Reese E Jones

List of Publications by Year
in descending order

74	2,385	218677 26	214800 47
papers	citations	h-index	g-index
75	75	75	2701
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Calculation of stress in atomistic simulation. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S319-S332.	2.0	379
2	Thin Film Thermoelectric Metalâ€"Organic Framework with High Seebeck Coefficient and Low Thermal Conductivity. Advanced Materials, 2015, 27, 3453-3459.	21.0	227
3	Oxygen solubility and transport in Liâ€"air battery electrolytes: establishing criteria and strategies for electrolyte design. Energy and Environmental Science, 2017, 10, 1167-1179.	30.8	103
4	Towards more accurate molecular dynamics calculation of thermal conductivity: Case study of GaN bulk crystals. Physical Review B, 2009, 79, .	3.2	94
5	Nanostructural control of methane release in kerogen and its implications to wellbore production decline. Scientific Reports, 2016, 6, 28053.	3.3	94
6	Chemo-mechanical coupling in kerogen gas adsorption/desorption. Physical Chemistry Chemical Physics, 2018, 20, 12390-12395.	2.8	76
7	Relationship of thermal boundary conductance to structure from an analytical model plus molecular dynamics simulations. Physical Review B, 2013, 87, .	3.2	71
8	A material frame approach for evaluating continuum variables in atomistic simulations. Journal of Computational Physics, 2010, 229, 2364-2389.	3.8	67
9	Firstâ€Principles Study of Hydrolysis Reaction Barriers in a Sodium Borosilicate Glass. International Journal of Applied Glass Science, 2013, 4, 395-407.	2.0	66
10	Investigation of size and electronic effects on Kapitza conductance with non-equilibrium molecular dynamics. Applied Physics Letters, 2013, 102, .	3.3	59
11	Revealing Transition States during the Hydration of Clay Minerals. Journal of Physical Chemistry Letters, 2019, 10, 3704-3709.	4.6	49
12	Adaptive Green-Kubo estimates of transport coefficients from molecular dynamics based on robust error analysis. Journal of Chemical Physics, 2012, 136, 154102.	3.0	48
13	Molecular Simulations of Carbon Dioxide and Water: Cation Solvation. Environmental Science & Technology, 2013, 47, 87-94.	10.0	47
14	Surface Structure and Stability of Partially Hydroxylated Silica Surfaces. Langmuir, 2017, 33, 3882-3891.	3.5	47
15	Thermal boundary conductance across metal-gallium nitride interfaces from 80 to 450â€‰K. Applied Physics Letters, 2014, 105, .	3.3	46
16	The construction and application of an atomistic J-integral via Hardy estimates of continuum fields. Journal of the Mechanics and Physics of Solids, 2010, 58, 1318-1337.	4.8	45
17	A homogeneous nonequilibrium molecular dynamics method for calculating thermal conductivity with a three-body potential. Journal of Chemical Physics, 2009, 130, 204106.	3.0	41
18	Molecular dynamics studies of material property effects on thermal boundary conductance. Physical Chemistry Chemical Physics, 2013, 15, 11078.	2.8	40

#	Article	IF	Citations
19	Interaction of NaOH solutions with silica surfaces. Journal of Colloid and Interface Science, 2018, 516, 128-137.	9.4	39
20	Crack propagation in silica from reactive classical molecular dynamics simulations. Journal of the American Ceramic Society, 2018, 101, 1488-1499.	3.8	36
21	A novel finite element formulation for frictionless contact problems. International Journal for Numerical Methods in Engineering, 1995, 38, 2603-2617.	2.8	35
22	Modeling Interfacial Glassâ€"Water Reactions: Recent Advances and Current Limitations. International Journal of Applied Glass Science, 2014, 5, 421-435.	2.0	34
23	Automated high-throughput tensile testing reveals stochastic process parameter sensitivity. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 772, 138632.	5.6	32
24	Molecular dynamics studies of defect formation during heteroepitaxial growth of InGaN alloys on (0001) GaN surfaces. Journal of Applied Physics, 2017, 121, 195301.	2.5	30
25	A novel threeâ€"dimensional contact finite element based on smooth pressure interpolations. International Journal for Numerical Methods in Engineering, 2001, 51, 791-811.	2.8	29
26	Chemical Effects on Subcritical Fracture in Silica From Molecular Dynamics Simulations. Journal of Geophysical Research: Solid Earth, 2018, 123, 9341-9354.	3.4	28
27	Metalâ€"organic frameworks for thermoelectric energy-conversion applications. MRS Bulletin, 2016, 41, 877-882.	3.5	26
28	Molecular dynamics prediction of thermal conductivity of GaN films and wires at realistic length scales. Physical Review B, 2010, 81, .	3.2	25
29	Electron transport enhanced molecular dynamics for metals and semiâ€"metals. International Journal for Numerical Methods in Engineering, 2010, 83, 940-967.	2.8	23
30	An atomistic J-integral at finite temperature based on Hardy estimates of continuum fields. Journal of Physics Condensed Matter, 2011, 23, 015002.	1.8	22
31	Enhanced Ion Adsorption on Mineral Nanoparticles. Langmuir, 2018, 34, 5926-5934.	3.5	22
32	A yield-limited Lagrange multiplier formulation for frictional contact. International Journal for Numerical Methods in Engineering, 2000, 48, 1127-1149.	2.8	21
33	Influence of crystallographic orientation and anisotropy on Kapitza conductance via classical molecular dynamics simulations. Journal of Applied Physics, 2012, 112, 093515.	2.5	21
34	A family of simple two-pass dual formulations for the finite element solution of contact problems. Computer Methods in Applied Mechanics and Engineering, 2007, 196, 782-802.	6.6	20
35	A Long-Range Electric Field Solver for Molecular Dynamics Based on Atomistic-to-Continuum Modeling. Journal of Chemical Theory and Computation, 2011, 7, 1736-1749.	5.3	20
36	The application of an atomistic J-integral to a ductile crack. Journal of Physics Condensed Matter, 2013, 25, 155402.	1.8	18

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37	Atomistic Structure of Mineral Nano-aggregates from Simulated Compaction and Dewatering. Scientific Reports, 2017, 7, 15286.	3.3	18
38	Molecular-level understanding of gibbsite particle aggregation in water. Journal of Colloid and Interface Science, 2021, 600, 310-317.	9.4	18
39	Simulating anisotropic frictional response using smoothly interpolated traction fields. Computer Methods in Applied Mechanics and Engineering, 2006, 195, 588-613.	6.6	17
40	Effects of cutoff functions of Tersoff potentials on molecular dynamics simulations of thermal transport. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 025004.	2.0	17
41	Prediction of the evolution of the stress field of polycrystals undergoing elastic-plastic deformation with a hybrid neural network model. Machine Learning: Science and Technology, 2020, 1, 035005.	5.0	17
42	Modeling strength and failure variability due to porosity in additively manufactured metals. Computer Methods in Applied Mechanics and Engineering, 2021, 373, 113471.	6.6	16
43	Generalization of the homogeneous nonequilibrium molecular dynamics method for calculating thermal conductivity to multibody potentials. Physical Review E, 2009, 80, 047702.	2.1	14
44	Analytical law for size effects on thermal conductivity of nanostructures. Physical Review B, 2010, 81, .	3.2	14
45	A homogeneous nonequilibrium molecular dynamics method for calculating the heat transport coefficient of mixtures and alloys. Journal of Chemical Physics, 2010, 133, 034122.	3.0	14
46	Estimates of crystalline LiF thermal conductivity at high temperature and pressure by a Green-Kubo method. Physical Review B, 2016, 94, .	3.2	14
47	Efficient non-reflecting boundary condition constructed via optimization of damped layers. Physical Review B, 2010, 81, .	3.2	13
48	Effects of nanoconfinement and surface charge on iron adsorption on mesoporous silica. Environmental Science: Nano, 2021, 8, 1992-2005.	4.3	13
49	Thermal boundary conductance between Al films and GaN nanowires investigated with molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 9403-9410.	2.8	11
50	Structural Properties of Aqueous Solutions at the (100) and (101) Goethite Surfaces by Molecular Dynamics Simulation. Langmuir, 2018, 34, 14498-14510.	3.5	10
51	Molecular dynamics studies of InGaN growth on nonpolar $(11\bar{2}0)$ GaN surfaces. Physical Review Materials, 2018, 2, .	2.4	10
52	Mechanisms of Silica Fracture in Aqueous Electrolyte Solutions. Frontiers in Materials, 2019, 6, .	2.4	9
53	Sensitivity of the strength and toughness of concrete to the properties of the interfacial transition zone. Construction and Building Materials, 2022, 336, 126875.	7.2	9
54	Correlating structure and transport behavior in Li^+ and O_2 containing pyrrolidinium ionic liquids. Physical Chemistry Chemical Physics, 2019, 21, 17176-17189.	2.8	8

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55	Bayesian modeling of inconsistent plastic response due to material variability. Computer Methods in Applied Mechanics and Engineering, 2019, 353, 183-200.	6.6	7
56	Inelastic relaxation in silica via reactive molecular dynamics. Journal of the American Ceramic Society, 2022, 105, 2517-2526.	3.8	7
57	Simulation of hardened cement degradation and estimation of uncertainty in predicted failure times with peridynamics. Construction and Building Materials, 2021, 286, 122927.	7.2	6
58	Assessing Electrolyte Transport Properties with Molecular Dynamics. Journal of the Electrochemical Society, 2017, 164, A1258-A1267.	2.9	5
59	Tuning the critical Li intercalation concentrations for Mo_X ( ). Physical Review Materials, 2021, 5, .	2.4	5
60	Spatial resolution of the electrical conductance of ionic fluids using a Green-Kubo method. Journal of Chemical Physics, 2014, 141, 184110.	3.0	4
61	Principles of Coarse-Graining and Coupling Using the Atom-to-Continuum Method. Springer Series in Materials Science, 2016, , 223-259.	0.6	4
62	Influence of defects on the thermal conductivity of compressed LiF. Physical Review B, 2018, 97, .	3.2	4
63	A minimally invasive, efficient method for propagation of full-field uncertainty in solid dynamics. International Journal for Numerical Methods in Engineering, 2021, 122, 6955-6983.	2.8	4
64	An atomic-scale evaluation of the fracture toughness of silica glass. Journal of Physics Condensed Matter, 2018, 30, 245901.	1.8	3
65	Fracture mechanisms of sodium silicate glasses. International Journal of Applied Glass Science, 2023, 14, 27-37.	2.0	3
66	Simulated Real-Time Detection of a Small Molecule on a Carbon Nanotube Cantilever. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1364-1384.	0.4	2
67	On the microscopic definitions of the dislocation density tensor. Mathematics and Mechanics of Solids, 2014, 19, 744-757.	2.4	2
68	Insight into hydrogen production through molecular simulation of an electrode-ionomer electrolyte system. Journal of Chemical Physics, 2019, 151, 034702.	3.0	2
69	Atomic-scale interaction of a crack and an infiltrating fluid. Chemical Physics Letters: X, 2019, 737, 100005.	2.1	2
70	Effects of Strain Rate and Temperature on the Mechanical Properties of Simulated Silica Ionogels. Journal of Physical Chemistry B, 2021, 125, 8659-8671.	2.6	1
71	Computational Study of the Structure and Transport in Pyrrolidinium-Li-TFSI-Silica Ionogels. Journal of Physical Chemistry B, 2021, 125, 13003-13014.	2.6	1
72	A heteroencoder architecture for prediction of failure locations in porous metals using variational inference. Computer Methods in Applied Mechanics and Engineering, 2022, 398, 115236.	6.6	1

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73	Sustainability: GEOCâ€™s Perspective. ACS Symposium Series, 2015, , 105-117.	0.5	0
74	Sensitivity of void mediated failure to geometric design features of porous metals. International Journal of Solids and Structures, 2022, 236-237, 111309.	2.7	0