Shuji Ogata

List of Publications by Year in descending order

59 papers	1,134 citations	516710 16 h-index	395702 33 g-index
60 all docs	60 docs citations	60 times ranked	945 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.	7.8	313
2	Hybrid finite-element/molecular-dynamics/electronic-density-functional approach to materials simulations on parallel computers. Computer Physics Communications, 2001, 138, 143-154.	7.5	136
3	Oxidation of aluminum nanoclusters. Physical Review B, 2005, 71, .	3.2	88
4	Hybrid quantum mechanical/molecular dynamics simulation on parallel computers: density functional theory on real-space multigrids. Computer Physics Communications, 2002, 149, 30-38.	7.5	56
5	Scalable and portable implementation of the fast multipole method on parallel computers. Computer Physics Communications, 2003, 153, 445-461.	7.5	49
6	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	45
7	Moisture-Induced Reduction of Adhesion Strength between Surface Oxidized Al and Epoxy Resin: Dynamics Simulation with Electronic Structure Calculation. Journal of Physical Chemistry C, 2016, 120, 13630-13637.	3.1	43
8	Buffered-cluster method for hybridization of density-functional theory and classical molecular dynamics: Application to stress-dependent reaction ofH2Oon nanostructured Si. Physical Review B, 2005, 72, .	3.2	38
9	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.	7.5	33
10	Unveiling the Chemical Reactions Involved in Moisture-Induced Weakening of Adhesion between Aluminum and Epoxy Resin. Journal of Physical Chemistry C, 2018, 122, 17748-17755.	3.1	29
11	Scalable Atomistic Simulation Algorithms for Materials Research. Scientific Programming, 2002, 10, 263-270.	0.7	27
12	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. International Journal of Fracture, 2003, 121, 71-79.	2.2	25
13	Linear scaling algorithm of real-space density functional theory of electrons with correlated overlapping domains. Computer Physics Communications, 2012, 183, 1664-1673.	7.5	25
14	A molecular dynamics study on thermal conductivity of thin epoxy polymer sandwiched between alumina fillers in heat-dissipation composite material. International Journal of Heat and Mass Transfer, 2015, 89, 714-723.	4.8	25
15	Multi-Thousand-Atom DFT Simulation of Li-Ion Transfer through the Boundary between the Solidâ€“Electrolyte Interface and Liquid Electrolyte in a Li-Ion Battery. Journal of Physical Chemistry C, 2013, 117, 17960-17968.	3.1	23
16	A hybrid electronic-density-functional/molecular-dynamics simulation scheme for multiscale simulation of materials on parallel computers: applications to silicon and alumina. Computational Materials Science, 2004, 30, 189-194.	3.0	19
17	Enhanced heat transfer through filler-polymer interface by surface-coupling agent in heat-dissipation material: A non-equilibrium molecular dynamics study. Journal of Applied Physics, 2013, 114, .	2.5	16
18	Combination of first-principles molecular dynamics and XANES simulations for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></m -electrolyte interfacial reactions in a lithium-ion battery. Physical Review B, 2017, 96, .	3.2	13

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19	Stress-induced nano-oxidation of silicon by diamond-tip in moisture environment: A hybrid quantum-classical simulation study. Journal of Applied Physics, 2010, 108, 064313.	2.5	12
20	Large-scale DFT simulation of quinone molecules encapsulated in single-walled carbon nanotube for novel Li-ion battery cathode. Computational Materials Science, 2020, 171, 109281.	3.0	11
21	Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers. Progress of Theoretical Physics Supplement, 2000, 138, 175-190.	0.1	10
22	Path-Integral Monte Carlo Simulations for Excitation Spectra of Cs in Superfluid He. Journal of the Physical Society of Japan, 1999, 68, 2153-2156.	1.6	8
23	A simple dynamical scaleâ€coupling method for concurrent simulation of hybridized atomistic/coarseâ€grainedâ€particle system. International Journal for Numerical Methods in Engineering, 2010, 83, 249-268.	2.8	8
24	Hybrid Quantum-Classical Simulation of Li Ion Dynamics and the Decomposition Reaction of Electrolyte Liquid at a Negative-Electrode/Electrolyte Interface. Journal of Physical Chemistry C, 2019, 123, 9673-9679.	3.1	8
25	First-Principles Calculations of the Protonation and Weakening of Epoxy Resin under Wet Conditions. Journal of Physical Chemistry B, 2021, 125, 8989-8996.	2.6	8
26	Activation Energy for Oxygen Diffusion in Strained Silicon: A Hybrid Quantum-Classical Simulation Study with the Nudged Elastic Band Method. Journal of the Physical Society of Japan, 2008, 77, 054708.	1.6	6
27	Enhanced Thermal Diffusion of Li in Graphite by Alternating Vertical Electric Field: A Hybrid Quantum-Classical Simulation Study. Journal of the Physical Society of Japan, 2012, 81, 023601.	1.6	6
28	Fast time-reversible algorithms for molecular dynamics of rigid-body systems. Journal of Chemical Physics, 2012, 136, 234105.	3.0	6
29	Efficient scheme for calculating work of adhesion between a liquid and polymer-grafted substrate. Journal of Chemical Physics, 2018, 149, 064703.	3.0	6
30	Fluctuating Local Recrystallization of Quasi-Liquid Layer of Sub-Micrometer-Scale Ice: A Molecular Dynamics Study. Journal of the Physical Society of Japan, 2014, 83, 083601.	1.6	4
31	Thermal diffusion of correlated Li-ions in graphite: A hybrid quantumâ€“classical simulation study. Computational Materials Science, 2015, 108, 250-257.	3.0	4
32	First-Principles Simulation Study on the Weakening of Silane Coupling to Silica under Alkaline Conditions. Journal of Physical Chemistry C, 2021, 125, 22907-22916.	3.1	4
33	Oxidation Dynamics of Nanophase Aluminum Clusters: A Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 1997, 481, 625.	0.1	3
34	Concurrent Coupling of Electronic-Density-Functional, Molecular Dynamics, and Coarse-Grained Particles Schemes for Multiscale Simulation of Nanostructured Materials. Materials Science Forum, 2005, 502, 33-38.	0.3	3
35	Enhanced Siâ€“O Bond Breaking in Silica Glass by Water Dimer: A Hybrid Quantumâ€“Classical Simulation Study. Journal of the Physical Society of Japan, 2016, 85, 054601.	1.6	3
36	Smart MD-Sampling Method for Interfacial Free Energy between Polymer-Grafted Substrate and Liquid. MRS Advances, 2018, 3, 519-524.	0.9	3

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37	Nonequilibrium molecular dynamics method based on coarse-graining formalism: Application to a nonuniform temperature field system. Physical Review E, 2021, 104, 065301.	2.1	3
38	Vacancy-assisted ferroelectric domain growth in BaTiO3 under an applied electric field: A molecular dynamics study. Journal of Applied Physics, 2022, 131, .	2.5	3
39	Classical and Hybrid Density-Functional/Classical Molecular Dynamics Study of Dislocation Core in Alumina Ceramic. Materials Transactions, 2009, 50, 1015-1018.	1.2	2
40	A Coupled Molecular Dynamics/Coarse-Grained-Particle Method for Dynamic Simulation of Crack Growth at Finite Temperatures. Materials Transactions, 2011, 52, 1603-1610.	1.2	2
41	A Monte Carlo Study of Host-Material Deformation Effect on Li Migration in Graphite. Journal of the Physical Society of Japan, 2013, 82, 094603.	1.6	2
42	Intercluster Interaction of TiO2 Nanoclusters Using Variable-Charge Interatomic Potentials. Materials Research Society Symposia Proceedings, 1999, 581, 667.	0.1	1
43	Exactly Time-Reversible Molecular Dynamics Algorithm for Rigid-Body Systems. Journal of the Physical Society of Japan, 2011, 80, 114002.	1.6	1
44	Large-Scale DFT Simulation of Li-atom Insertion and Extraction in Quinons@SWCNT Rechargeable Battery Cathodes. MRS Advances, 2018, 3, 1229-1234.	0.9	1
45	FE-CLIP: A tool for the calculation of the solidâ€“liquid interfacial free energy. Computer Physics Communications, 2020, 254, 107252.	7.5	1
46	Simulation Analysis of Effect of Vacancies on Ferroic Domain Growth of BaTiO^3. International Journal of Circuits, Systems and Signal Processing, 2022, 15, 1828-1832.	0.3	1
47	Protonation and weakening of an epoxy resinâ€“SiO2 composite with silane coupling agents under moist conditions. MRS Communications, 0, , 1.	1.8	1
48	Initial Stages of Sintering of TiO2 Nanoparticles: Variable-Charge Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2000, 634, 761.	0.1	0
49	Hybrid Electronic-density-functional/molecular-dynamics Simulation on Parallel Computers: Oxidation of Si Surface. Materials Research Society Symposia Proceedings, 2000, 653, .	0.1	0
50	Mechanisms of Stress Corrosion Cracking in Si: A Hybrid Quantum-Mechanical/Molecular-Dynamics Simulation. Materials Research Society Symposia Proceedings, 2002, 750, 1.	0.1	0
51	Hybrid Simulations for Desinging of Nano-Interfacial Structures. Solid State Phenomena, 2007, 127, 57-62.	0.3	0
52	A Suite of Hybrid Simulation Schemes for Nano-to-Micrometer Scale Processes at Solid-Fluid Interfaces. Progress of Theoretical Physics Supplement, 2009, 178, 149-156.	0.1	0
53	Hybrid Electronic-density-functional/molecular-dynamics Simulation on Parallel Computers: Oxidation of Si Surface. Materials Research Society Symposia Proceedings, 2000, 653, 1.	0.1	0
54	Moisture effects of crack initiation in nanocrystalline silicon: a hybrid density-functional/molecular-dynamics study. Materials Research Society Symposia Proceedings, 2002, 737, 695.	0.1	0

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55	VIRTUALIZATION-AWARE APPLICATION FRAMEWORK FOR HIERARCHICAL MULTISCALE SIMULATIONS ON A GRID. Lecture Notes Series, Institute for Mathematical Sciences, 2005, , 229-243.	0.2	0
56	Theoretical mechanical properties of silica glass. Transactions of the Materials Research Society of Japan, 2011, 36, 35-40.	0.2	0
57	Concurrent Hybrid Simulation of Fracture Dynamics of Suspended Graphene at Finite Temperatures. Transactions of the Materials Research Society of Japan, 2012, 37, 7-10.	0.2	0
58	2105 Order-N, real-space grid implementation of density-functional theory for hybrid QM-CL simulation : DC-RGDFT. The Proceedings of the Computational Mechanics Conference, 2012, 2012.25, 180-181.	0.0	0
59	Effects of Mono/Di-Vacancies on Domain Growth of BaTiO3: An Atomistic Computer Simulation Study. , 2021, , .		0