Artem Oganov

List of Publications by Year
in descending order

304	27,347	7561 77	6465 157
papers	citations	h-index	g-index

333	333	333	14502
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. Science, 2015, 350, 1513-1516.	6.0	2,047
2	Crystal structure prediction usingab initioevolutionary techniques: Principles and applications. Journal of Chemical Physics, 2006, 124, 244704.	1.2	2,044
3	New developments in evolutionary structure prediction algorithm USPEX. Computer Physics Communications, 2013, 184, 1172-1182.	3.0	1,031
4	USPEXâ€"Evolutionary crystal structure prediction. Computer Physics Communications, 2006, 175, 713-720.	3.0	946
5	How Evolutionary Crystal Structure Prediction Worksâ€"and Why. Accounts of Chemical Research, 2011, 44, 227-237.	7.6	940
6	Theoretical and experimental evidence for a post-perovskite phase of MgSiO3 in Earth's Dâ€³ layer. Nature, 2004, 430, 445-448.	13.7	914
7	Ionic high-pressure form of elemental boron. Nature, 2009, 457, 863-867.	13.7	803
8	Transparent dense sodium. Nature, 2009, 458, 182-185.	13.7	710
9	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. Physical Review Letters, 2014, 112, .	2.9	497
10	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5â€“6â€“7 Carbon Rings with Distorted Dirac Cones. Nano Letters, 2015, 15, 6182-6186.	4.5	482
11	Superhard Monoclinic Polymorph of Carbon. Physical Review Letters, 2009, 102, 175506.	2.9	480
12	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
13	Structure prediction drives materials discovery. Nature Reviews Materials, 2019, 4, 331-348.	23.3	402
14	Unexpected Stable Stoichiometries of Sodium Chlorides. Science, 2013, 342, 1502-1505.	6.0	394
15	High-pressure phases of CaCO3: Crystal structure prediction and experiment. Earth and Planetary Science Letters, 2006, 241, 95-103.	1.8	318
16	A stable compound of helium and sodium at high pressure. Nature Chemistry, 2017, 9, 440-445.	6.6	276
17	Rational design of all organic polymer dielectrics. Nature Communications, 2014, 5, 4845.	5.8	259
18	A little bit of lithium does a lot for hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 17640-17643.	3.3	245

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19	Evolutionary search for superhard materials: Methodology and applications to forms of carbon and TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2011, 84, .	1.1	229
20	Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning. Physical Review B, 2019, 99, .	1.1	229
21	Novel High Pressure Structures of Polymeric Nitrogen. Physical Review Letters, 2009, 102, 065501.	2.9	226
22	Superconducting High Pressure Phase of Germane. Physical Review Letters, 2008, 101, 107002.	2.9	224
23	Anisotropy of Earth's Dâ€³ layer and stacking faults in the MgSiO3 post-perovskite phase. Nature, 2005, 438, 1142-1144.	13.7	219
24	Ruby, metals, andMgOas alternative pressure scales: A semiempirical description of shock-wave, ultrasonic, x-ray, and thermochemical data at high temperatures and pressures. Physical Review B, 2007, 75, .	1.1	211
25	Novel high-pressure structures of MgCO3, CaCO3 and CO2 and their role in Earth's lower mantle. Earth and Planetary Science Letters, 2008, 273, 38-47.	1.8	211
26	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. Nature Materials, 2006, 5, 623-626.	13.3	198
27	Anomalous Highâ€Temperature Superconductivity in YH₆. Advanced Materials, 2021, 33, e2006832.	11.1	196
28	The elastic constants of MgSiO3 perovskite at pressures and temperatures of the Earth's mantle. Nature, 2001, 411, 934-937.	13.7	190
29	Superconductivity at 161â€K in thorium hydride ThH10: Synthesis and properties. Materials Today, 2020, 33, 36-44.	8.3	187
30	Evolutionary Crystal Structure Prediction as a Method for the Discovery of Minerals and Materials. Reviews in Mineralogy and Geochemistry, 2010, 71, 271-298.	2.2	182
31	How to quantify energy landscapes of solids. Journal of Chemical Physics, 2009, 130, 104504.	1.2	172
32	High-pressure crystal structures and superconductivity of Stannane (SnH ₄). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1317-1320.	3.3	168
33	How to predict very large and complex crystal structures. Computer Physics Communications, 2010, 181, 1623-1632.	3.0	162
34	All-electron and pseudopotential study of MgO: Equation of state, anharmonicity, and stability. Physical Review B, 2003, 67, .	1.1	151
35	Structural stability of silica at high pressures and temperatures. Physical Review B, 2005, 71, .	1.1	146
36	Novel Structures and Superconductivity of Silane under Pressure. Physical Review Letters, 2009, 102, 087005.	2.9	146

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37	Constrained evolutionary algorithm for structure prediction of molecular crystals: methodology and applications. Acta Crystallographica Section B: Structural Science, 2012, 68, 215-226.	1.8	146
38	Ab initio lattice dynamics and structural stability of MgO. Journal of Chemical Physics, 2003, 118, 10174-10182.	1.2	144
39	Thermochemical electronegativities of the elements. Nature Communications, 2021, 12, 2087.	5.8	141
40	In situ observations of phase transition between perovskite and CaIrO-type phase in MgSiO and pyrolitic mantle composition. Earth and Planetary Science Letters, 2005, 236, 914-932.	1.8	138
41	Simple and accurate model of fracture toughness of solids. Journal of Applied Physics, 2019, 125, .	1.1	136
42	Ab initio elasticity and thermal equation of state of MgSiO3 perovskite. Earth and Planetary Science Letters, 2001, 184, 555-560.	1.8	133
43	A model of hardness and fracture toughness of solids. Journal of Applied Physics, 2019, 126, .	1.1	133
44	High-pressure structures of lithium, potassium, and rubidium predicted by anab initioevolutionary algorithm. Physical Review B, 2008, 78, .	1.1	132
45	Graphane sheets and crystals under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6833-6837.	3.3	126
46	Phase stability, chemical bonding and mechanical properties of titanium nitrides: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 11763-11769.	1.3	126
47	Boron: a hunt for superhard polymorphs. Journal of Superhard Materials, 2009, 31, 285-291.	0.5	125
48	On the hardness of a new boron phase, orthorhombic Î³-B28. Journal of Superhard Materials, 2008, 30, 428-429.	0.5	121
49	Superconductivity at 253â€¯K in lanthanumâ€“yttrium ternary hydrides. Materials Today, 2021, 48, 18-28.	8.3	119
50	Denser than diamond:Ab initiosearch for superdense carbon allotropes. Physical Review B, 2011, 83, .	1.1	118
51	Stability of xenon oxides at high pressures. Nature Chemistry, 2013, 5, 61-65.	6.6	118
52	Synthesis of clathrate cerium superhydride CeH9 at 80-100 GPa with atomic hydrogen sublattice. Nature Communications, 2019, 10, 4453.	5.8	117
53	Valence state and spin transitions of iron in Earth's mantle silicates. Earth and Planetary Science Letters, 2006, 249, 436-443.	1.8	116
54	Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure. Physical Review B, 2008, 77, .	1.1	112

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55	High-Temperature Superconducting Phases in Cerium Superhydride with a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>T</mml:mi></mml:mrow><mml:mrow><mml:mi>c</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> up to 115ÂK below a Pressure of 1ÂMegabar. Physical Review Letters, 2021, 127, 117001.	2.9	112
56	The high-pressure phase of alumina and implications for Earth's D'' layer. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10828-10831.	3.3	110
57	Comparative study of quasiharmonic lattice dynamics, molecular dynamics and Debye model applied to MgSiO3 perovskite. Physics of the Earth and Planetary Interiors, 2000, 122, 277-288.	0.7	108
58	Structure of the metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î¶</mml:mi></mml:math>-phase of oxygen and isosymmetric nature of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Îµ</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>Î¶</mml:mi></mml:mrow></mml:math>pha transition:Ab initiosimulations. Physical Review B, 2007, 76, .	1.1	107
59	On Distribution of Superconductivity in Metal Hydrides. Current Opinion in Solid State and Materials Science, 2020, 24, 100808.	5.6	104
60	Novel stable compounds in the Mgâ€“O system under high pressure. Physical Chemistry Chemical Physics, 2013, 15, 7696.	1.3	102
61	Dissociation of methane under high pressure. Journal of Chemical Physics, 2010, 133, 144508.	1.2	101
62	Two-dimensional magnetic boron. Physical Review B, 2016, 93, .	1.1	101
63	Structure, Bonding, and Mineralogy of Carbon at Extreme Conditions. Reviews in Mineralogy and Geochemistry, 2013, 75, 47-77.	2.2	100
64	Actinium Hydrides AcH₁₀, AcH₁₂, and AcH₁₆ as High-Temperature Conventional Superconductors. Journal of Physical Chemistry Letters, 2018, 9, 1920-1926.	2.1	100
65	Evolutionary method for predicting surface reconstructions with variable stoichiometry. Physical Review B, 2013, 87, .	1.1	99
66	Superconducting praseodymium superhydrides. Science Advances, 2020, 6, eaax6849.	4.7	99
67	Hydrogen sulfide at high pressure: Change in stoichiometry. Physical Review B, 2016, 93, .	1.1	97
68	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	3.7	97
69	High-Temperature Superconductivity in a Thâ€“H System under Pressure Conditions. ACS Applied Materials & Interfaces, 2018, 10, 43809-43816.	4.0	95
70	Evolutionary crystal structure prediction as a tool in materials design. Journal of Physics Condensed Matter, 2008, 20, 064210.	0.7	89
71	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. Chemistry of Materials, 2020, 32, 6947-6957.	3.2	89
72	Exotic behavior and crystal structures of calcium under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 7646-7651.	3.3	86

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73	Understanding the nature of â€œsuperhard graphiteâ€•. Scientific Reports, 2012, 2, 471.	1.6	86
74	Pressure-stabilized hafnium nitrides and their properties. Physical Review B, 2017, 95, .	1.1	85
75	The performance of minima hopping and evolutionary algorithms for cluster structure prediction. Journal of Chemical Physics, 2009, 130, 144108.	1.2	83
76	Systematic search for low-enthalpy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:mrow allotropes using evolutionary metadynamics. Physical Review B, 2012, 85, .	1.1	82
77	Uranium polyhydrides at moderate pressures: Prediction, synthesis, and expected superconductivity. Science Advances, 2018, 4, eaat9776.	4.7	82
78	Compressed carbon nanotubes: A family of new multifunctional carbon allotropes. Scientific Reports, 2013, 3, 1331.	1.6	80
79	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
80	The phase diagram and hardness of carbon nitrides. Scientific Reports, 2015, 5, 9870.	1.6	78
81	Stability and compressibility of the high-pressure phases of Al2O3 up to 200 GPa: Implications for the electrical conductivity of the base of the lower mantle. Earth and Planetary Science Letters, 2006, 246, 326-335.	1.8	77
82	Pressure-Induced Stabilization and Insulator-Superconductor Transition of BH. Physical Review Letters, 2013, 110, 165504.	2.9	76
83	Emergence of Novel Polynitrogen Molecule-like Species, Covalent Chains, and Layers in Magnesiumâ€“Nitrogen Mg_xN_y Phases under High Pressure. Journal of Physical Chemistry C, 2017, 121, 11037-11046.	1.5	76
84	Crystal fingerprint space â€“ a novel paradigm for studying crystal-structure sets. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 507-517.	0.3	74
85	Resorcinol Crystallization from the Melt: A New Ambient Phase and New â€œRiddlesâ€•. Journal of the American Chemical Society, 2016, 138, 4881-4889.	6.6	74
86	Intrinsic anharmonicity in equations of state and thermodynamics of solids. Journal of Physics Condensed Matter, 2004, 16, 1351-1360.	0.7	72
87	Feâ€“C and Feâ€“H systems at pressures of the Earth's inner core. Physics-Uspekhi, 2012, 55, 489-497.	0.8	71
88	Variable cell nudged elastic band method for studying solidâ€“solid structural phase transitions. Computer Physics Communications, 2013, 184, 2111-2118.	3.0	71
89	Towards the theory of hardness of materials. Journal of Superhard Materials, 2010, 32, 143-147.	0.5	70
90	Investigation of exotic stable calcium carbides using theory and experiment. Nature Communications, 2015, 6, 6974.	5.8	70

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91	Topology-based crystal structure generator. Computer Physics Communications, 2019, 236, 1-7.	3.0	67
92	Novel lithium-nitrogen compounds at ambient and high pressures. Scientific Reports, 2015, 5, 14204.	1.6	66
93	Synthesis of molecular metallic barium superhydride: pseudocubic BaH12. Nature Communications, 2021, 12, 273.	5.8	66
94	Ab initio study of the high-pressure behavior of CaSiO3 perovskite. Physics and Chemistry of Minerals, 2005, 32, 146-153.	0.3	65
95	Novel High Pressure Structures and Superconductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ca</mml:mi><mml:msub><mml:mi>Li</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2010, 104, 177005.	2.9	64
96	Evolutionary metadynamics: a novel method to predict crystal structures. CrystEngComm, 2012, 14, 3596.	1.3	62
97	Computational Search for Novel Hard Chromium-Based Materials. Journal of Physical Chemistry Letters, 2017, 8, 755-764.	2.1	62
98	Superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaH</mml:mi><mml:mn>10</mml:mn></mml:msub></mml and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaH</mml:mi><mml:mn>16</mml:mn></mml:msub></mml polyhydrides. Physical Review B, 2020, 101, .	1.1	62
99	New Reconstructions of the (110) Surface of Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> by an Evolutionary Method. Physical Review Letters, 2014, 113, 266101.	2.9	61
100	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. Journal of Physical Chemistry Letters, 2018, 9, 3470-3477.	2.1	61
101	Superconductivity of lithium-doped hydrogen under high pressure. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 104-111.	0.2	59
102	High-Pressure Synthesis of Magnetic Neodymium Polyhydrides. Journal of the American Chemical Society, 2020, 142, 2803-2811.	6.6	59
103	Ultra-incompressible phases of tungsten dinitride predicted from first principles. Physical Review B, 2009, 79, .	1.1	58
104	Grain boundary phases in bcc metals. Nanoscale, 2018, 10, 8253-8268.	2.8	55
105	Crystal structure prediction: reflections on present status and challenges. Faraday Discussions, 2018, 211, 643-660.	1.6	55
106	Rhombohedral superhard structure of BC2N. Journal of Applied Physics, 2009, 105, 053514.	1.1	54
107	Raman spectroscopy and x-ray diffraction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="italic">sp</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msup><mml:mspace width="4pt" /><mml:mi>CaC</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> at lower mantle pressures. Physical Review B, 2017, 96, .	1.1	54
108	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	3.7	54

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109	Effects of carbon vacancies on the structures, mechanical properties, and chemical bonding of zirconium carbides: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 12299-12306.	1.3	53
110	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B, 2013, 88, .	1.1	51
111	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. Earth and Planetary Science Letters, 2008, 272, 481-487.	1.8	50
112	Phase transitions and equation of state of forsterite to 90 GPa from single-crystal X-ray diffraction and molecular modeling. American Mineralogist, 2014, 99, 35-43.	0.9	50
113	Energy-free machine learning force field for aluminum. Scientific Reports, 2017, 7, 8512.	1.6	50
114	Variable-composition structural optimization and experimental verification of MnB₃and MnB₄. Physical Chemistry Chemical Physics, 2014, 16, 15866-15873.	1.3	49
115	Machine learning scheme for fast extraction of chemically interpretable interatomic potentials. AIP Advances, 2016, 6, .	0.6	49
116	High-pressure phases in the Al 2 SiO 5 system and the problem of aluminous phase in the Earth's lower mantle: ab initio calculations. Physics and Chemistry of Minerals, 2000, 27, 430-439.	0.3	48
117	Iron Superhydrides FeH₅ and FeH₆: Stability, Electronic Properties, and Superconductivity. Journal of Physical Chemistry C, 2018, 122, 4731-4736.	1.5	48
118	Application of machine learning methods for predicting new superhard materials. Journal of Applied Physics, 2020, 128, .	1.1	48
119	Ab initiomolecular dynamics study ofCaSiO3perovskite atPâ^Tconditions of Earthâ€™s lower mantle. Physical Review B, 2006, 73, .	1.1	47
120	Superconducting high-pressure phase of platinum hydride from first principles. Physical Review B, 2011, 84, .	1.1	47
121	First-Principles Determination of the Structure of Magnesium Borohydride. Physical Review Letters, 2012, 109, 245503.	2.9	47
122	Imaging Domain Reversal in an Ultrathin Van der Waals Ferromagnet. Advanced Materials, 2020, 32, e2003314.	11.1	47
123	Computational discovery of hard and superhard materials. Journal of Applied Physics, 2019, 126, .	1.1	46
124	From four- to six-coordinated silica: Transformation pathways from metadynamics. Physical Review B, 2007, 76, .	1.1	45
125	First-principles study of Zrâ€“N crystalline phases: phase stability, electronic and mechanical properties. RSC Advances, 2017, 7, 4697-4703.	1.7	45
126	Evolutionary search for new high-kdielectric materials: methodology and applications to hafnia-based oxides. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 76-84.	0.2	44

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127	Pressure-induced novel compounds in the Hf-O system from first-principles calculations. Physical Review B, 2015, 92, .	1.1	44
128	Novel superhard Bâ€“Câ€“O phases predicted from first principles. Physical Chemistry Chemical Physics, 2016, 18, 1859-1863.	1.3	44
129	New two-dimensional phase of tin chalcogenides: Candidates for high-performance thermoelectric materials. Physical Review Materials, 2019, 3, .	0.9	44
130	Absence of superconductivity in the high-pressure polymorph of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2009, 79, .	1.1	43
131	Prediction of novel stable compounds in the Mg-Si-O system under exoplanet pressures. Scientific Reports, 2016, 5, 18347.	1.6	43
132	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. Nano Letters, 2016, 16, 4236-4242.	4.5	42
133	Predicting polymeric crystal structures by evolutionary algorithms. Journal of Chemical Physics, 2014, 141, 154102.	1.2	41
134	Novel Hydrogen Hydrate Structures under Pressure. Scientific Reports, 2014, 4, 5606.	1.6	41
135	Synthesis of Ultra-incompressible sp³-Hybridized Carbon Nitride with 1:1 Stoichiometry. Chemistry of Materials, 2016, 28, 6925-6933.	3.2	41
136	Synthesis of Î²-Mg2C3: A Monoclinic High-Pressure Polymorph of Magnesium Sesquicarbide. Inorganic Chemistry, 2014, 53, 7020-7027.	1.9	40
137	Exploring the Real Ground-State Structures of Molybdenum Dinitride. Journal of Physical Chemistry C, 2016, 120, 11060-11067.	1.5	39
138	Superconductivity of novel tin hydrides (SnnHm) under pressure. Scientific Reports, 2016, 6, 22873.	1.6	39
139	The high-pressure phase of boron, Î³-B28: Disputes and conclusions of 5 years after discovery. Journal of Superhard Materials, 2011, 33, 363-379.	0.5	38
140	Backbone NxH compounds at high pressures. Journal of Chemical Physics, 2015, 142, 214308.	1.2	38
141	Exotic Two-Dimensional Structure: The First Case of Hexagonal NaCl. Journal of Physical Chemistry Letters, 2020, 11, 3821-3827.	2.1	38
142	Ab initio theory of planetary materials. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	37
143	Pressure-driven formation and stabilization of superconductive chromium hydrides. Scientific Reports, 2015, 5, 17764.	1.6	37
144	Explaining stability of transition metal carbides â€“ and why TcC does not exist. RSC Advances, 2016, 6, 16197-16202.	1.7	37

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145	Atomic-scale observation and analysis of chemical ordering in M3B2 and M5B3 borides. Acta Materialia, 2018, 149, 274-284.	3.8	37
146	Ionic high-pressure form of elemental boron. Nature, 2009, 460, 292-292.	13.7	34
147	Method for Simultaneous Prediction of Atomic Structure and Stability of Nanoclusters in a Wide Area of Compositions. Journal of Physical Chemistry Letters, 2019, 10, 102-106.	2.1	34
148	Crystal structure prediction and simulations of structural transformations: metadynamics and evolutionary algorithms. Phase Transitions, 2007, 80, 277-298.	0.6	33
149	Boron phosphide under pressure: In situ study by Raman scattering and X-ray diffraction. Journal of Applied Physics, 2014, 116, .	1.1	33
150	Generalized evolutionary metadynamics for sampling the energy landscapes and its applications. Physical Review B, 2015, 92, .	1.1	33
151	Novel Strongly Correlated Europium Superhydrides. Journal of Physical Chemistry Letters, 2021, 12, 32-40.	2.1	33
152	Mechanisms of Al3+ incorporation in MgSiO3 post-perovskite at high pressures. Earth and Planetary Science Letters, 2006, 248, 69-76.	1.8	32
153	Lattice Dynamics of MgO at High Pressure: Theory and Experiment. Physical Review Letters, 2006, 96, 035507.	2.9	32
154	dâ€AO spherical aromaticity in Ce₆O₈. Journal of Computational Chemistry, 2016, 37, 103-109.	1.5	32
155	Novel high-pressure calcium carbonates. Physical Review B, 2018, 98, .	1.1	32
156	Prediction of a new ground state of superhard compound B6O at ambient conditions. Scientific Reports, 2016, 6, 31288.	1.6	31
157	Fermi surface nesting and phonon instabilities in simple cubic calcium. High Pressure Research, 2008, 28, 443-448.	0.4	30
158	Stable magnesium peroxide at high pressure. Scientific Reports, 2015, 5, 13582.	1.6	30
159	Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO2. Scientific Reports, 2017, 7, 10357.	1.6	30
160	Unexpected stable phases of tungsten borides. Physical Chemistry Chemical Physics, 2018, 20, 24665-24670.	1.3	30
161	Structure, Stability, and Mechanical Properties of Boron-Rich Moâ€“B Phases: A Computational Study. Journal of Physical Chemistry Letters, 2020, 11, 2393-2401.	2.1	30
162	A Revisited Mechanism of the Graphite-to-Diamond Transition at High Temperature. Matter, 2020, 3, 864-878.	5.0	30

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163	Theoretical investigation of metastable Al2SiO5polymorphs. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 548-557.	0.3	29
164	Unexpected Reconstruction of theÎ±-Boron (111) Surface. Physical Review Letters, 2014, 113, 176101.	2.9	29
165	Novel compounds in the Zrâ€“O system, their crystal structures and mechanical properties. Physical Chemistry Chemical Physics, 2015, 17, 17301-17310.	1.3	29
166	Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations. Scientific Reports, 2014, 4, 5889.	1.6	29
167	Superconductivity and equation of state of lanthanum at megabar pressures. Physical Review B, 2020, 102, .	1.1	29
168	Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied usingab initiocalculations. Physical Review B, 2007, 75, .	1.1	28
169	Phase diagram of uranium fromab initiocalculations and machine learning. Physical Review B, 2019, 100, .	1.1	28
170	Prediction of Novel van der Waals Boron Oxides with Superior Deepâ€Ultraviolet Nonlinear Optical Performance. Angewandte Chemie - International Edition, 2021, 60, 10791-10797.	7.2	28
171	Superconducting high-pressure phase of cesium iodide. Physical Review B, 2009, 79, .	1.1	27
172	Prediction of a stable post-post-perovskite structure from first principles. Physical Review B, 2015, 91, .	1.1	27
173	Diverse Chemistry of Stable Hydronitrogens, and Implications for Planetary and Materials Sciences. Scientific Reports, 2016, 6, 25947.	1.6	27
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