of MoO<sub>3</sub> Surfaces Using Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 7494-7503. | 1.5 | 41 |
| 58 | Molecular-dynamics simulations of Coulombic systems on distributed-memory MIMD machines. Computer Physics Communications, 1993, 74, 316-326. | 3.0 | 38 |
| 59 | The nature of free-carrier transport in organometal halide perovskites. Scientific Reports, 2016, 6, 19599. | 1.6 | 38 |
| 60 | Simultaneous Observation of Carrier-Specific Redistribution and Coherent Lattice Dynamics in 2H-MoTe<sub>2</sub> with Femtosecond Core-Level Spectroscopy. ACS Nano, 2020, 14, 15829-15840. | 7.3 | 38 |
| 61 | Fast reaction mechanism of a core(Al)-shell (Al2O3) nanoparticle in oxygen. Applied Physics Letters, 2009, 95, . | 1.5 | 37 |
| 62 | Telluride-Based Atomically Thin Layers of Ternary Two-Dimensional Transition Metal Dichalcogenide Alloys. Chemistry of Materials, 2018, 30, 7262-7268. | 3.2 | 37 |
| 63 | 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 |
| 64 | Defect migration and recombination in nanoindentation of silica glass. Applied Physics Letters, 2011, 99, . | 1.5 | 36 |
| 65 | Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. Journal of Applied Physics, 2000, 87, 7708-7711. | 1.1 | 34 |
| 66 | 1,3,5-trinitro-1,3,5-triazine decomposition and chemisorption on Al(111) surface: First-principles molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234702. | 1.2 | 34 |
| 67 | Kinetic Monte Carlo Simulations and Molecular Conductance Measurements of the Bacterial Decaheme Cytochrome MtrF. ChemElectroChem, 2014, 1, 1932-1939. | 1.7 | 34 |
| 68 | Semiconductorâ€“metal structural phase transformation in MoTe<sub>2</sub> monolayers by electronic excitation. Nanoscale, 2018, 10, 2742-2747. | 2.8 | 34 |
| 69 | A scalable molecular-dynamics algorithm suite for materials simulations: design-space diagram on 1024 Cray T3E processors. Future Generation Computer Systems, 2000, 17, 279-291. | 4.9 | 33 |
| 70 | Large nonadiabatic quantum molecular dynamics simulations on parallel computers. Computer Physics Communications, 2013, 184, 1-8. | 3.0 | 33 |
| 71 | Nanoscopic mechanisms of singlet fission in amorphous molecular solid. Applied Physics Letters, 2013, 102, . | 1.5 | 33 |
| 72 | Hydrogen-on-Demand Using Metallic Alloy Nanoparticles in Water. Nano Letters, 2014, 14, 4090-4096. | 4.5 | 33 |

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| 73 | Atomistic processes during nanoindentation of amorphous silicon carbide. Applied Physics Letters, 2005, 86, 021915. | 1.5 | 32 |
| 74 | QXMD: An open-source program for nonadiabatic quantum molecular dynamics. SoftwareX, 2019, 10, 100307. | 1.2 | 32 |
| 75 | Two-Dimensional Lateral Epitaxy of 2H (MoSe<sub>2</sub>)â€"1Tâ€² (ReSe<sub>2</sub>) Phases. Nano Letters, 2019, 19, 6338-6345. | 4.5 | 30 |
| 76 | Pressure-induced structural transformation in GaAs:â€ƒA molecular-dynamics study. Physical Review B, 2002, 65, . | 1.1 | 29 |
| 77 | Immersive and Interactive Exploration of Billion-Atom Systems. Presence: Teleoperators and Virtual Environments, 2003, 12, 85-95. | 0.3 | 29 |
| 78 | Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study. Applied Physics Letters, 2008, 92, . | 1.5 | 29 |
| 79 | Molecular control of photoexcited charge transfer and recombination at a quaterthiophene/zinc oxide interface. Applied Physics Letters, 2012, 100, . | 1.5 | 29 |
| 80 | 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 |
| 81 | Nanoductility induced brittle fracture in shocked high performance ceramics. Applied Physics Letters, 2010, 97, . | 1.5 | 28 |
| 82 | Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering. Nature Photonics, 2019, 13, 425-430. | 15.6 | 28 |
| 83 | Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations. Journal of Chemical Information and Modeling, 2021, 61, 2175-2186. | 2.5 | 28 |
| 84 | Scalable Atomistic Simulation Algorithms for Materials Research. Scientific Programming, 2002, 10, 263-270. | 0.5 | 27 |
| 85 | Structural, mechanical, and vibrational properties of Ga1â^'xInxAs alloys: A molecular dynamics study. Applied Physics Letters, 2003, 82, 1057-1059. | 1.5 | 27 |
| 86 | Optical Control of Non-Equilibrium Phonon Dynamics. Nano Letters, 2019, 19, 4981-4989. | 4.5 | 27 |
| 87 | Hypervelocity impact induced deformation modes in Î±-alumina. Applied Physics Letters, 2007, 91, 071906. | 1.5 | 26 |
| 88 | Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. Langmuir, 2020, 36, 7658-7668. | 1.6 | 26 |
| 89 | Multistage reaction pathways in detonating high explosives. Applied Physics Letters, 2014, 105, . | 1.5 | 25 |
| 90 | Multiobjective genetic training and uncertainty quantification of reactive force fields. Npj Computational Materials, 2018, 4, . | 3.5 | 25 |

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| 92 | An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. Computer Physics Communications, 2015, 192, 91-96. | 3.0 | 24 |
| 93 | Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. Journal of Applied Physics, 2018, 123, . | 1.1 | 24 |
| 94 | Effects of oxide-shell structures on the dynamics of oxidation of Al nanoparticles. Applied Physics Letters, 2010, 96, 181906. | 1.5 | 23 |
| 95 | Towards simulation of the dynamics of materials on quantum computers. Physical Review B, 2020, 101, . | 1.1 | 23 |
| 96 | Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers. Journal of Nanoparticle Research, 2003, 5, 119-135. | 0.8 | 22 |
| 97 | 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 |
| 98 | Plane shock loading on mono- and nano-crystalline silicon carbide. Applied Physics Letters, 2018, 112, . | 1.5 | 22 |
| 99 | Thermal conductivity of MoS2 monolayers from molecular dynamics simulations. AIP Advances, 2019, 9, . | 0.6 | 22 |
| 100 | Multiresolution load balancing in curved space: the wavelet representation. Concurrency and Computation: Practice and Experience, 1999, 11, 343-353. | 0.6 | 21 |
| 101 | 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 |
| 102 | Pressure-induced structural transformations in cadmium selenide nanorods. Applied Physics Letters, 2006, 89, 093101. | 1.5 | 20 |
| 103 | Fracture initiation mechanisms in Î±-alumina under hypervelocity impact. Applied Physics Letters, 2007, 91, 121911. | 1.5 | 20 |
| 104 | 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 |
| 105 | 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 |
| 106 | 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 |
| 107 | Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters. Journal of Supercomputing, 2012, 62, 946-966. | 2.4 | 19 |
| 108 | Decaheme Cytochrome MtrF Adsorption and Electron Transfer on Gold Surface. Journal of Physical Chemistry Letters, 2016, 7, 929-936. | 2.1 | 19 |

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| 109 | Facile Five-Step Heteroepitaxial Growth of GaAs Nanowires on Silicon Substrates and the Twin Formation Mechanism. ACS Nano, 2016, 10, 2424-2435. | 7.3 | 19 |
| 110 | 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 |
| 111 | Molecular Simulation of MoS2 Exfoliation. Scientific Reports, 2018, 8, 16761. | 1.6 | 19 |
| 112 | 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 |
| 113 | Defect Healing in Layered Materials: A Machine Learning-Assisted Characterization of MoS<sub>2</sub> Crystal Phases. Journal of Physical Chemistry Letters, 2019, 10, 2739-2744. | 2.1 | 19 |
| 114 | Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study. Applied Physics Letters, 2014, 104, . | 1.5 | 18 |
| 115 | Universal stretched exponential relaxation in nanoconfined water. Applied Physics Letters, 2014, 105, . | 1.5 | 17 |
| 116 | Picosecond amorphization of SiO <sub>2</sub> stishovite under tension. Science Advances, 2017, 3, e1602339. | 4.7 | 17 |
| 117 | Simulation of many-electron correlations in a resonant-tunneling diode. Physical Review B, 1991, 43, 9066-9069. | 1.1 | 16 |
| 118 | Bonding and Structure of Ceramic-Ceramic Interfaces. Physical Review Letters, 2013, 111, 066103. | 2.9 | 16 |
| 119 | Enhanced charge recombination due to surfaces and twin defects in GaAs nanostructures. Journal of Applied Physics, 2015, 117, 054307. | 1.1 | 16 |
| 120 | Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in MoSe<sub>2</sub> Monolayer. Nano Letters, 2018, 18, 4653-4658. | 4.5 | 16 |
| 121 | Growth Kinetics and Atomistic Mechanisms of Native Oxidation of ZrS<sub>x</sub>Se<sub>2â€“x</sub> and MoS<sub>2</sub> Crystals. Nano Letters, 2020, 20, 8592-8599. | 4.5 | 16 |
| 122 | Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics. Physical Review Letters, 2021, 126, 216403. | 2.9 | 16 |
| 123 | Simulation of correlated electron tunneling and a Coulomb blockade in a quantum-dot diode. Physical Review B, 1991, 44, 8121-8128. | 1.1 | 15 |
| 124 | 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 |
| 125 | Nanocarbon synthesis by high-temperature oxidation of nanoparticles. Scientific Reports, 2016, 6, 24109. | 1.6 | 15 |
| 126 | RXMD: A scalable reactive molecular dynamics simulator for optimized time-to-solution. SoftwareX, 2020, 11, 100389. | 1.2 | 15 |

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| 127 | 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 |
| 128 | Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials. Journal of Propulsion and Power, 2007, 23, 688-692. | 1.3 | 14 |
| 129 | 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 |
| 130 | Meteorite Impact-Induced Rapid NH3 Production on Early Earth: Ab Initio Molecular Dynamics Simulation. Scientific Reports, 2016, 6, 38953. | 1.6 | 14 |
| 131 | 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 |
| 132 | Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials. Npj Computational Materials, 2021, 7, . | 3.5 | 14 |
| 133 | InAs/GaAs square nanomesas: Multimillion-atom molecular dynamics simulations on parallel computers. Journal of Applied Physics, 2003, 94, 6762-6773. | 1.1 | 13 |
| 134 | Grid applications---Sustainable adaptive grid supercomputing. , 2006, , . | | 13 |
| 135 | A core/shell mechanism for stacking-fault generation in GaAs nanowires. Applied Physics Letters, 2012, 100, 163103. | 1.5 | 13 |
| 136 | Crystalline anisotropy of shock-induced phenomena: Omni-directional multiscale shock technique. Applied Physics Letters, 2016, 108, . | 1.5 | 13 |
| 137 | Faceting, Grain Growth, and Crack Healing in Alumina. ACS Nano, 2018, 12, 9005-9010. | 7.3 | 13 |
| 138 | Sulfurization of MoO<sub>3</sub> in the Chemical Vapor Deposition Synthesis of MoS<sub>2</sub> Enhanced by an H<sub>2</sub>S/H<sub>2</sub> Mixture. Journal of Physical Chemistry Letters, 2021, 12, 1997-2003. | 2.1 | 13 |
| 139 | Autonomous reinforcement learning agent for stretchable kirigami design of 2D materials. Npj Computational Materials, 2021, 7, . | 3.5 | 13 |
| 140 | Core/shell structural transformation and brittle-to-ductile transition in nanowires. Applied Physics Letters, 2012, 100, . | 1.5 | 12 |
| 141 | Quantum Molecular Dynamics in the Post-Petaflops Era. Computer, 2015, 48, 33-41. | 1.2 | 12 |
| 142 | Photoexcitation Induced Ultrafast Nonthermal Amorphization in Sb<sub>2</sub>Te<sub>3</sub>. Journal of Physical Chemistry Letters, 2020, 11, 10242-10249. | 2.1 | 12 |
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| 144 | Massively parallel algorithms for computational nanoelectronics based on quantum molecular dynamics. Computer Physics Communications, 1994, 83, 181-196. | 3.0 | 11 |

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| 145 | Sustainable Adaptive Grid Supercomputing: Multiscale Simulation of Semiconductor Processing across the Pacific. , 2006, , . | | 11 |
| 146 | Effects of solvation shells and cluster size on the reaction of aluminum clusters with water. AIP Advances, 2011, 1, . | 0.6 | 11 |
| 147 | Collective oxidation behavior of aluminum nanoparticle aggregate. Applied Physics Letters, 2013, 102, 221904. | 1.5 | 11 |
| 148 | A crossover in anisotropic nanomechanochemistry of van der Waals crystals. Applied Physics Letters, 2015, 107, . | 1.5 | 11 |
| 149 | Game-Engine-Assisted Research platform for Scientific computing (GEARS) in Virtual Reality. SoftwareX, 2019, 9, 112-116. | 1.2 | 11 |
| 150 | Review of strategies toward the development of alloy two-dimensional (2D) transition metal dichalcogenides. IScience, 2021, 24, 103532. | 1.9 | 11 |
| 151 | Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers. Progress of Theoretical Physics Supplement, 2000, 138, 175-190. | 0.2 | 10 |
| 152 | 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 |
| 153 | Exploiting hierarchical parallelisms for molecular dynamics simulation on multicore clusters. Journal of Supercomputing, 2011, 57, 20-33. | 2.4 | 10 |
| 154 | Atomistic mechanisms of rapid energy transport in light-harvesting molecules. Applied Physics Letters, 2011, 98, 113302. | 1.5 | 10 |
| 155 | Enhanced charge transfer by phenyl groups at a rubrene/C60 interface. Journal of Chemical Physics, 2012, 136, 184705. | 1.2 | 10 |
| 156 | Role of H Transfer in the Gas-Phase Sulfidation Process of MoO<sub>3</sub>: A Quantum Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2018, 9, 6517-6523. | 2.1 | 10 |
| 157 | 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 |
| 158 | Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, . | 1.1 | 10 |
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| 160 | Differences in Sb2Te3 growth by pulsed laser and sputter deposition. Acta Materialia, 2020, 200, 811-820. | 3.8 | 10 |
| 161 | Phononâ€induced electron localization and magneticâ€field effects in a double quantum dot. Applied Physics Letters, 1993, 62, 3470-3472. | 1.5 | 9 |
| 162 | Reactivity of Sulfur Molecules on MoO<sub>3</sub> (010) Surface. Journal of Physical Chemistry Letters, 2017, 8, 6206-6210. | 2.1 | 9 |

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| 163 | Effects of chemical defects on anisotropic dielectric response of polyethylene. AIP Advances, 2019, 9, . | 0.6 | 9 |
| 164 | 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 |
| 165 | Scalable and portable visualization of large atomistic datasets. Computer Physics Communications, 2004, 163, 53-64. | 3.0 | 8 |
| 166 | Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand. , 2014, , . | | 8 |
| 167 | Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals. Applied Physics Letters, 2018, 112, . | 1.5 | 8 |
| 168 | Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. Journal of Physical Chemistry Letters, 2019, 10, 3937-3943. | 2.1 | 8 |
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| 170 | Lattice thermal transport in two-dimensional alloys and fractal heterostructures. Scientific Reports, 2021, 11, 1656. | 1.6 | 8 |
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