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	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
2	Extending the Time Scale in Atomistic Simulation of Materials. Annual Review of Materials Research, 2002, 32, 321-346.	4.3	614
3	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
4	Microscopic View of Structural Phase Transitions Induced by Shock Waves. Science, 2002, 296, 1681-1684.	6.0	435
5	Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities. Chemical Reviews, 2019, 119, 11980-12031.	23.0	242
6	Orientation Dependence in Molecular Dynamics Simulations of Shocked Single Crystals. Physical Review Letters, 2000, 84, 5351-5354.	2.9	196
7	Atomistic simulations of shock-induced transformations and their orientation dependence in bcc Fe single crystals. Physical Review B, 2005, 72, .	1.1	174
8	Shock-induced spall in solid and liquid Cu at extreme strain rates. Journal of Applied Physics, 2009, 106, .	1.1	156
9	Shock Waves in Polycrystalline Iron. Physical Review Letters, 2007, 98, 135701.	2.9	138
10	Rational Design of Highly Stable and Active MXeneâ€Based Bifunctional ORR/OER Doubleâ€Atom Catalysts. Advanced Materials, 2021, 33, e2102595.	11.1	137
11	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
12	Dislocation nucleation mechanisms from fcc/bcc incoherent interfaces. Scripta Materialia, 2011, 65, 1022-1025.	2.6	125
13	Atomic-scale study of nucleation of dislocations from fccâ€“bcc interfaces. Acta Materialia, 2012, 60, 2855-2865.	3.8	117
14	TRILLION-ATOM MOLECULAR DYNAMICS BECOMES A REALITY. International Journal of Modern Physics C, 2008, 19, 1315-1319.	0.8	100
15	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
16	Atomistic Mechanism for Hot Spot Initiation. Physical Review Letters, 2002, 89, 285501.	2.9	97
17	On the ultimate tensile strength of tantalum. Acta Materialia, 2017, 126, 313-328.	3.8	90
18	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

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19	Atomistic simulations of shock-induced alloying reactions in Niâˆ•Al nanolaminates. Journal of Chemical Physics, 2006, 125, 164707.	1.2	83
20	Effect of loading direction on grain boundary failure under shock loading. Acta Materialia, 2014, 64, 113-122.	3.8	82
21	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
22	Structure and shear deformation of metallic crystallineâ€“amorphous interfaces. Acta Materialia, 2013, 61, 3600-3611.	3.8	77
23	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
24	Anisotropic shock response of columnar nanocrystalline Cu. Journal of Applied Physics, 2010, 107, .	1.1	74
25	Molecular dynamics simulations of shock-induced plasticity in tantalum. High Energy Density Physics, 2014, 10, 9-15.	0.4	74
26	Spall damage of copper under supported and decaying shock loading. Journal of Applied Physics, 2009, 106, .	1.1	73
27	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
28	LARGE-SCALE MOLECULAR-DYNAMICS SIMULATION OF 19 BILLION PARTICLES. International Journal of Modern Physics C, 2004, 15, 193-201.	0.8	69
29	Atomistic methods in fluid simulation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 1547-1560.	1.6	66
30	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
31	Role of interfaces in shock-induced plasticity in Cu/Nb nanolaminates. Philosophical Magazine, 2011, 91, 4172-4185.	0.7	62
32	Encapsulation kinetics and dynamics of carbon monoxide in clathrate hydrate. Nature Communications, 2014, 5, 4128.	5.8	62
33	Orientation dependent spall strength of tantalum single crystals. Acta Materialia, 2018, 159, 241-248.	3.8	60
34	Twinning in bcc metals under shock loading: a challenge to empirical potentials. Philosophical Magazine Letters, 2011, 91, 731-740.	0.5	54
35	Layer size effect on the shock compression behavior of fccâ€“bcc nanolaminates. Acta Materialia, 2014, 79, 74-83.	3.8	53
36	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

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37	Early stage dynamic damage and the role of grain boundary type. Scripta Materialia, 2012, 66, 638-641.	2.6	48
38	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
39	Shock induced damage and fracture in SiC at elevated temperature and high strain rate. Acta Materialia, 2019, 167, 51-70.	3.8	48
40	Strain rate and orientation dependencies of the strength of single crystalline copper under compression. Physical Review B, 2012, 86, .	1.1	47
41	Shock Loading of Granular Ni/Al Composites. Part 1: Mechanics of Loading. Journal of Physical Chemistry C, 2014, 118, 26377-26386.	1.5	47
42	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	5.8	47
43	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
44	Manipulating dislocation nucleation and shear resistance of bimetal interfaces by atomic steps. Acta Materialia, 2016, 113, 194-205.	3.8	44
45	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>â^•</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
46	Molecular dynamics simulation of dynamical response of perfect and porousNiâ^•Alnanolaminates under shock loading. Physical Review B, 2007, 76, .	1.1	39
47	INFLUENCE OF SHOCKWAVE PROFILE ON EJECTA. AIP Conference Proceedings, 2009, , .	0.3	39
48	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
49	Symmetric tilt boundaries in body-centered cubic tantalum. Scripta Materialia, 2016, 116, 108-111.	2.6	39
50	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
51	Shock Loading of Granular Ni/Al Composites. Part 2: Shock-Induced Chemistry. Journal of Physical Chemistry C, 2016, 120, 6804-6813.	1.5	35
52	Stronger and more failure-resistant with three-dimensional serrated bimetal interfaces. Acta Materialia, 2019, 166, 231-245.	3.8	35
53	Surface Electrochemical Stability and Strainâ€Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides. Advanced Functional Materials, 2018, 28, 1804867.	7.8	33
54	School dismissal as a pandemic influenza response: When, where and for how long?. Epidemics, 2019, 28, 100348.	1.5	32

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55	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
56	First-principles design of strong solids: Approaches and applications. Physics Reports, 2019, 826, 1-49.	10.3	31
57	The effect of vacancies on dynamic response of single crystal Cu to shock waves. Journal of Applied Physics, 2010, 107, .	1.1	30
58	Graph-based linear scaling electronic structure theory. Journal of Chemical Physics, 2016, 144, 234101.	1.2	29
59	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
60	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
61	Modeling and scale-bridging using machine learning: nanoconfinement effects in porous media. Scientific Reports, 2020, 10, 13312.	1.6	24
62	Spatial adaptive sampling in multiscale simulation. Computer Physics Communications, 2014, 185, 1857-1864.	3.0	23
63	Distributed Database Kriging for Adaptive Sampling (D2KAS). Computer Physics Communications, 2015, 192, 138-147.	3.0	23
64	Large-Scale Molecular Dynamics Simulations of Ejecta Formation in Copper. AIP Conference Proceedings, 2004, , .	0.3	22
65	High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength. Carbon, 2018, 137, 156-164.	5.4	22
66	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
67	Interface facilitated transformation of voids directly into stacking fault tetrahedra. Acta Materialia, 2020, 188, 623-634.	3.8	21
68	Scaling of atomistic fluid dynamics simulations. Physical Review E, 2008, 78, 045301.	0.8	18
69	Mesodynamics with implicit degrees of freedom. Journal of Chemical Physics, 2014, 141, 064107.	1.2	18
70	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
71	Molecular dynamics simulations of ejecta formation in helium-implanted copper. Scripta Materialia, 2020, 178, 114-118.	2.6	18
72	Shock-induced plasticity in nanocrystalline iron: Large-scale molecular dynamics simulations. Physical Review B, 2020, 102, .	1.1	18

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73	Molecular dynamics simulations of detonation instability. Physical Review E, 2008, 78, 046710.	0.8	16
74	A quantum chemistry study of Dielsâ€“Alder dimerizations in benzene and anthracene. Journal of Chemical Physics, 2009, 131, 024313.	1.2	16
75	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
76	Large-scale molecular dynamics simulations of shock induced plasticity in tantalum single crystals. AIP Conference Proceedings, 2012, , .	0.3	15
77	Shock-induced phase transformations in gallium single crystals by atomistic methods. Physical Review B, 2013, 88, .	1.1	15
78	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
79	Two-Dimensional Carbonitride MXenes as an Efficient Electrocatalyst for Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 4477-4488.	1.5	13
80	Influence of interatomic bonding potentials on detonation properties. Physical Review E, 2007, 76, 026318.	0.8	12
81	Non-equilibrium molecular dynamics simulations of spall in single crystal tantalum. AIP Conference Proceedings, 2017, , .	0.3	12
82	HIGH STRAIN RATES EFFECTS IN QUASI-ISENTROPIC COMPRESSION OF SOLIDS. AIP Conference Proceedings, 2009, , .	0.3	11
83	Large-scale molecular dynamics simulations of hyperthermal cluster impact. International Journal of Impact Engineering, 2006, 33, 285-293.	2.4	10
84	369 Tflop/s molecular dynamics simulations on the Roadrunner general-purpose heterogeneous supercomputer. , 2008, , .		10
85	Interaction potential for atomic simulations of conventional high explosives. Physical Review E, 2008, 78, 046709.	0.8	10
86	Entropic Stabilization of Nanoscale Voids in Materials under Tension. Physical Review Letters, 2013, 110, 206001.	2.9	10
87	Mechanistic understanding of the size effect on shock facilitated dislocation nucleation at semicoherent interfaces. Scripta Materialia, 2020, 178, 457-462.	2.6	10
88	Evaluating diffusion and the thermodynamic factor for binary ionic mixtures. Physics of Plasmas, 2020, 27, .	0.7	10
89	Grain Boundary Motion under Dynamic Loading: Mechanism and Large-Scale Molecular Dynamics Simulations. Materials Research Letters, 2013, 1, 220-227.	4.1	9
90	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

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91	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
92	LARGE-SCALE CLASSICAL MOLECULAR DYNAMICS SIMULATIONS OF SHOCK-INDUCED PLASTICITY IN BCC NIOBIUM. , 2009, , .		8
93	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
94	Directional-Dependence in Shock-Induced Melting of FCC Metals. AIP Conference Proceedings, 2006, , .	0.3	7
95	The kinetics study of the S + S2â†' S3reaction by the chaperone mechanism. Journal of Chemical Physics, 2011, 134, 154508.	1.2	7
96	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
97	The role of grain boundary orientation on void nucleation in tantalum. AIP Conference Proceedings, 2018, , .	0.3	7
98	Machine learning of consistent thermodynamic models using automatic differentiation. Physical Review E, 2022, 105, 045301.	0.8	7
99	Predicting EXAFS signals from shock compressed iron by use of molecular dynamics simulations. High Energy Density Physics, 2009, 5, 44-50.	0.4	6
100	Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites. AIP Conference Proceedings, 2012, , .	0.3	6
101	Richtmyer-Meshkov instability examinedwith large-scalemolecular dynamics simulations. AIP Conference Proceedings, 2012, , .	0.3	6
102	Database assisted distribution to improve fault tolerance for multiphysics applications. , 2015, , .		6
103	Defect reversibility regulates dynamic tensile strength in silicon carbide at high strain rates. Scripta Materialia, 2022, 213, 114593.	2.6	6
104	Atomistic Simulations of Shock-Induced Melting in Fe. AIP Conference Proceedings, 2006, , .	0.3	5
105	Cooperative roles of stacking fault energies on dislocation nucleation at bimetal interface through tunable potentials. Computational Materials Science, 2021, 193, 110416.	1.4	5
106	SHOCK-INDUCED SPALL IN COPPER: THE EFFECTS OF ANISOTROPY, TEMPERATURE, DEFECTS AND LOADING PULSE. , 2009, , .		4
107	Isomorphic phase transformation in shocked Cerium using molecular dynamics. EPJ Web of Conferences, 2010, 10, 00009.	0.1	4
108	The role of the structure of grain boundary interfaces during shock loading. AIP Conference Proceedings, 2012, , .	0.3	4

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109	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
110	BlueGene/L applications: Parallelism On a Massive Scale. International Journal of High Performance Computing Applications, 2008, 22, 33-51.	2.4	3
111	Large-scale atomistic studies of sliding friction in polycrystalline aluminum interfaces. Journal of Applied Physics, 2022, 131, .	1.1	3
112	Nanoscale Structure and High Velocity Sliding at Cu/Ag Interfaces. Materials Research Society Symposia Proceedings, 2004, 821, 216.	0.1	2
113	Sensitivity effects of void density and arrangement in a REBO high explosive. EPJ Web of Conferences, 2010, 10, 00024.	0.1	2
114	Molecular Dynamics Simulations of Shock-Induced Chemical, Mechanical, and Thermal Processes in Ni/Al Nanolaminates. AIP Conference Proceedings, 2006, , .	0.3	1
115	Interplay of Shock-induced Melting and Alloying in Nanostructured Multilayer Films. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	1
116	ATOMISTIC SIMULATIONS OF SHOCK-INDUCED PHASE TRANSFORMATIONS IN POLYCRYSTALLINE IRON. , 2008, , .		1
117	SIMULATION OF FLUID INSTABILITIES USING ATOMISTIC METHODS. AIP Conference Proceedings, 2008, , .	0.3	1
118	Finite size effects at high speed frictional interfaces. , 2012, , .		1
119	Shock loading and release of a small angle tilt grain boundary in CU. , 2012, , .		1
120	Adaptive Physics Refinement at the Microstructure Scale. , 2020, , 1153-1171.		1
121	Large-Scale Molecular Dynamics Simulations of Shock-Induced Plasticity, Phase Transformations, and Detonation. AIP Conference Proceedings, 2002, , .	0.3	0
122	A Molecular Dynamics Study of Solid Gallium Using a Modified Embedded Atom Model. AIP Conference Proceedings, 2006, , .	0.3	0
123	SIMULATING EXAFS PATTERNS OF SHOCKED CRYSTALS. , 2008, , .		0
124	THE EFFECTS OF DEFECTS ON MELTING OF COPPER. , 2009, , .		0
125	LARGE-SCALE MOLECULAR DYNAMICS SIMULATIONS OF THE FCC-FCC VOLUME COLLAPSE TRANSITION IN SHOCKED CESIUM. , 2009, , .		0
126	Molecular dynamics simulations of detonation on the roadrunner supercomputer. , 2012, , .		0

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127	Adaptive Physics Refinement at the Microstructure Scale. , 2018, , 1-19.		0