Timothy C Germann

List of Publications by Year
in descending order

127 papers	7,190 citations	57719 44 h-index	58549 82 g-index
132 all docs	132 docs citations	132 times ranked	5648 citing authors

#	Article	IF	Citations
1	Machine learning of consistent thermodynamic models using automatic differentiation. Physical Review E, 2022, 105, 045301.	0.8	7
2	Defect reversibility regulates dynamic tensile strength in silicon carbide at high strain rates. Scripta Materialia, 2022, 213, 114593.	2.6	6
3	Large-scale atomistic studies of sliding friction in polycrystalline aluminum interfaces. Journal of Applied Physics, 2022, 131, .	1.1	3
4	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	5.8	47
5	Two-Dimensional Carbonitride MXenes as an Efficient Electrocatalyst for Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 4477-4488.	1.5	13
6	Rate dependence and anisotropy of SiC response to ramp and wave-free quasi-isentropic compression. International Journal of Plasticity, 2021, 138, 102923.	4.1	15
7	Cooperative roles of stacking fault energies on dislocation nucleation at bimetal interface through tunable potentials. Computational Materials Science, 2021, 193, 110416.	1.4	5
8	Rational Design of Highly Stable and Active MXeneâ€Based Bifunctional ORR/OER Doubleâ€Atom Catalysts. Advanced Materials, 2021, 33, e2102595.	11.1	137
9	Mechanistic understanding of the size effect on shock facilitated dislocation nucleation at semicoherent interfaces. Scripta Materialia, 2020, 178, 457-462.	2.6	10
10	Molecular dynamics simulations of ejecta formation in helium-implanted copper. Scripta Materialia, 2020, 178, 114-118.	2.6	18
11	Evaluating diffusion and the thermodynamic factor for binary ionic mixtures. Physics of Plasmas, 2020, 27, .	0.7	10
12	On the grain size dependence of shock responses in nanocrystalline sic ceramics at high strain rates. Acta Materialia, 2020, 200, 632-651.	3.8	32
13	Shock-induced plasticity in nanocrystalline iron: Large-scale molecular dynamics simulations. Physical Review B, 2020, 102, .	1.1	18
14	Modeling and scale-bridging using machine learning: nanoconfinement effects in porous media. Scientific Reports, 2020, 10, 13312.	1.6	24
15	Interface facilitated transformation of voids directly into stacking fault tetrahedra. Acta Materialia, 2020, 188, 623-634.	3.8	21
16	Adaptive Physics Refinement at the Microstructure Scale. , 2020, , 1153-1171.		1
17	Designing Flexible Quantum Spin Hall Insulators through 2D Ordered Hybrid Transition-Metal Carbides. Journal of Physical Chemistry C, 2019, 123, 20664-20674.	1.5	4
18	School dismissal as a pandemic influenza response: When, where and for how long?. Epidemics, 2019, 28, 100348.	1.5	32

#	Article	IF	Citations
19	First-principles design of strong solids: Approaches and applications. Physics Reports, 2019, 826, 1-49.	10.3	31
20	Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities. Chemical Reviews, 2019, 119, 11980-12031.	23.0	242
21	Shock induced damage and fracture in SiC at elevated temperature and high strain rate. Acta Materialia, 2019, 167, 51-70.	3.8	48
22	Stronger and more failure-resistant with three-dimensional serrated bimetal interfaces. Acta Materialia, 2019, 166, 231-245.	3.8	35
23	Atomistic insight into the dislocation nucleation at crystalline/crystalline and crystalline/amorphous interfaces without full symmetry. Acta Materialia, 2019, 162, 255-267.	3.8	18
24	Mechanistic Quantification of Thermodynamic Stability and Mechanical Strength for Two-Dimensional Transition-Metal Carbides. Journal of Physical Chemistry C, 2018, 122, 4710-4722.	1.5	28
25	Phonon-mediated stabilization and softening of 2D transition metal carbides: case studies of Ti₂CO₂ and Mo₂CO₂. Physical Chemistry Chemical Physics, 2018, 20, 14608-14618.	1.3	8
26	Effect of dynamic evolution of misfit dislocation pattern on dislocation nucleation and shear sliding at semi-coherent bimetal interfaces. Acta Materialia, 2018, 143, 107-120.	3.8	48
27	A synergetic stabilization and strengthening strategy for two-dimensional ordered hybrid transition metal carbides. Physical Chemistry Chemical Physics, 2018, 20, 29684-29692.	1.3	9
28	The role of grain boundary orientation on void nucleation in tantalum. AIP Conference Proceedings, 2018, , .	0.3	7
29	Adaptive Physics Refinement at the Microstructure Scale. , 2018, , 1-19.		0
30	Surface Electrochemical Stability and Strainâ€Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides. Advanced Functional Materials, 2018, 28, 1804867.	7.8	33
31	Orientation dependent spall strength of tantalum single crystals. Acta Materialia, 2018, 159, 241-248.	3.8	60
32	High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength. Carbon, 2018, 137, 156-164.	5.4	22
33	On the ultimate tensile strength of tantalum. Acta Materialia, 2017, 126, 313-328.	3.8	90
34	Non-equilibrium molecular dynamics simulations of spall in single crystal tantalum. AIP Conference Proceedings, 2017, , .	0.3	12
35	Designing flexible 2D transition metal carbides with strain-controllable lithium storage. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E11082-E11091.	3.3	51
36	Graph-based linear scaling electronic structure theory. Journal of Chemical Physics, 2016, 144, 234101.	1.2	29

#	Article	IF	Citations
37	Manipulating dislocation nucleation and shear resistance of bimetal interfaces by atomic steps. Acta Materialia, 2016, 113, 194-205.	3.8	44
38	Symmetric tilt boundaries in body-centered cubic tantalum. Scripta Materialia, 2016, 116, 108-111.	2.6	39
39	Shock Loading of Granular Ni/Al Composites. Part 2: Shock-Induced Chemistry. Journal of Physical Chemistry C, 2016, 120, 6804-6813.	1.5	35
40	Database assisted distribution to improve fault tolerance for multiphysics applications. , 2015, , .		6
41	Distributed Database Kriging for Adaptive Sampling (D2KAS). Computer Physics Communications, 2015, 192, 138-147.	3.0	23
42	New insight into the helium-induced damage in MAX phase Ti3AlC2 by first-principles studies. Journal of Chemical Physics, 2015, 143, 114707.	1.2	26
43	Encapsulation kinetics and dynamics of carbon monoxide in clathrate hydrate. Nature Communications, 2014, 5, 4128.	5.8	62
44	Mesodynamics with implicit degrees of freedom. Journal of Chemical Physics, 2014, 141, 064107.	1.2	18
45	Effect of loading direction on grain boundary failure under shock loading. Acta Materialia, 2014, 64, 113-122.	3.8	82
46	Molecular dynamics simulations of shock-induced plasticity in tantalum. High Energy Density Physics, 2014, 10, 9-15.	0.4	74
47	Layer size effect on the shock compression behavior of fccâ€“bcc nanolaminates. Acta Materialia, 2014, 79, 74-83.	3.8	53
48	Shock Loading of Granular Ni/Al Composites. Part 1: Mechanics of Loading. Journal of Physical Chemistry C, 2014, 118, 26377-26386.	1.5	47
49	Crystal structure and encapsulation dynamics of ice II-structured neon hydrate. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10456-10461.	3.3	36
50	Spatial adaptive sampling in multiscale simulation. Computer Physics Communications, 2014, 185, 1857-1864.	3.0	23
51	Shock-induced phase transformations in gallium single crystals by atomistic methods. Physical Review B, 2013, 88, .	1.1	15
52	Structure and shear deformation of metallic crystallineâ€“amorphous interfaces. Acta Materialia, 2013, 61, 3600-3611.	3.8	77
53	Role of interface structure on the plastic response of Cu/Nb nanolaminates under shock compression: Non-equilibrium molecular dynamics simulations. Scripta Materialia, 2013, 68, 114-117.	2.6	81
54	Entropic Stabilization of Nanoscale Voids in Materials under Tension. Physical Review Letters, 2013, 110, 206001.	2.9	10

#	Article	IF	Citations
55	Grain Boundary Motion under Dynamic Loading: Mechanism and Large-Scale Molecular Dynamics Simulations. Materials Research Letters, 2013, 1, 220-227.	4.1	9
56	Finite size effects at high speed frictional interfaces. , 2012, , .		1
57	Molecular dynamics simulations of detonation on the roadrunner supercomputer. , 2012, , .		0
58	Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites. AIP Conference Proceedings, 2012, , .	0.3	6
59	Shock loading and release of a small angle tilt grain boundary in CU. , 2012, , .		1
60	Richtmyer-Meshkov instability examinedwith large-scalemolecular dynamics simulations. AIP Conference Proceedings, 2012, , .	0.3	6
61	The role of the structure of grain boundary interfaces during shock loading. AIP Conference Proceedings, 2012, , .	0.3	4
62	Atomic-scale study of nucleation of dislocations from fccâ€“bcc interfaces. Acta Materialia, 2012, 60, 2855-2865.	3.8	117
63	Large-scale molecular dynamics simulations of shock induced plasticity in tantalum single crystals. AIP Conference Proceedings, 2012, , .	0.3	15
64	Strain rate and orientation dependencies of the strength of single crystalline copper under compression. Physical Review B, 2012, 86, .	1.1	47
65	Early stage dynamic damage and the role of grain boundary type. Scripta Materialia, 2012, 66, 638-641.	2.6	48
66	Transmission electron microscopy study of the role of interface structure at 1 0 0/1 1 1 boundaries in a shocked copper multicrystal. Scripta Materialia, 2012, 67, 412-415.	2.6	7
67	Twinning in bcc metals under shock loading: a challenge to empirical potentials. Philosophical Magazine Letters, 2011, 91, 731-740.	0.5	54
68	Role of interfaces in shock-induced plasticity in Cu/Nb nanolaminates. Philosophical Magazine, 2011, 91, 4172-4185.	0.7	62
69	Dislocation nucleation mechanisms from fcc/bcc incoherent interfaces. Scripta Materialia, 2011, 65, 1022-1025.	2.6	125
70	The kinetics study of the S + S2â†' S3reaction by the chaperone mechanism. Journal of Chemical Physics, 2011, 134, 154508.	1.2	7
71	Isomorphic phase transformation in shocked Cerium using molecular dynamics. EPJ Web of Conferences, 2010, 10, 00009.	0.1	4
72	Sensitivity effects of void density and arrangement in a REBO high explosive. EPJ Web of Conferences, 2010, 10, 00024.	0.1	2

#	Article	IF	Citations
73	The influence of dilute heats of mixing on the atomic structures, defect energetics and mechanical properties of fccâ€“bcc interfaces. Acta Materialia, 2010, 58, 4549-4557.	3.8	45
74	Anisotropic shock response of columnar nanocrystalline Cu. Journal of Applied Physics, 2010, 107, .	1.1	74
75	Effects of void size, density, and arrangement on deflagration and detonation sensitivity of a reactive empirical bond order high explosive. Physical Review B, 2010, 82, .	1.1	39
76	Shock wave loading and spallation of copper bicrystals with asymmetric Î£3âŸ¨110âŸ© tilt grain boundaries. Journal of Applied Physics, 2010, 108, .	1.1	62
77	Atomistic methods in fluid simulation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 1547-1560.	1.6	66
78	Dynamic response of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mn>46</mml:m glass to high-strain-rate shock loading: Plasticity, spall, and atomic-level structures. Physical Review B, 2010, 81, .	1.1	85
79	The effect of vacancies on dynamic response of single crystal Cu to shock waves. Journal of Applied Physics, 2010, 107, .	1.1	30
80	Spall damage of copper under supported and decaying shock loading. Journal of Applied Physics, 2009, 106, .	1.1	73
81	A quantum chemistry study of Dielsâ€“Alder dimerizations in benzene and anthracene. Journal of Chemical Physics, 2009, 131, 024313.	1.2	16
82	369 Tflop/s molecular dynamics simulations on the petaflop hybrid supercomputer â€˜Roadrunnerâ€™. Concurrency Computation Practice and Experience, 2009, 21, 2143-2159.	1.4	15
83	Predicting EXAFS signals from shock compressed iron by use of molecular dynamics simulations. High Energy Density Physics, 2009, 5, 44-50.	0.4	6
84	Shock-induced spall in solid and liquid Cu at extreme strain rates. Journal of Applied Physics, 2009, 106, .	1.1	156
85	HIGH STRAIN RATES EFFECTS IN QUASI-ISENTROPIC COMPRESSION OF SOLIDS. AIP Conference Proceedings, 2009, , .	0.3	11
86	INFLUENCE OF SHOCKWAVE PROFILE ON EJECTA. AIP Conference Proceedings, 2009, , .	0.3	39
87	SHOCK-INDUCED SPALL IN COPPER: THE EFFECTS OF ANISOTROPY, TEMPERATURE, DEFECTS AND LOADING PULSE. , 2009, , .		4
88	THE EFFECTS OF DEFECTS ON MELTING OF COPPER. , 2009, , .		0
89	LARGE-SCALE MOLECULAR DYNAMICS SIMULATIONS OF THE FCC-FCC VOLUME COLLAPSE TRANSITION IN SHOCKED CESIUM. , 2009, , .		0
90	LARGE-SCALE CLASSICAL MOLECULAR DYNAMICS SIMULATIONS OF SHOCK-INDUCED PLASTICITY IN BCC NIOBIUM. , 2009, , .		8

#	Article	IF	Citations
91	Simulating picosecond x-ray diffraction from shocked crystals using post-processing molecular dynamics calculations. Journal of Physics Condensed Matter, 2008, 20, 505203.	0.7	21
92	369 Tflop/s molecular dynamics simulations on the Roadrunner general-purpose heterogeneous supercomputer. , 2008, , .		10
93	TRILLION-ATOM MOLECULAR DYNAMICS BECOMES A REALITY. International Journal of Modern Physics C, 2008, 19, 1315-1319.	0.8	100
94	BlueGene/L applications: Parallelism On a Massive Scale. International Journal of High Performance Computing Applications, 2008, 22, 33-51.	2.4	3
95	Modeling targeted layered containment of an influenza pandemic in the United States. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 4639-4644.	3.3	570
96	Molecular dynamics simulations of detonation instability. Physical Review E, 2008, 78, 046710.	0.8	16
97	Interaction potential for atomic simulations of conventional high explosives. Physical Review E, 2008, 78, 046709.	0.8	10
98	Scaling of atomistic fluid dynamics simulations. Physical Review E, 2008, 78, 045301.	0.8	18
99	ATOMISTIC SIMULATIONS OF SHOCK-INDUCED PHASE TRANSFORMATIONS IN POLYCRYSTALLINE IRON. , 2008, , .		1
100	SIMULATION OF FLUID INSTABILITIES USING ATOMISTIC METHODS. AIP Conference Proceedings, 2008, , .	0.3	1
101	SIMULATING EXAFS PATTERNS OF SHOCKED CRYSTALS. , 2008, , .		0
102	Molecular Dynamics Characterization of the Response of Ni/Al Nanolaminates Under Dynamic Loading. Journal of Propulsion and Power, 2007, 23, 693-697.	1.3	8
103	Melting and alloying of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ni</mml:mi><mml:mo>âˆ•</mml:mo><mml:mi mathvariant="normal">Al</mml:mi></mml:mrow></mml:math>nanolaminates induced by shock loading: A molecular dynamics simulation study. Physical Review B, 2007, 76, .	1.1	42
104	Influence of interatomic bonding potentials on detonation properties. Physical Review E, 2007, 76, 026318.	0.8	12
105	The importance of fluctuations in fluid mixing. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7741-7745.	3.3	76
106	Molecular dynamics simulation of dynamical response of perfect and porousNiâˆ•Alnanolaminates under shock loading. Physical Review B, 2007, 76, .	1.1	39
107	Shock Waves in Polycrystalline Iron. Physical Review Letters, 2007, 98, 135701.	2.9	138
108	MOLECULAR DYNAMICS COMES OF AGE: 320 BILLION ATOM SIMULATION ON BlueGene/L. International Journal of Modern Physics C, 2006, 17, 1755-1761.	0.8	126

#	Article	IF	Citations
109	Large-scale molecular dynamics simulations of hyperthermal cluster impact. International Journal of Impact Engineering, 2006, 33, 285-293.	2.4	10
110	A Molecular Dynamics Study of Solid Gallium Using a Modified Embedded Atom Model. AIP Conference Proceedings, 2006, , .	0.3	0
111	Atomistic Simulations of Shock-Induced Melting in Fe. AIP Conference Proceedings, 2006, , .	0.3	5
112	Directional-Dependence in Shock-Induced Melting of FCC Metals. AIP Conference Proceedings, 2006, , .	0.3	7
113	Molecular Dynamics Simulations of Shock-Induced Chemical, Mechanical, and Thermal Processes in Ni/Al Nanolaminates. AIP Conference Proceedings, 2006, , .	0.3	1
114	Atomistic simulations of shock-induced alloying reactions in Niâˆ•Al nanolaminates. Journal of Chemical Physics, 2006, 125, 164707.	1.2	83
115	Interplay of Shock-induced Melting and Alloying in Nanostructured Multilayer Films. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	1
116	Mitigation strategies for pandemic influenza in the United States. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 5935-5940.	3.3	904
117	Atomistic simulations of shock-induced transformations and their orientation dependence in bcc Fe single crystals. Physical Review B, 2005, 72, .	1.1	174
118	Nanoscale Structure and High Velocity Sliding at Cu/Ag Interfaces. Materials Research Society Symposia Proceedings, 2004, 821, 216.	0.1	2
119	Nanohydrodynamics simulations: An atomistic view of the Rayleigh-Taylor instability. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5851-5855.	3.3	98
120	Dislocation structure behind a shock front in fcc perfect crystals: Atomistic simulation results. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2004, 35, 2609-2615.	1.1	71
121	LARGE-SCALE MOLECULAR-DYNAMICS SIMULATION OF 19 BILLION PARTICLES. International Journal of Modern Physics C, 2004, 15, 193-201.	0.8	69
122	Large-Scale Molecular Dynamics Simulations of Ejecta Formation in Copper. AIP Conference Proceedings, 2004, , .	0.3	22
123	Large-Scale Molecular Dynamics Simulations of Shock-Induced Plasticity, Phase Transformations, and Detonation. AIP Conference Proceedings, 2002, , .	0.3	0
124	Atomistic Mechanism for Hot Spot Initiation. Physical Review Letters, 2002, 89, 285501.	2.9	97
125	Microscopic View of Structural Phase Transitions Induced by Shock Waves. Science, 2002, 296, 1681-1684.	6.0	435
126	Extending the Time Scale in Atomistic Simulation of Materials. Annual Review of Materials Research, 2002, 32, 321-346.	4.3	614

#	Article	IF	Citations
127	Orientation Dependence in Molecular Dynamics Simulations of Shocked Single Crystals. Physical Review Letters, 2000, 84, 5351-5354.	2.9	196