

# Shuji Ogata

## List of Publications by Year in descending order

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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	Simulation Analysis of Effect of Vacancies on Ferroic Domain Growth of BaTiO <sup>3</sup> . International Journal of Circuits, Systems and Signal Processing, 2022, 15, 1828-1832.	0.3	1
2	Vacancy-assisted ferroelectric domain growth in BaTiO <sub>3</sub> under an applied electric field: A molecular dynamics study. Journal of Applied Physics, 2022, 131, .	2.5	3
3	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
4	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
5	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
6	Effects of Mono/Di-Vacancies on Domain Growth of BaTiO <sub>3</sub> : An Atomistic Computer Simulation Study. , 2021, , .		0
7	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
8	FE-CLIP: A tool for the calculation of the solid-liquid interfacial free energy. Computer Physics Communications, 2020, 254, 107252.	7.5	1
9	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
10	Efficient scheme for calculating work of adhesion between a liquid and polymer-grafted substrate. Journal of Chemical Physics, 2018, 149, 064703.	3.0	6
11	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
12	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
13	Smart MD-Sampling Method for Interfacial Free Energy between Polymer-Grafted Substrate and Liquid. MRS Advances, 2018, 3, 519-524.	0.9	3
14	Combination of first-principles molecular dynamics and XANES simulations for $\text{LiCoO}_2$ -electrolyte interfacial reactions in a lithium-ion battery. Physical Review B, 2017, 96, .		1
15	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
16	Enhanced Si-O Bond Breaking in Silica Glass by Water Dimer: A Hybrid Quantum-Classical Simulation Study. Journal of the Physical Society of Japan, 2016, 85, 054601.	1.6	3
17	Thermal diffusion of correlated Li-ions in graphite: A hybrid quantum-classical simulation study. Computational Materials Science, 2015, 108, 250-257.	3.0	4
18	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

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19	Fluctuating Local Recrystallization of Quasi-Liquid Layer of Sub-Micrometer-Scale Ice: A Molecular Dynamics Study. <i>Journal of the Physical Society of Japan</i> , 2014, 83, 083601.	1.6	4
20	Multi-Thousand-Atom DFT Simulation of Li-Ion Transfer through the Boundary between the Solid-Electrolyte Interface and Liquid Electrolyte in a Li-Ion Battery. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17960-17968.	3.1	23
21	Enhanced heat transfer through filler-polymer interface by surface-coupling agent in heat-dissipation material: A non-equilibrium molecular dynamics study. <i>Journal of Applied Physics</i> , 2013, 114, .	2.5	16
22	A Monte Carlo Study of Host-Material Deformation Effect on Li Migration in Graphite. <i>Journal of the Physical Society of Japan</i> , 2013, 82, 094603.	1.6	2
23	Enhanced Thermal Diffusion of Li in Graphite by Alternating Vertical Electric Field: A Hybrid Quantum-Classical Simulation Study. <i>Journal of the Physical Society of Japan</i> , 2012, 81, 023601.	1.6	6
24	Fast time-reversible algorithms for molecular dynamics of rigid-body systems. <i>Journal of Chemical Physics</i> , 2012, 136, 234105.	3.0	6
25	Linear scaling algorithm of real-space density functional theory of electrons with correlated overlapping domains. <i>Computer Physics Communications</i> , 2012, 183, 1664-1673.	7.5	25
26	Concurrent Hybrid Simulation of Fracture Dynamics of Suspended Graphene at Finite Temperatures. <i>Transactions of the Materials Research Society of Japan</i> , 2012, 37, 7-10.	0.2	0
27	2105 Order-N, real-space grid implementation of density-functional theory for hybrid QM-CL simulation : DC-RGDFT. <i>The Proceedings of the Computational Mechanics Conference</i> , 2012, 2012.25, 180-181.	0.0	0
28	A Coupled Molecular Dynamics/Coarse-Grained-Particle Method for Dynamic Simulation of Crack Growth at Finite Temperatures. <i>Materials Transactions</i> , 2011, 52, 1603-1610.	1.2	2
29	Exactly Time-Reversible Molecular Dynamics Algorithm for Rigid-Body Systems. <i>Journal of the Physical Society of Japan</i> , 2011, 80, 114002.	1.6	1
30	Theoretical mechanical properties of silica glass. <i>Transactions of the Materials Research Society of Japan</i> , 2011, 36, 35-40.	0.2	0
31	A simple dynamical scale-coupling method for concurrent simulation of hybridized atomistic/coarse-grained-particle system. <i>International Journal for Numerical Methods in Engineering</i> , 2010, 83, 249-268.	2.8	8
32	Stress-induced nano-oxidation of silicon by diamond-tip in moisture environment: A hybrid quantum-classical simulation study. <i>Journal of Applied Physics</i> , 2010, 108, 064313.	2.5	12
33	A Suite of Hybrid Simulation Schemes for Nano-to-Micrometer Scale Processes at Solid-Fluid Interfaces. <i>Progress of Theoretical Physics Supplement</i> , 2009, 178, 149-156.	0.1	0
34	Classical and Hybrid Density-Functional/Classical Molecular Dynamics Study of Dislocation Core in Alumina Ceramic. <i>Materials Transactions</i> , 2009, 50, 1015-1018.	1.2	2
35	Activation Energy for Oxygen Diffusion in Strained Silicon: A Hybrid Quantum-Classical Simulation Study with the Nudged Elastic Band Method. <i>Journal of the Physical Society of Japan</i> , 2008, 77, 054708.	1.6	6
36	Hybrid Simulations for Desinging of Nano-Interfacial Structures. <i>Solid State Phenomena</i> , 2007, 127, 57-62.	0.3	0

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37	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
38	Oxidation of aluminum nanoclusters. Physical Review B, 2005, 71, .	3.2	88
39	Buffered-cluster method for hybridization of density-functional theory and classical molecular dynamics: Application to stress-dependent reaction of H <sub>2</sub> O on nanostructured Si. Physical Review B, 2005, 72, .	3.2	38
40	VIRTUALIZATION-AWARE APPLICATION FRAMEWORK FOR HIERARCHICAL MULTISCALE SIMULATIONS ON A GRID. Lecture Notes Series, Institute for Mathematical Sciences, 2005, , 229-243.	0.2	0
41	Environmental effects of H <sub>2</sub> O on fracture initiation in silicon: A hybrid electronic-density-functional/molecular-dynamics study. Journal of Applied Physics, 2004, 95, 5316-5323.	2.5	45
42	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
43	Multiresolution atomistic simulations of dynamic fracture in nanostructured ceramics and glasses. International Journal of Fracture, 2003, 121, 71-79.	2.2	25
44	Scalable and portable implementation of the fast multipole method on parallel computers. Computer Physics Communications, 2003, 153, 445-461.	7.5	49
45	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
46	Scalable Atomistic Simulation Algorithms for Materials Research. Scientific Programming, 2002, 10, 263-270.	0.7	27
47	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
48	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
49	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
50	Initial Stages of Sintering of TiO <sub>2</sub> Nanoparticles: Variable-Charge Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2000, 634, 761.	0.1	0
51	Hybrid Electronic-density-functional/molecular-dynamics Simulation on Parallel Computers: Oxidation of Si Surface. Materials Research Society Symposia Proceedings, 2000, 653, .	0.1	0
52	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
53	Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers. Progress of Theoretical Physics Supplement, 2000, 138, 175-190.	0.1	10
54	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

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55	Dynamics of Oxidation of Aluminum Nanoclusters using Variable Charge Molecular-Dynamics Simulations on Parallel Computers. <i>Physical Review Letters</i> , 1999, 82, 4866-4869.	7.8	313
56	Path-Integral Monte Carlo Simulations for Excitation Spectra of Cs in Superfluid He. <i>Journal of the Physical Society of Japan</i> , 1999, 68, 2153-2156.	1.6	8
57	Intercluster Interaction of TiO <sub>2</sub> Nanoclusters Using Variable-Charge Interatomic Potentials. <i>Materials Research Society Symposia Proceedings</i> , 1999, 581, 667.	0.1	1
58	Oxidation Dynamics of Nanophase Aluminum Clusters: A Molecular Dynamics Study. <i>Materials Research Society Symposia Proceedings</i> , 1997, 481, 625.	0.1	3
59	Protonation and weakening of an epoxy resin/SiO <sub>2</sub> composite with silane coupling agents under moist conditions. <i>MRS Communications</i> , 0, , 1.	1.8	1