Vladimir V Stegailov

List of Publications by Year
in descending order

118	2,162	186209	276775
papers	citations	28 h-index	41 g-index

120	120	120	1205
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Stochastic theory of the classical molecular dynamics method. Mathematical Models and Computer Simulations, 2013, 5, 305-333.	0.1	130
2	Standards for molecular dynamics modelling and simulation of relaxation. Molecular Simulation, 2005, 31, 1005-1017.	0.9	82
3	Theory and molecular dynamics modeling of spall fracture in liquids. Physical Review B, 2010, 82, .	1.1	80
4	A ternary EAM interatomic potential for Uâ€“Mo alloys with xenon. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 035011.	0.8	71
5	Atomistic simulation of laser ablation of gold: Effect of pressure relaxation. Journal of Experimental and Theoretical Physics, 2012, 114, 792-800.	0.2	66
6	Melting and superheating of sI methane hydrate: Molecular dynamics study. Journal of Chemical Physics, 2012, 136, 044523.	1.2	64
7	Molecular-dynamics simulation of edge-dislocation dynamics in aluminum. Doklady Physics, 2008, 53, 287-291.	0.2	62
8	Radiation-induced damage and evolution of defects in Mo. Physical Review B, 2011, 84, .	1.1	53
9	Atomistic Modeling of Warm Dense Matter in the Twoâ€Temperature State. Contributions To Plasma Physics, 2013, 53, 129-139.	0.5	52
10	High temperature pure carbon nanoparticle formation: Validation of AIREBO and ReaxFF reactive molecular dynamics. Carbon, 2020, 170, 606-620.	5.4	51
11	Atomistic simulation of the premelting of iron and aluminum: Implications for high-pressure melting-curve measurements. Physical Review B, 2009, 80, .	1.1	46
12	Molecular dynamics simulations of the relaxation processes in the condensed matter on GPUs. Computer Physics Communications, 2011, 182, 1974-1978.	3.0	46
13	Angara interconnect makes GPU-based Desmos supercomputer an efficient tool for molecular dynamics calculations. International Journal of High Performance Computing Applications, 2019, 33, 507-521.	2.4	45
14	Nanomodification of gold surface by picosecond soft x-ray laser pulse. Journal of Applied Physics, 2012, 112, .	1.1	44
15	GPU-accelerated molecular dynamics: State-of-art software performance and porting from Nvidia CUDA to AMD HIP. International Journal of High Performance Computing Applications, 2021, 35, 312-324.	2.4	43
16	Self-consistent molecular dynamics calculation of diffusion in higher n-alkanes. Journal of Chemical Physics, 2016, 145, 204504.	1.2	40
17	Graphite melting: Atomistic kinetics bridges theory and experiment. Carbon, 2015, 87, 358-364.	5.4	39
18	Stability of LiF Crystal in the Warm Dense Matter State. Contributions To Plasma Physics, 2010, 50, 31-34.	0.5	38

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19	Simulation of Ideal Crystal Superheating and Decay. Molecular Simulation, 2004, 30, 397-406.	0.9	37
20	Toward Determination of the New Hydrogen Hydrate Clathrate Structures. Journal of Physical Chemistry Letters, 2013, 4, 3560-3564.	2.1	37
21	Interatomic potential for uranium in a wide range of pressures and temperatures. Journal of Physics Condensed Matter, 2012, 24, 015702.	0.7	36
22	Development of the advanced mechanistic fuel performance and safety code using the multi-scale approach. Nuclear Engineering and Design, 2015, 295, 116-126.	0.8	35
23	HPC Hardware Efficiency for Quantum and Classical Molecular Dynamics. Lecture Notes in Computer Science, 2015, , 469-473.	1.0	33
24	Atomistic modeling of the self-diffusion in Î³-U and Î³-U-Mo. Physics of Metals and Metallography, 2015, 116, 445-455.	0.3	31
25	Optimization of neighbor list techniques in liquid matter simulations. Journal of Molecular Liquids, 2006, 125, 197-203.	2.3	30
26	The phase diagram and spinodal decomposition of metastable states of Lennard-Jones system. High Temperature, 2007, 45, 37-48.	0.1	30
27	Dynamic fracture kinetics, influence of temperature and microstructure in the atomistic model of aluminum. International Journal of Fracture, 2010, 162, 127-136.	1.1	30
28	Cavitation in liquid metals under negative pressures. Molecular dynamics modeling and simulation. Journal of Physics Condensed Matter, 2008, 20, 114113.	0.7	28
29	Atomistic simulation of plasticity and fracture of nanocrystalline copper under high-rate tension. Physics of the Solid State, 2008, 50, 2069-2075.	0.2	27
30	Atomic positions and diffusion paths of h and he in the Î±-Ti lattice. Physics of the Solid State, 2013, 55, 367-372.	0.2	26
31	Homogeneous nucleation in a superheated crystal. Molecular-dynamic simulation. Doklady Physics, 2002, 47, 667-671.	0.2	25
32	Laser ablation of gold: Experiment and atomistic simulation. JETP Letters, 2011, 93, 642-647.	0.4	25
33	Atomistic Modelling and Simulation of Warm Dense Matter. Conductivity and Reflectivity. Contributions To Plasma Physics, 2013, 53, 300-310.	0.5	25
34	Plasmaâ€Plasma and Liquidâ€Liquid Firstâ€Order Phase Transitions. Contributions To Plasma Physics, 2015, 55, 215-221.	0.5	25
35	Influence of plastic deformation on fracture of an aluminum single crystal under shock-wave loading. Physics of the Solid State, 2010, 52, 1619-1624.	0.2	24
36	Structural transformations in single-crystal iron during shock-wave compression and tension: Molecular dynamics simulation. Journal of Experimental and Theoretical Physics, 2007, 104, 928-935.	0.2	23

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37	Surface melting of superheated crystals. Atomistic simulation study. Computer Physics Communications, 2007, 177, 34-37.	3.0	22
38	Anomalous kinetic energy of a system of dust particles in a gas discharge plasma. Journal of Experimental and Theoretical Physics, 2011, 113, 887-900.	0.2	22
39	Molecular dynamics simulation of graphite melting. High Temperature, 2014, 52, 198-204.	0.1	22
40	Reactive molecular-dynamics study of onion-like carbon nanoparticle formation. Diamond and Related Materials, 2019, 94, 14-20.	1.8	21
41	Interatomic potential for uranium in a wide range of pressures and temperatures. Journal of Physics Condensed Matter, 2012, 24, 149501.	0.7	20
42	Ab initiocalculation of shocked xenon reflectivity. Physical Review E, 2015, 91, 023105.	0.8	20
43	Stochastic and dynamic properties of molecular dynamics systems: Simple liquids, plasma and electrolytes, polymers. Computer Physics Communications, 2002, 147, 678-683.	3.0	18
44	Homogeneous and heterogeneous mechanisms of superheated solid melting and decay. Computer Physics Communications, 2005, 169, 247-250.	3.0	17
45	VASP hits the memory wall: Processors efficiency comparison. Concurrency Computation Practice and Experience, 2019, 31, e5136.	1.4	17
46	Floating-point performance of ARM cores and their efficiency in classical molecular dynamics. Journal of Physics: Conference Series, 2016, 681, 012049.	0.3	16
47	Efficiency of the Tegra K1 and X1 systems-on-chip for classical molecular dynamics. , 2016, , .		16
48	A kinetic model of fracture of simple liquids. High Temperature, 2010, 48, 511-517.	0.1	15
49	Relaxation and transport properties of liquid n-triacontane. Journal of Physics: Conference Series, 2015, 653, 012107.	0.3	14
50	Pressure in electronically excited warm dense metals. Contributions To Plasma Physics, 2015, 55, 164-171.	0.5	14
51	Derivation of kinetic coefficients by atomistic methods for studying defect behavior in Mo. Journal of Nuclear Materials, 2012, 425, 41-47.	1.3	13
52	Efficiency of classical molecular dynamics algorithms on supercomputers. Mathematical Models and Computer Simulations, 2016, 8, 734-743.	0.1	13
53	Atomistic simulation of the interaction of an electrolyte with graphite nanostructures in perspective supercapacitors. High Temperature, 2010, 48, 837-845.	0.1	12
54	New interatomic potential for computation of mechanical and thermodynamic properties of uranium in a wide range of pressures and temperatures. Physics of Metals and Metallography, 2012, 113, 107-116.	0.3	12

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55	Nanobubbles diffusion in bcc uranium: Theory and atomistic modelling. Journal of Nuclear Materials, 2020, 533, 152110.	1.3	12
56	Performance and Scalability of Materials Science and Machine Learning Codes on the State-of-Art Hybrid Supercomputer Architecture. Communications in Computer and Information Science, 2019, , 597-609.	0.4	12
57	Excited States of Warm Dense Matter. Contributions To Plasma Physics, 2011, 51, 411-418.	0.5	11
58	Anomalous diffusion of guest molecules in hydrogen gas hydrates. High Temperature, 2015, 53, 829-836.	0.1	11
59	Cavitation and the stability region of liquid lead at negative pressures: Molecular dynamics study. Doklady Physics, 2005, 50, 570-576.	0.2	10
60	Molecular-dynamics based insights into the problem of graphite melting. Journal of Physics: Conference Series, 2015, 653, 012090.	0.3	10
61	Early Performance Evaluation of the Hybrid Cluster with Torus Interconnect Aimed at Molecular-Dynamics Simulations. Lecture Notes in Computer Science, 2018, , 327-336.	1.0	10
62	Microscopic mechanisms of diffusion of higher alkanes. Polymer Science - Series A, 2016, 58, 825-836.	0.4	9
63	Porting CUDA-Based Molecular Dynamics Algorithms to AMD ROCm Platform Using HIP Framework: Performance Analysis. Communications in Computer and Information Science, 2019, , 121-130.	0.4	9
64	GPU Acceleration of Four-Site Water Models in LAMMPS. Advances in Parallel Computing, 2020, , .	0.3	9
65	The modeling of high-rate tension of crystalline iron by the method of molecular dynamics. High Temperature, 2007, 45, 164-172.	0.1	8
66	Kinetics of graphite melting. Doklady Physics, 2015, 60, 109-113.	0.2	8
67	Formation free energies of point defects and thermal expansion of bcc U and Mo. Journal of Physics Condensed Matter, 2019, 31, 235704.	0.7	8
68	Molecular dynamics simulation of cavitation in a lead melt at negative pressures. Russian Journal of Physical Chemistry A, 2006, 80, S90-S97.	0.1	7
69	Atomistic simulation of laser ablation of gold: The effect of electronic pressure. , 2012, , .		7
70	Warm dense gold: effective ionâ€“ion interaction and ionisation. Molecular Physics, 0, , 1-10.	0.8	7
71	Simulation of the adhesion properties of the polyethylene/carbon nanotube interface. Polymer Science - Series A, 2016, 58, 476-486.	0.4	7
72	Nonadiabatic effects and excitonlike states during the insulator-to-metal transition in warm dense hydrogen. Physical Review B, 2020, 101, .	1.1	7

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73	Performance of Supercomputers Based onÂAngara Interconnect and Novel AMD CPUs/GPUs. Communications in Computer and Information Science, 2021, , 401-416.	0.4	7
74	Abnormal Kinetic Energy of Charged Dust Particles in Plasmas. Contributions To Plasma Physics, 2010, 50, 104-108.	0.5	6
75	Atomistic Simulation of Clustering and Annihilation of Point Defects in Molybdenum. Defect and Diffusion Forum, 0, 323-325, 95-100.	0.4	6
76	Ab initio calculations of thermal conductivity of metals with hot electrons. Doklady Physics, 2013, 58, 334-338.	0.2	6
77	GPU-Accelerated Molecular Dynamics: Energy Consumption and Performance. Communications in Computer and Information Science, 2016, , 78-90.	0.4	6
78	Pseudopotential for electronic structure calculations of uranium compounds. Lobachevskii Journal of Mathematics, 2017, 38, 974-977.	0.1	6
79	Efficiency Analysis of Intel and AMD x86_64 Architectures for Ab Initio Calculations: A Case Study of VASP. Communications in Computer and Information Science, 2017, , 430-441.	0.4	6
80	Efficiency Analysis of Intel, AMD and Nvidia 64-Bit Hardware forÂMemory-Bound Problems: A Case Study of Ab Initio Calculations with VASP. Lecture Notes in Computer Science, 2018, , 81-90.	1.0	5
81	Premelting of iron at high pressures under conditions of contact with amorphous argon. High Temperature, 2008, 46, 795-799.	0.1	4
82	Molecular simulation as a scientific base of nanotechnologies in power engineering. Journal of Engineering Thermophysics, 2009, 18, 197-226.	0.6	4
83	Application of the density-functional theory to calculation of the reflectivity from shocked xenon. Doklady Physics, 2013, 58, 277-281.	0.2	4
84	First-principles calculation of the reflectance of shock-compressed xenon. Journal of Experimental and Theoretical Physics, 2015, 120, 894-904.	0.2	4
85	Domain-Decomposition Parallelization for Molecular Dynamics Algorithm with Short-Ranged Potentials on Epiphany Architecture. Lobachevskii Journal of Mathematics, 2018, 39, 1228-1238.	0.1	4
86	Hybrid Supercomputer Desmos withÂTorus Angara Interconnect: Efficiency Analysis and Optimization. Communications in Computer and Information Science, 2018, , 77-91.	0.4	4
87	Energy Consumption of MD Calculations on Hybrid and CPU-Only Supercomputers with Air and Immersion Cooling. Advances in Parallel Computing, 2020, , .	0.3	4
88	ATOMISTIC SIMULATION OF PLASTICITY AND FRACTURE OF CRYSTALLINE AND POLYCRYSTALLINE METALS UNDER HIGH STRAIN RATE. AIP Conference Proceedings, 2008, , .	0.3	3
89	Atomistic Modeling and Simulation for Solving Gas Extraction Problems. Molecular Modeling and Simulation, 2016, , 137-151.	0.2	3
90	Hybrid Codes for Atomistic Simulations on the Desmos Supercomputer: GPU-acceleration, Scalability and Parallel I/O. Communications in Computer and Information Science, 2019, , 218-229.	0.4	3

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91	Matrix-Matrix Multiplication Using Multiple GPUs Connected by Nvlink. , 2020, , .		3
92	Ultrafast diffusion of overpressurized gas filled nanobubbles in UO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Journal of Nuclear Materials, 2021, 551, 152942.	1.3	3
93	Description of mechanical properties of carbon nanotubes. Tube wall thickness problem. Size effect. Part 1. Letters on Materials, 2011, 1, 185-189.	0.2	3
94	Fracture of crystalline iron subjected to high-rate tension. Molecular dynamics simulation. Doklady Physics, 2005, 50, 509-513.	0.2	2
95	Cavitation in liquid Pb and Li under negative pressures. Computer Physics Communications, 2007, 177, 41.	3.0	2
96	Performance of MD-Algorithms on Hybrid Systems-on-Chip Nvidia Tegra K1 & X1. Communications in Computer and Information Science, 2016, , 199-211.	0.4	2
97	Tuning ofÂaÂMatrix-Matrix Multiplication Algorithm forÂSeveral GPUs Connected byÂFast Communication Links. Communications in Computer and Information Science, 2022, , 158-171.	0.4	2
98	Atomistic simulations of structure transitions and fracture in Fe and Al single crystals. Computer Physics Communications, 2007, 177, 48.	3.0	1
99	On thermodynamic similarity of the stability boundaries of metastable metal states. Russian Journal of Physical Chemistry A, 2007, 81, 1016-1024.	0.1	1
100	MODELING OF Al CRYSTAL FRACTURE UNDER HIGH-RATE STRAIN BASED ON ATOMISTIC SIMULATIONS. , 2008, , .		1
101	Molecular-dynamics simulation of iron premelting at high pressures. Doklady Physics, 2009, 54, 1-5.	0.2	1
102	MOLECULAR DYNAMIC MODELING OF PLASTICITY OF Al AND Al-Cu ALLOYS UNDER DYNAMIC LOADING. , 2009, , .		1
103	MICROSCOPIC THEORY AND KINETIC MODEL OF SPALL IN LIQUIDS. , 2009, , .		1
104	Atomistic and Kinetic Simulations of Radiation Damage in Molybdenum. Materials Research Society Symposia Proceedings, 2012, 1444, 15.	0.1	1
105	Nano-meter scale modifications on material surfaces induced by soft x-ray laser pulse irradiations. Proceedings of SPIE, 2013, , .	0.8	1
106	Hydration structure of Na+ and Clâ˜ ions in Tip3P water model. Lobachevskii Journal of Mathematics, 2017, 38, 971-973.	0.1	1
107	Theoretical Study of Electronic Structure of Charged Fullerenes. Journal of Nanomaterials, 2021, 2021, 1-10.	1.5	1
108	Performance and Portability of State-of-Art Molecular Dynamics Software on Modern GPUs. Lecture Notes in Computer Science, 2020, , 324-334.	1.0	1

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109	System for accumulation and processing of spectrometric data from the YASNAPP-2 facility. European Physical Journal D, 1999, 49, 249-252.	0.4	0
110	Standard of Molecular Dynamics Modeling and Simulation of Relaxation in Dense Media. Lecture Notes in Computer Science, 2004, , 596-603.	1.0	0
111	On similarity relations for the stability limits of metastable metals. Doklady Physics, 2007, 52, 173-178.	0.2	0
112	ATOMISTIC STUDY OF NANOPRECIPITATES INFLUENCE ON PLASTICITY AND FRACTURE OF CRYSTALLINE METALS. , 2008, , .		0
113	ATOMISTIC SIMULATIONS OF FRACTURE IN NANOCRYSTALLINE COPPER UNDER HIGH STRAIN RATES. , 2008, , .		0
114	INFLUENCE OF TEMPERATURE ON SPALL STRENGTH: ATOMISTIC SIMULATION. , 2009, , .		0
115	Performance of Elbrus Processors forÂComputational Materials Science Codes and Fast Fourier Transform. Communications in Computer and Information Science, 2018, , 92-103.	0.4	0
116	Deploying Elbrus VLIW CPU Ecosystem for Materials Science Calculations: Performance and Problems. Communications in Computer and Information Science, 2019, , 543-553.	0.4	0
117	Dynamic and Stochastic Properties of Molecular Systems: From Simple Liquids to Enzymes. Lecture Notes in Computer Science, 2002, , 1137-1146.	1.0	0
118	Determinism and Chaos in Decay of Metastable States. Lecture Notes in Computer Science, 2002, , 1147-1153.	1.0	0