Ivan I Oleynik

List of Publications by Year
in descending order

111	5,315	109264	85498
papers	citations	35 h-index	71 g-index

111	111	111	6577
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Crystal structure of silver pentazolates AgN5 and AgN6. Dalton Transactions, 2021, 50, 16364-16370.	1.6	6
2	Billion atom molecular dynamics simulations of carbon at extreme conditions and experimental time and length scales. , 2021, , .		18
3	Correlating structural, electronic, and magnetic properties of epitaxial VSe2 thin films. Physical Review B, 2020, 102, .	1.1	25
4	Predictive simulations of metastable phases of carbon at high compression. AIP Conference Proceedings, 2020, , .	0.3	1
5	Quantum accurate SNAP carbon potential for MD shock simulations. AIP Conference Proceedings, 2020, , .	0.3	4
6	First principles molecular dynamics simulations of high-pressure melting of diamond. AIP Conference Proceedings, 2020, , .	0.3	1
7	Monolayer Modification of VTe₂ and Its Charge Density Wave. Journal of Physical Chemistry Letters, 2019, 10, 4987-4993.	2.1	43
8	Charge Density Wave State Suppresses Ferromagnetic Ordering in VSe₂ Monolayers. Journal of Physical Chemistry C, 2019, 123, 14089-14096.	1.5	144
9	Computational Discovery of New High-Nitrogen Energetic Materials. Challenges and Advances in Computational Chemistry and Physics, 2019, , 25-52.	0.6	5
10	Novel phases and superconductivity of tin sulfide compounds. Journal of Chemical Physics, 2018, 148, 194701.	1.2	17
11	Tinâ€“Selenium Compounds at Ambient and High Pressures. Journal of Physical Chemistry C, 2018, 122, 18274-18281.	1.5	13
12	First principles investigation of nitrogen-rich energetic materials. AIP Conference Proceedings, 2018, , .	0.3	1
13	Cesium pentazolate: A new nitrogen-rich energetic material. AIP Conference Proceedings, 2017, , .	0.3	8
14	First-principles investigation of iron pentacarbonyl molecular solid phases at high pressure. AIP Conference Proceedings, 2017, , .	0.3	0
15	Vibrational and thermal properties of Î²-HMX and TATB from dispersion corrected density functional theory. AIP Conference Proceedings, 2017, , .	0.3	12
16	Pentazole and Ammonium Pentazolate: Crystalline Hydro-Nitrogens at High Pressure. Journal of Physical Chemistry A, 2017, 121, 1808-1813.	1.1	56
17	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
18	Sensor Effect in Oxide Films with a Large Concentration of Conduction Electrons. Journal of Physical Chemistry C, 2017, 121, 6940-6945.	1.5	11

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19	High-Pressure Synthesis of a Pentazolate Salt. Chemistry of Materials, 2017, 29, 735-741.	3.2	170
20	Novel Potassium Polynitrides at High Pressures. Journal of Physical Chemistry A, 2017, 121, 8955-8961.	1.1	56
21	Ternary Inorganic Compounds Containing Carbon, Nitrogen, and Oxygen at High Pressures. Inorganic Chemistry, 2017, 56, 13321-13328.	1.9	24
22	Force distribution in a granular medium under dynamic loading. Physical Review E, 2017, 96, 012906.	0.8	5
23	Vibrational and thermophysical properties of PETN from first principles. AIP Conference Proceedings, 2017, , .	0.3	4
24	New crystal phase of ammonium nitrate: First-principles prediction and characterization. AIP Conference Proceedings, 2017, , .	0.3	1
25	Novel rubidium poly-nitrogen materials at high pressure. Journal of Chemical Physics, 2017, 147, 234701.	1.2	46
26	Layer-dependent properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">SnS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">SnSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>two-dimensional materials. Physical Review B, 2016, 94, .	1.1	267
27	Sodium pentazolate: A nitrogen rich high energy density material. Chemical Physics Letters, 2016, 643, 21-26.	1.2	115
28	New phase of ammonium nitrate: A monoclinic distortion of AN-IV. Journal of Chemical Physics, 2015, 143, 234705.	1.2	6
29	Inhomogeneous Charge Distribution in Semiconductor Nanoparticles. Journal of Physical Chemistry C, 2015, 119, 16286-16292.	1.5	29
30	Surface nanodeformations caused by ultrashort laser pulse. Engineering Failure Analysis, 2015, 47, 328-337.	1.8	26
31	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
32	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
33	Density functional theory investigation of sodium azide at high pressure. Journal of Physics: Conference Series, 2014, 500, 162005.	0.3	4
34	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
35	Elastic-plastic collapse of super-elastic shock waves in face-centered-cubic solids. Journal of Physics: Conference Series, 2014, 500, 172007.	0.3	11
36	Ammonium azide under hydrostatic compression. Journal of Physics: Conference Series, 2014, 500, 162006.	0.3	3

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37	Ammonium Azide under High Pressure: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry A, 2014, 118, 8695-8700.	1.1	19
38	Effect of Temperature and Nanoparticle Size on Sensor Properties of Nanostructured Tin Dioxide Films. Journal of Physical Chemistry C, 2014, 118, 11440-11444.	1.5	35
39	From laminar to turbulent detonations in energetic materials from molecular dynamics simulations. Journal of Physics: Conference Series, 2014, 500, 172005.	0.3	0
40	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
41	Ultrafast lasers and solids in highly excited states: results of hydrodynamics and molecular dynamics simulations. Journal of Physics: Conference Series, 2014, 510, 012041.	0.3	23
42	Nano-scale spinning detonation in a condensed phase energetic material. Journal of Physics: Conference Series, 2014, 500, 172006.	0.3	0
43	Screened environment-dependent reactive empirical bond-order potential for atomistic simulations of carbon materials. Physical Review B, 2013, 88, .	1.1	34
44	Electronâ€Ion Relaxation, Phase Transitions, and Surface Nanoâ€Structuring Produced by Ultrashort Laser Pulses in Metals. Contributions To Plasma Physics, 2013, 53, 796-810.	0.5	36
45	Ultrashort shock waves in nickel induced by femtosecond laser pulses. Physical Review B, 2013, 87, .	1.1	76
46	Theory of Sensing Response of Nanostructured Tin-Dioxide Thin Films to Reducing Hydrogen Gas. Journal of Physical Chemistry C, 2013, 117, 11562-11568.	1.5	27
47	Ultrashort laser-matter interaction at moderate intensities: two-temperature relaxation, foaming of stretched melt, and freezing of evolving nanostructures. Proceedings of SPIE, 2013, , .	0.8	5
48	Shock-induced phase transition in diamond. , 2012, , .		4
49	Effect of reactive chemistry on mechanisms of condensed phase detonation. , 2012, , .		0
50	Evolution of metastable elastic shockwaves in nickel. , 2012, , .		5
51	First-principles thermodynamics of energetic materials. , 2012, , .		2
52	A new nickel EAM potential for atomistic simulations of ablation, spallation, and shockwave phenomena. AIP Conference Proceedings, 2012, , .	0.3	6
53	Shock-induced phase transitions in metals: Recrystallization of supercooled melt and melting of overheated solids. , 2012, , .		4
54	Evolution of Shock-Induced Orientation-Dependent Metastable States in Crystalline Aluminum. Physical Review Letters, 2012, 109, 125505.	2.9	57

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55	Strength of metals in liquid and solid states at extremely high tension produced by femtosecond laser heating. AIP Conference Proceedings, 2012, , .	0.3	14
56	Shock compression of diamond: Molecular dynamics simulations using different interatomic potentials. , 2012, , .		8
57	Single two-zone elastic-plastic shock waves in solids. , 2012, , .		6
58	Two-temperature thermodynamic and kinetic properties of transition metals irradiated by femtosecond lasers. , 2012, , .		34
59	Vibrational excitation of a molecule by a resonance current. Journal of Experimental and Theoretical Physics, 2012, 115, 759-768.	0.2	4
60	MD simulations of laser-induced ultrashort shock waves in nickel. , 2012, , .		5
61	Ultrashort elastic and plastic shockwaves in aluminum. , 2012, , .		8
62	Super-elastic response of metals to laser-induced shock waves. , 2012, , .		5
63	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
64	Atomic and electronic structure of simple metal/graphene and complex metal/graphene/metal interfaces. Physical Review B, 2012, 85, .	1.1	72
65	Formation of nanocavities in the surface layer of an aluminum target irradiated by a femtosecond laser pulse. JETP Letters, 2012, 95, 176-181.	0.4	102
66	Graphene growth and stability at nickel surfaces. New Journal of Physics, 2011, 13, 025001.	1.2	107
67	Graphene Growth on Ni(111) by Transformation of a Surface Carbide. Nano Letters, 2011, 11, 518-522.	4.5	182
68	Two-Zone Elastic-Plastic Single Shock Waves in Solids. Physical Review Letters, 2011, 107, 135502.	2.9	90
69	Molecular Dynamics Simulations of Femtosecond Laser Ablation and Spallation of Gold. , 2010, , .		5
70	An extended defect in graphene as a metallic wire. Nature Nanotechnology, 2010, 5, 326-329.	15.6	909
71	Hydrostatic and uniaxial compression studies of 1,3,5-triamino- 2,4,6-trinitrobenzene using density functional theory with van der Waals correction. Journal of Applied Physics, 2010, 107, .	1.1	39
72	Equations of state for energetic materials from density functional theory with van der Waals, thermal, and zero-point energy corrections. Applied Physics Letters, 2010, 97, .	1.5	67

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73	Prediction of Isothermal Equation of State of an Explosive Nitrate Ester by van der Waals Density Functional Theory. Journal of Physical Chemistry Letters, 2010, 1, 346-348.	2.1	5
74	Electron-plasmon interactions in resonant molecular tunnel junctions. Physical Review B, 2010, 81, .	1.1	2
75	Ablation and spallation of gold films irradiated by ultrashort laser pulses. Physical Review B, 2010, 82, .	1.1	122
76	Rectification and stability of a single molecular diode with controlled orientation. Nature Chemistry, 2009, 1, 635-641.	6.6	517
77	Density Functional Theory Calculations of Solid Nitromethane under Hydrostatic and Uniaxial Compressions with Empirical van der Waals Correction. Journal of Physical Chemistry A, 2009, 113, 3610-3614.	1.1	38
78	Reactive Molecular Dynamics of Hypervelocity Collisions of PETN Molecules. Journal of Physical Chemistry A, 2009, 113, 12094-12104.	1.1	26
79	Computational Nanomechanics of Graphene Membranes. Materials Research Society Symposia Proceedings, 2009, 1185, 55.	0.1	0
80	A mechanism for crystal twinning in the growth of diamond by chemical vapour deposition. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2008, 366, 295-311.	1.6	90
81	First-principles investigation of anisotropic constitutive relationships in pentaerythritol tetranitrate. Physical Review B, 2008, 77, .	1.1	46
82	Shear stresses in shock-compressed diamond from density functional theory. Physical Review B, 2008, 78, .	1.1	6
83	First-principles anisotropic constitutive relationships in Î²-cyclotetramethylene tetranitramine (Î²-HMX). Journal of Applied Physics, 2008, 104, 053506.	1.1	36
84	Density functional theory calculations of anisotropic constitutive relationships in alpha-cyclotrimethylenetrinitramine. Journal of Applied Physics, 2008, 104, .	1.1	17
85	Interface effects in spin-dependent tunneling. Progress in Materials Science, 2007, 52, 401-420.	16.0	92
86	Bound states of tunneling electrons in molecular chains. Physical Review B, 2006, 74, .	1.1	7
87	Rectification Mechanism in Diblock Oligomer Molecular Diodes. Physical Review Letters, 2006, 96, 096803.	2.9	90
88	Tunneling and resonant conductance in one-dimensional molecular structures. Chemical Physics, 2005, 319, 368-379.	0.9	18
89	Positive spin polarization inCoâ^•Al2O3â^•Cotunnel junctions driven by oxygen adsorption. Physical Review B, 2005, 71, .	1.1	32
90	Metal-Oxide Interfaces in Magnetic Tunnel Junctions. Journal of Materials Science, 2004, 12, 105-116.	1.2	13

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91	Spin-dependent tunneling from clean and oxidized Co surfaces. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 1954-1955.	1.0	2
92	Interatomic bond-order potentials and structural prediction. Progress in Materials Science, 2004, 49, 285-312.	16.0	18
93	Effect of interface bonding on spin-dependent tunneling from the oxidized Co surface. Physical Review B, 2004, 69, .	1.1	74
94	Atomic, electronic, and magnetic properties of magnetic tunnel junctions. Journal of Applied Physics, 2003, 93, 6429-6431.	1.1	9
95	Spin injection into amorphous semiconductors. Physical Review B, 2002, 66, .	1.1	14
96	Analytic bond-order potential for open and close-packed phases. Physical Review B, 2002, 65, .	1.1	64
97	Bond-order potentials: bridging the electronic to atomistic modelling hierarchies. Computational Materials Science, 2002, 23, 33-37.	1.4	35
98	Atomic and electronic structure ofCo/SrTiO3/Comagnetic tunnel junctions. Physical Review B, 2001, 65, .	1.1	96
99	Bonding and Cohesive Properties of Cobalt/Alumina Magnetic Tunnel Junctions. Materials Research Society Symposia Proceedings, 2000, 616, 171.	0.1	0
100	Oxygen-induced positive spin polarization from Fe into the vacuum barrier. Journal of Applied Physics, 2000, 87, 5230-5232.	1.1	49
101	Diamond CVD Growth Mechanisms and Reaction Rates From First-Principles. Materials Research Society Symposia Proceedings, 2000, 616, 123.	0.1	1
102	Bounded Analytic Bond-Order Potentials forÏƒandÏ€Bonds. Physical Review Letters, 2000, 84, 4124-4127.	2.9	102
103	Structural and electronic properties ofCo/Al2O3/Comagnetic tunnel junction from first principles. Physical Review B, 2000, 62, 3952-3959.	1.1	138
104	Theoretical study of chemical reactions on CVD diamond surfaces. Diamond and Related Materials, 2000, 9, 241-245.	1.8	19
105	Etching effects during the chemical vapor deposition of (100) diamond. Journal of Chemical Physics, 1999, 111, 4291-4299.	1.2	72
106	Analytic bond-order potentials beyond Tersoff-Brenner. II. Application to the hydrocarbons. Physical Review B, 1999, 59, 8500-8507.	1.1	72
107	Analytic bond-order potentials beyond Tersoff-Brenner. I. Theory. Physical Review B, 1999, 59, 8487-8499.	1.1	183
108	Surface Chemistry of CVD Diamond: Linking the Nanoscale and Mesoscale Modelling Hierarchies. Materials Research Society Symposia Proceedings, 1998, 538, 275.	0.1	0

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109	Tunneling dynamics of electrons and effective tunneling potential. Surface Science, 1996, 363, 360-367.	0.8	2
110	Direct and inverse problems in the theory of scanning tunneling microscopy. Surface Science, 1995, 331-333, 1191-1196.	0.8	4
111	An extended defect in graphene as a metallic wire. , 0, .		1