

Ivan I Oleynik

List of Publications by Year in descending order

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111
papers

5,315
citations

109264

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h-index

85498

71
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111
all docs

111
docs citations

111
times ranked

6577
citing authors

#	ARTICLE	IF	CITATIONS
1	An extended defect in graphene as a metallic wire. <i>Nature Nanotechnology</i> , 2010, 5, 326-329.	15.6	909
2	Rectification and stability of a single molecular diode with controlled orientation. <i>Nature Chemistry</i> , 2009, 1, 635-641.	6.6	517
3	Layer-dependent properties of SnS two-dimensional materials. <i>Physical Review B</i> , 2016, 94.	1.1	267
4	Analytic bond-order potentials beyond Tersoff-Brenner. I. Theory. <i>Physical Review B</i> , 1999, 59, 8487-8499.	1.1	183
5	Graphene Growth on Ni(111) by Transformation of a Surface Carbide. <i>Nano Letters</i> , 2011, 11, 518-522.	4.5	182
6	High-Pressure Synthesis of a Pentazolate Salt. <i>Chemistry of Materials</i> , 2017, 29, 735-741.	3.2	170
7	Charge Density Wave State Suppresses Ferromagnetic Ordering in VSe_2 Monolayers. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14089-14096.	1.5	144
8	Structural and electronic properties of $\text{Co}/\text{Al}_2\text{O}_3/\text{Co}$ magnetic tunnel junction from first principles. <i>Physical Review B</i> , 2000, 62, 3952-3959.	1.1	138
9	Ablation and spallation of gold films irradiated by ultrashort laser pulses. <i>Physical Review B</i> , 2010, 82, .	1.1	122
10	Sodium pentazolate: A nitrogen rich high energy density material. <i>Chemical Physics Letters</i> , 2016, 643, 21-26.	1.2	115
11	Graphene growth and stability at nickel surfaces. <i>New Journal of Physics</i> , 2011, 13, 025001.	1.2	107
12	Bounded Analytic Bond-Order Potentials for f and d Bonds. <i>Physical Review Letters</i> , 2000, 84, 4124-4127.	2.9	102
13	Formation of nanocavities in the surface layer of an aluminum target irradiated by a femtosecond laser pulse. <i>JETP Letters</i> , 2012, 95, 176-181.	0.4	102
14	Atomic and electronic structure of $\text{Co}/\text{SrTiO}_3/\text{Co}$ magnetic tunnel junctions. <i>Physical Review B</i> , 2001, 65, .	1.1	96
15	Interface effects in spin-dependent tunneling. <i>Progress in Materials Science</i> , 2007, 52, 401-420.	16.0	92
16	Rectification Mechanism in Diblock Oligomer Molecular Diodes. <i>Physical Review Letters</i> , 2006, 96, 096803.	2.9	90
17	A mechanism for crystal twinning in the growth of diamond by chemical vapour deposition. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2008, 366, 295-311.	1.6	90
18	Two-Zone Elastic-Plastic Single Shock Waves in Solids. <i>Physical Review Letters</i> , 2011, 107, 135502.	2.9	90

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19	Ultrashort shock waves in nickel induced by femtosecond laser pulses. <i>Physical Review B</i> , 2013, 87, .	1.1	76
20	Effect of interface bonding on spin-dependent tunneling from the oxidized Co surface. <i>Physical Review B</i> , 2004, 69, .	1.1	74
21	Etching effects during the chemical vapor deposition of (100) diamond. <i>Journal of Chemical Physics</i> , 1999, 111, 4291-4299.	1.2	72
22	Analytic bond-order potentials beyond Tersoff-Brenner. II. Application to the hydrocarbons. <i>Physical Review B</i> , 1999, 59, 8500-8507.	1.1	72
23	Atomic and electronic structure of simple metal/graphene and complex metal/graphene/metal interfaces. <i>Physical Review B</i> , 2012, 85, .	1.1	72
24	Equations of state for energetic materials from density functional theory with van der Waals, thermal, and zero-point energy corrections. <i>Applied Physics Letters</i> , 2010, 97, .	1.5	67
25	Analytic bond-order potential for open and close-packed phases. <i>Physical Review B</i> , 2002, 65, .	1.1	64
26	Evolution of Shock-Induced Orientation-Dependent Metastable States in Crystalline Aluminum. <i>Physical Review Letters</i> , 2012, 109, 125505.	2.9	57
27	Pentazole and Ammonium Pentazolate: Crystalline Hydro-Nitrogens at High Pressure. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1808-1813.	1.1	56
28	Novel Potassium Polynitrides at High Pressures. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8955-8961.	1.1	56
29	Oxygen-induced positive spin polarization from Fe into the vacuum barrier. <i>Journal of Applied Physics</i> , 2000, 87, 5230-5232.	1.1	49
30	First-principles investigation of anisotropic constitutive relationships in pentaerythritol tetranitrate. <i>Physical Review B</i> , 2008, 77, .	1.1	46
31	Novel rubidium poly-nitrogen materials at high pressure. <i>Journal of Chemical Physics</i> , 2017, 147, 234701.	1.2	46
32	Monolayer Modification of VTe_2 and Its Charge Density Wave. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4987-4993.	2.1	43
33	Hydrostatic and uniaxial compression studies of 1,3,5-triamino-2,4,6-trinitrobenzene using density functional theory with van der Waals correction. <i>Journal of Applied Physics</i> , 2010, 107, .	1.1	39
34	Density Functional Theory Calculations of Solid Nitromethane under Hydrostatic and Uniaxial Compressions with Empirical van der Waals Correction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3610-3614.	1.1	38
35	First-principles anisotropic constitutive relationships in $\hat{\Gamma}^2$ -cyclotetramethylene tetranitramine ($\hat{\Gamma}^2$ -HMX). <i>Journal of Applied Physics</i> , 2008, 104, 053506.	1.1	36
36	Electron Relaxation, Phase Transitions, and Surface Nanostructuring Produced by Ultrashort Laser Pulses in Metals. <i>Contributions To Plasma Physics</i> , 2013, 53, 796-810.	0.5	36

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37	Bond-order potentials: bridging the electronic to atomistic modelling hierarchies. <i>Computational Materials Science</i> , 2002, 23, 33-37.	1.4	35
38	Effect of Temperature and Nanoparticle Size on Sensor Properties of Nanostructured Tin Dioxide Films. <i>Journal of Physical Chemistry C</i> , 2014, 118, 11440-11444.	1.5	35
39	Two-temperature thermodynamic and kinetic properties of transition metals irradiated by femtosecond lasers. , 2012, , .		34
40	Screened environment-dependent reactive empirical bond-order potential for atomistic simulations of carbon materials. <i>Physical Review B</i> , 2013, 88, .	1.1	34
41	Positive spin polarization in $\text{Co}/\text{Al}_2\text{O}_3/\text{Co}$ tunnel junctions driven by oxygen adsorption. <i>Physical Review B</i> , 2005, 71, .	1.1	32
42	Inhomogeneous Charge Distribution in Semiconductor Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16286-16292.	1.5	29
43	Theory of Sensing Response of Nanostructured Tin-Dioxide Thin Films to Reducing Hydrogen Gas. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11562-11568.	1.5	27
44	Reactive Molecular Dynamics of Hypervelocity Collisions of PETN Molecules. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12094-12104.	1.1	26
45	Surface nanodeformations caused by ultrashort laser pulse. <i>Engineering Failure Analysis</i> , 2015, 47, 328-337.	1.8	26
46	Correlating structural, electronic, and magnetic properties of epitaxial VSe ₂ thin films. <i>Physical Review B</i> , 2020, 102, .	1.1	25
47	Ternary Inorganic Compounds Containing Carbon, Nitrogen, and Oxygen at High Pressures. <i>Inorganic Chemistry</i> , 2017, 56, 13321-13328.	1.9	24
48	Ultrafast lasers and solids in highly excited states: results of hydrodynamics and molecular dynamics simulations. <i>Journal of Physics: Conference Series</i> , 2014, 510, 012041.	0.3	23
49	Theoretical study of chemical reactions on CVD diamond surfaces. <i>Diamond and Related Materials</i> , 2000, 9, 241-245.	1.8	19
50	Ammonium Azide under High Pressure: A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8695-8700.	1.1	19
51	Interatomic bond-order potentials and structural prediction. <i>Progress in Materials Science</i> , 2004, 49, 285-312.	16.0	18
52	Tunneling and resonant conductance in one-dimensional molecular structures. <i>Chemical Physics</i> , 2005, 319, 368-379.	0.9	18
53	Billion atom molecular dynamics simulations of carbon at extreme conditions and experimental time and length scales. , 2021, , .		18
54	Density functional theory calculations of anisotropic constitutive relationships in alpha-cyclotrimethylenetrinitramine. <i>Journal of Applied Physics</i> , 2008, 104, .	1.1	17

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55	Atomic and electronic structure of graphene/Sn-Ni(111) and graphene/Sn-Cu(111) surface alloy interfaces. Applied Physics Letters, 2012, 101, 051602.	1.5	17
56	Novel phases and superconductivity of tin sulfide compounds. Journal of Chemical Physics, 2018, 148, 194701.	1.2	17
57	Evolution of elastic precursor and plastic shock wave in copper via molecular dynamics simulations. Journal of Physics: Conference Series, 2014, 500, 172008.	0.3	16
58	Surface nano-structuring produced by spallation of metal irradiated by an ultrashort laser pulse. Journal of Physics: Conference Series, 2014, 500, 112070.	0.3	15
59	Spin injection into amorphous semiconductors. Physical Review B, 2002, 66, .	1.1	14
60	Strength of metals in liquid and solid states at extremely high tension produced by femtosecond laser heating. AIP Conference Proceedings, 2012, , .	0.3	14
61	Metal-Oxide Interfaces in Magnetic Tunnel Junctions. Journal of Materials Science, 2004, 12, 105-116.	1.2	13
62	Structural and spectroscopic studies of nitrogen-carbon monoxide mixtures: Photochemical response and observation of a novel phase. Journal of Chemical Physics, 2017, 146, 184309.	1.2	13
63	Tin Selenide Compounds at Ambient and High Pressures. Journal of Physical Chemistry C, 2018, 122, 18274-18281.	1.5	13
64	Vibrational and thermal properties of β -HMX and TATB from dispersion corrected density functional theory. AIP Conference Proceedings, 2017, , .	0.3	12
65	Elastic-plastic collapse of super-elastic shock waves in face-centered-cubic solids. Journal of Physics: Conference Series, 2014, 500, 172007.	0.3	11
66	Sensor Effect in Oxide Films with a Large Concentration of Conduction Electrons. Journal of Physical Chemistry C, 2017, 121, 6940-6945.	1.5	11
67	Laminar, cellular, transverse, and multiheaded pulsating detonations in condensed phase energetic materials from molecular dynamics simulations. Physical Review E, 2014, 90, 033312.	0.8	10
68	Two-temperature hydrodynamic expansion and coupling of strong elastic shock with supersonic melting front produced by ultrashort laser pulse. Journal of Physics: Conference Series, 2014, 500, 192023.	0.3	10
69	Atomic, electronic, and magnetic properties of magnetic tunnel junctions. Journal of Applied Physics, 2003, 93, 6429-6431.	1.1	9
70	Shock compression of diamond: Molecular dynamics simulations using different interatomic potentials. , 2012, , .		8
71	Ultrashort elastic and plastic shockwaves in aluminum. , 2012, , .		8
72	Cesium pentazolate: A new nitrogen-rich energetic material. AIP Conference Proceedings, 2017, , .	0.3	8

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73	Bound states of tunneling electrons in molecular chains. <i>Physical Review B</i> , 2006, 74, .	1.1	7
74	Shear stresses in shock-compressed diamond from density functional theory. <i>Physical Review B</i> , 2008, 78, .	1.1	6
75	A new nickel EAM potential for atomistic simulations of ablation, spallation, and shockwave phenomena. <i>AIP Conference Proceedings</i> , 2012, , .	0.3	6
76	Single two-zone elastic-plastic shock waves in solids. , 2012, , .		6
77	New phase of ammonium nitrate: A monoclinic distortion of AN-IV. <i>Journal of Chemical Physics</i> , 2015, 143, 234705.	1.2	6
78	Crystal structure of silver pentazolates AgN5 and AgN6. <i>Dalton Transactions</i> , 2021, 50, 16364-16370.	1.6	6
79	Molecular Dynamics Simulations of Femtosecond Laser Ablation and Spallation of Gold. , 2010, , .		5
80	Prediction of Isothermal Equation of State of an Explosive Nitrate Ester by van der Waals Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 346-348.	2.1	5
81	Evolution of metastable elastic shockwaves in nickel. , 2012, , .		5
82	MD simulations of laser-induced ultrashort shock waves in nickel. , 2012, , .		5
83	Super-elastic response of metals to laser-induced shock waves. , 2012, , .		5
84	Ultrashort laser-matter interaction at moderate intensities: two-temperature relaxation, foaming of stretched melt, and freezing of evolving nanostructures. <i>Proceedings of SPIE</i> , 2013, , .	0.8	5
85	Force distribution in a granular medium under dynamic loading. <i>Physical Review E</i> , 2017, 96, 012906.	0.8	5
86	Computational Discovery of New High-Nitrogen Energetic Materials. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 25-52.	0.6	5
87	Direct and inverse problems in the theory of scanning tunneling microscopy. <i>Surface Science</i> , 1995, 331-333, 1191-1196.	0.8	4
88	Shock-induced phase transition in diamond. , 2012, , .		4
89	Shock-induced phase transitions in metals: Recrystallization of supercooled melt and melting of overheated solids. , 2012, , .		4
90	Vibrational excitation of a molecule by a resonance current. <i>Journal of Experimental and Theoretical Physics</i> , 2012, 115, 759-768.	0.2	4

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91	Density functional theory investigation of sodium azide at high pressure. Journal of Physics: Conference Series, 2014, 500, 162005.	0.3	4
92	Vibrational and thermophysical properties of PETN from first principles. AIP Conference Proceedings, 2017, , .	0.3	4
93	Quantum accurate SNAP carbon potential for MD shock simulations. AIP Conference Proceedings, 2020, , .	0.3	4
94	Ammonium azide under hydrostatic compression. Journal of Physics: Conference Series, 2014, 500, 162006.	0.3	3
95	Tunneling dynamics of electrons and effective tunneling potential. Surface Science, 1996, 363, 360-367.	0.8	2
96	Spin-dependent tunneling from clean and oxidized Co surfaces. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 1954-1955.	1.0	2
97	Electron-plasmon interactions in resonant molecular tunnel junctions. Physical Review B, 2010, 81, .	1.1	2
98	First-principles thermodynamics of energetic materials. , 2012, , .		2
99	Diamond CVD Growth Mechanisms and Reaction Rates From First-Principles. Materials Research Society Symposia Proceedings, 2000, 616, 123.	0.1	1
100	New crystal phase of ammonium nitrate: First-principles prediction and characterization. AIP Conference Proceedings, 2017, , .	0.3	1
101	First principles investigation of nitrogen-rich energetic materials. AIP Conference Proceedings, 2018, , .	0.3	1
102	Predictive simulations of metastable phases of carbon at high compression. AIP Conference Proceedings, 2020, , .	0.3	1
103	An extended defect in graphene as a metallic wire. , 0, .		1
104	First principles molecular dynamics simulations of high-pressure melting of diamond. AIP Conference Proceedings, 2020, , .	0.3	1
105	Surface Chemistry of CVD Diamond: Linking the Nanoscale and Mesoscale Modelling Hierarchies. Materials Research Society Symposia Proceedings, 1998, 538, 275.	0.1	0
106	Bonding and Cohesive Properties of Cobalt/Alumina Magnetic Tunnel Junctions. Materials Research Society Symposia Proceedings, 2000, 616, 171.	0.1	0
107	Computational Nanomechanics of Graphene Membranes. Materials Research Society Symposia Proceedings, 2009, 1185, 55.	0.1	0
108	Effect of reactive chemistry on mechanisms of condensed phase detonation. , 2012, , .		0

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109	From laminar to turbulent detonations in energetic materials from molecular dynamics simulations. Journal of Physics: Conference Series, 2014, 500, 172005.	0.3	0
110	Nano-scale spinning detonation in a condensed phase energetic material. Journal of Physics: Conference Series, 2014, 500, 172006.	0.3	0
111	First-principles investigation of iron pentacarbonyl molecular solid phases at high pressure. AIP Conference Proceedings, 2017, , .	0.3	0