Vladimir V Stegailov

List of Publications by Year in Descending Order

113 papers	1,723 citations	24 h-index	35 g-index
120 ext. papers	1,921 ext. citations	1.7 avg, IF	5.24 L-index

#	Paper	IF	Citations
113	Tuning of a Matrix-Matrix Multiplication Algorithm for Several GPUs Connected by Fast Communication Links. *Communications in Computer and Information Science*, **2022**, 158-171	0.3	1
112	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	1.8	13
111	Theoretical Study of Electronic Structure of Charged Fullerenes. *Journal of Nanomaterials*, **2021**, 2021, 1-10	3.2	
110	Performance of Supercomputers Based on Angara Interconnect and Novel AMD CPUs/GPUs. *Communications in Computer and Information Science*, **2021**, 401-416	0.3	1
109	Ultrafast diffusion of overpressurized gas filled nanobubbles in UO2. *Journal of Nuclear Materials*, **2021**, 551, 152942	3.3	0
108	Matrix-Matrix Multiplication Using Multiple GPUs Connected by Nvlink **2020**,		2
107	Nonadiabatic effects and excitonlike states during the insulator-to-metal transition in warm dense hydrogen. *Physical Review B*, **2020**, 101,	3.3	3
106	Nanobubbles diffusion in bcc uranium: Theory and atomistic modelling. *Journal of Nuclear Materials* , **2020**, 533, 152110	3.3	7
105	Performance and Portability of State-of-Art Molecular Dynamics Software on Modern GPUs. *Lecture Notes in Computer Science*, **2020**, 324-334	0.9	1
104	High temperature pure carbon nanoparticle formation: Validation of AIREBO and ReaxFF reactive molecular dynamics. *Carbon*, **2020**, 170, 606-620	10.4	17
103	Energy Consumption of MD Calculations on Hybrid and CPU-Only Supercomputers with Air and Immersion Cooling. *Advances in Parallel Computing*, **2020**,	1.1	3
102	VASP hits the memory wall: Processors efficiency comparison. *Concurrency Computation Practice and Experience*, **2019**, 31, e5136	1.4	8
101	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	1.8	23
100	Formation free energies of point defects and thermal expansion of bcc U and Mo. *Journal of Physics Condensed Matter*, **2019**, 31, 235704	1.8	4
99	Porting CUDA-Based Molecular Dynamics Algorithms to AMD ROCm Platform Using HIP Framework: Performance Analysis. *Communications in Computer and Information Science*, **2019**, 121-130	0.3	5
98	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	0.3	9
97	Reactive molecular-dynamics study of onion-like carbon nanoparticle formation. *Diamond and Related Materials*, **2019**, 94, 14-20	3.5	13

96	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	0.3	3
95	Deploying Elbrus VLIW CPU Ecosystem for Materials Science Calculations: Performance and Problems. *Communications in Computer and Information Science*, **2019**, 543-553	0.3	
94	Early Performance Evaluation of the Hybrid Cluster with Torus Interconnect Aimed at Molecular-Dynamics Simulations. *Lecture Notes in Computer Science*, **2018**, 327-336	0.9	9
93	Efficiency Analysis of Intel, AMD and Nvidia 64-Bit Hardware for Memory-Bound Problems: A Case Study of Ab Initio Calculations with VASP. *Lecture Notes in Computer Science*, **2018**, 81-90	0.9	4
92	Domain-Decomposition Parallelization for Molecular Dynamics Algorithm with Short-Ranged Potentials on Epiphany Architecture. *Lobachevskii Journal of Mathematics*, **2018**, 39, 1228-1238	0.9	3
91	Hybrid Supercomputer Desmos with Torus Angara Interconnect: Efficiency Analysis and Optimization. *Communications in Computer and Information Science*, **2018**, 77-91	0.3	4
90	Performance of Elbrus Processors for Computational Materials Science Codes and Fast Fourier Transform. *Communications in Computer and Information Science*, **2018**, 92-103	0.3	
89	Hydration structure of Na+ and Cl□ions in Tip3P water model. *Lobachevskii Journal of Mathematics*, **2017**, 38, 971-973	0.9	1
88	Pseudopotential for electronic structure calculations of uranium compounds. *Lobachevskii Journal of Mathematics*, **2017**, 38, 974-977	0.9	5
87	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	0.3	6
86	Simulation of the adhesion properties of the polyethylene/carbon nanotube interface. *Polymer Science - Series A*, **2016**, 58, 476-486	1.2	6
85	Atomistic Modeling and Simulation for Solving Gas Extraction Problems. *Molecular Modeling and Simulation*, **2016**, 137-151		3
84	Floating-point performance of ARM cores and their efficiency in classical molecular dynamics. *Journal of Physics: Conference Series*, **2016**, 681, 012049	0.3	10
83	Performance of MD-Algorithms on Hybrid Systems-on-Chip Nvidia Tegra K1 & X1. *Communications in Computer and Information Science*, **2016**, 199-211	0.3	2
82	GPU-Accelerated Molecular Dynamics: Energy Consumption and Performance. *Communications in Computer and Information Science*, **2016**, 78-90	0.3	5
81	Efficiency of classical molecular dynamics algorithms on supercomputers. *Mathematical Models and Computer Simulations*, **2016**, 8, 734-743	0.8	12
80	Self-consistent molecular dynamics calculation of diffusion in higher n-alkanes. *Journal of Chemical Physics*, **2016**, 145, 204504	3.9	33
79	Efficiency of the Tegra K1 and X1 systems-on-chip for classical molecular dynamics **2016**,		12

78	Microscopic mechanisms of diffusion of higher alkanes. *Polymer Science - Series A*, **2016**, 58, 825-836	1.2	6
77	Graphite melting: Atomistic kinetics bridges theory and experiment. *Carbon*, **2015**, 87, 358-364	10.4	35
76	Ab initio calculation of shocked xenon reflectivity. *Physical Review E*, **2015**, 91, 023105	2.4	19
75	Kinetics of graphite melting. *Doklady Physics*, **2015**, 60, 109-113	0.8	8
74	HPC Hardware Efficiency for Quantum and Classical Molecular Dynamics. *Lecture Notes in Computer Science*, **2015**, 469-473	0.9	33
73	First-principles calculation of the reflectance of shock-compressed xenon. *Journal of Experimental and Theoretical Physics*, **2015**, 120, 894-904	1	4
72	Development of the advanced mechanistic fuel performance and safety code using the multi-scale approach. *Nuclear Engineering and Design*, **2015**, 295, 116-126	1.8	24
71	Warm dense gold: effective ion□bn interaction and ionisation. *Molecular Physics*, **2015**, 1-10	1.7	5
70	Plasma-Plasma and Liquid-Liquid First-Order Phase Transitions. *Contributions To Plasma Physics*, **2015**, 55, 215-221	1.4	20
69	Molecular-dynamics based insights into the problem of graphite melting. *Journal of Physics: Conference Series*, **2015**, 653, 012090	0.3	9
68	Relaxation and transport properties of liquid n-triacontane. *Journal of Physics: Conference Series*, **2015**, 653, 012107	0.3	11
67	Atomistic modeling of the self-diffusion in □U and □U-Mo. *Physics of Metals and Metallography*, **2015**, 116, 445-455	1.2	26
66	Anomalous diffusion of guest molecules in hydrogen gas hydrates. *High Temperature*, **2015**, 53, 829-836	0.8	10
65	Pressure in electronically excited warm dense metals. *Contributions To Plasma Physics*, **2015**, 55, 164-171	1.4	11
64	Molecular dynamics simulation of graphite melting. *High Temperature*, **2014**, 52, 198-204	0.8	18
63	Nano-meter Size Modification of Metal Surfaces Induced by Soft X-Ray Laser Single Pulse. *Springer Proceedings in Physics*, **2014**, 121-124	0.2	
62	Stochastic theory of the classical molecular dynamics method. *Mathematical Models and Computer Simulations*, **2013**, 5, 305-333	0.8	109
61	Application of the density-functional theory to calculation of the reflectivity from shocked xenon. *Doklady Physics*, **2013**, 58, 277-281	0.8	4

60	Toward Determination of the New Hydrogen Hydrate Clathrate Structures. *Journal of Physical Chemistry Letters*, **2013**, 4, 3560-3564	6.4	30
59	Ab initio calculations of thermal conductivity of metals with hot electrons. *Doklady Physics*, **2013**, 58, 334-338	0.8	6
58	Atomistic Modeling of Warm Dense Matter in the Two-Temperature State. *Contributions To Plasma Physics*, **2013**, 53, 129-139	1.4	34
57	A ternary EAM interatomic potential for U–Mo alloys with xenon. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 035011	2	57
56	Atomistic Modelling and Simulation of Warm Dense Matter. Conductivity and Reflectivity. *Contributions To Plasma Physics*, **2013**, 53, 300-310	1.4	22
55	Atomic positions and diffusion paths of h and he in the □Ti lattice. *Physics of the Solid State*, **2013**, 55, 367-372	0.8	21
54	Nano-meter scale modifications on material surfaces induced by soft x-ray laser pulse irradiations **2013**,		1
53	Derivation of kinetic coefficients by atomistic methods for studying defect behavior in Mo. *Journal of Nuclear Materials*, **2012**, 425, 41-47	3.3	11
52	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	1.2	9
51	Atomistic simulation of laser ablation of gold: Effect of pressure relaxation. *Journal of Experimental and Theoretical Physics*, **2012**, 114, 792-800	1	53
50	Atomistic simulation of laser ablation of gold: The effect of electronic pressure **2012**,		3
49	Interatomic potential for uranium in a wide range of pressures and temperatures. *Journal of Physics Condensed Matter*, **2012**, 24, 015702	1.8	22
48	Interatomic potential for uranium in a wide range of pressures and temperatures. *Journal of Physics Condensed Matter*, **2012**, 24, 149501	1.8	18
47	Melting and superheating of sI methane hydrate: molecular dynamics study. *Journal of Chemical Physics*, **2012**, 136, 044523	3.9	53
46	Nanomodification of gold surface by picosecond soft x-ray laser pulse. *Journal of Applied Physics*, **2012**, 112, 013104	2.5	37
45	Atomistic Simulation of Clustering and Annihilation of Point Defects in Molybdenum. *Defect and Diffusion Forum*, **2012**, 323-325, 95-100	0.7	6
44	Atomistic and Kinetic Simulations of Radiation Damage in Molybdenum. *Materials Research Society Symposia Proceedings*, **2012**, 1444, 15		1
43	Laser ablation of gold: Experiment and atomistic simulation. *JETP Letters*, **2011**, 93, 642-647	1.2	21

42	Anomalous kinetic energy of a system of dust particles in a gas discharge plasma. *Journal of Experimental and Theoretical Physics*, **2011**, 113, 887-900	1	20
41	Radiation-induced damage and evolution of defects in Mo. *Physical Review B*, **2011**, 84,	3.3	48
40	Molecular dynamics simulations of the relaxation processes in the condensed matter on GPUs. *Computer Physics Communications*, **2011**, 182, 1974-1978	4.2	40
39	Excited States of Warm Dense Matter. *Contributions To Plasma Physics*, **2011**, 51, 411-418	1.4	10
38	Description of mechanical properties of carbon nanotubes. Tube wall thickness problem. Size effect. Part 1. *Letters on Materials*, **2011**, 1, 185-189	0.9	3
37	A kinetic model of fracture of simple liquids. *High Temperature*, **2010**, 48, 511-517	0.8	14
36	Atomistic simulation of the interaction of an electrolyte with graphite nanostructures in perspective supercapacitors. *High Temperature*, **2010**, 48, 837-845	0.8	10
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	0.8	19
34	Theory and molecular dynamics modeling of spall fracture in liquids. *Physical Review B*, **2010**, 82,	3.3	71
33	Dynamic fracture kinetics, influence of temperature and microstructure in the atomistic model of aluminum. *International Journal of Fracture*, **2010**, 162, 127-136	2.3	25
32	Stability of LiF Crystal in the Warm Dense Matter State. *Contributions To Plasma Physics*, **2010**, 50, 31-34	1.4	32
31	Abnormal Kinetic Energy of Charged Dust Particles in Plasmas. *Contributions To Plasma Physics*, **2010**, 50, 104-108	1.4	6
30	Molecular simulation as a scientific base of nanotechnologies in power engineering. *Journal of Engineering Thermophysics*, **2009**, 18, 197-226	1.4	3
29	Molecular-dynamics simulation of iron premelting at high pressures. *Doklady Physics*, **2009**, 54, 1-5	0.8	1
28	Atomistic simulation of the premelting of iron and aluminum: Implications for high-pressure melting-curve measurements. *Physical Review B*, **2009**, 80,	3.3	42
27	MOLECULAR DYNAMIC MODELING OF PLASTICITY OF Al AND Al-Cu ALLOYS UNDER DYNAMIC LOADING **2009**,		1
26	Premelting of iron at high pressures under conditions of contact with amorphous argon. *High Temperature*, **2008**, 46, 795-799	0.8	4
25	ATOMISTIC SIMULATION OF PLASTICITY AND FRACTURE OF CRYSTALLINE AND POLYCRYSTALLINE METALS UNDER HIGH STRAIN RATE **2008**,		3

24	Cavitation in liquid metals under negative pressures. Molecular dynamics modeling and simulation. *Journal of Physics Condensed Matter*, **2008**, 20, 114113	1.8	25
23	Molecular-dynamics simulation of edge-dislocation dynamics in aluminum. *Doklady Physics*, **2008**, 53, 287-291	0.8	55
22	Atomistic simulation of plasticity and fracture of nanocrystalline copper under high-rate tension. *Physics of the Solid State*, **2008**, 50, 2069-2075	0.8	22
21	Cavitation in liquid Pb and Li under negative pressures. *Computer Physics Communications*, **2007**, 177, 41	4.2	2
20	Atomistic simulations of structure transitions and fracture in Fe and Al single crystals. *Computer Physics Communications*, **2007**, 177, 48	4.2	1
19	The phase diagram and spinodal decomposition of metastable states of Lennard-Jones system. *High Temperature*, **2007**, 45, 37-48	0.8	27
18	The modeling of high-rate tension of crystalline iron by the method of molecular dynamics. *High Temperature*, **2007**, 45, 164-172	0.8	7
17	On thermodynamic similarity of the stability boundaries of metastable metal states. *Russian Journal of Physical Chemistry A*, **2007**, 81, 1016-1024	0.7	1
16	On similarity relations for the stability limits of metastable metals. *Doklady Physics*, **2007**, 52, 173-178	0.8	
15	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	1	18
14	Surface melting of superheated crystals. Atomistic simulation study. *Computer Physics Communications*, **2007**, 177, 34-37	4.2	19
13	Optimization of neighbor list techniques in liquid matter simulations. *Journal of Molecular Liquids*, **2006**, 125, 197-203	6	21
12	Molecular dynamics simulation of cavitation in a lead melt at negative pressures. *Russian Journal of Physical Chemistry A*, **2006**, 80, S90-S97	0.7	6
11	Standards for molecular dynamics modelling and simulation of relaxation. *Molecular Simulation*, **2005**, 31, 1005-1017	2	74
10	Homogeneous and heterogeneous mechanisms of superheated solid melting and decay. *Computer Physics Communications*, **2005**, 169, 247-250	4.2	16
9	Fracture of crystalline iron subjected to high-rate tension. Molecular dynamics simulation. *Doklady Physics*, **2005**, 50, 509-513	0.8	2
8	Cavitation and the stability region of liquid lead at negative pressures: Molecular dynamics study. *Doklady Physics*, **2005**, 50, 570-576	0.8	9
7	Standard of Molecular Dynamics Modeling and Simulation of Relaxation in Dense Media. *Lecture Notes in Computer Science*, **2004**, 596-603	0.9	

6	Simulation of Ideal Crystal Superheating and Decay. *Molecular Simulation*, **2004**, 30, 397-406	2	35
5	Homogeneous nucleation in a superheated crystal. Molecular-dynamic simulation. *Doklady Physics*, **2002**, 47, 667-671	0.8	24
4	Stochastic and dynamic properties of molecular dynamics systems: Simple liquids, plasma and electrolytes, polymers. *Computer Physics Communications*, **2002**, 147, 678-683	4.2	15
3	Dynamic and Stochastic Properties of Molecular Systems: From Simple Liquids to Enzymes. *Lecture Notes in Computer Science*, **2002**, 1137-1146	0.9	
2	Determinism and Chaos in Decay of Metastable States. *Lecture Notes in Computer Science*, **2002**, 1147-1153	0.9	
1	System for accumulation and processing of spectrometric data from the YASNAPP-2 facility. *European Physical Journal D*, **1999**, 49, 249-252		