Artem Oganov

List of Publications by Citations

310 papers	20,817 citations	66 h-index	138 g-index
333 ext. papers	24,143 ext. citations	6.8 avg, IF	7.29 L-index

#	Paper	IF	Citations
310	Crystal structure prediction using ab initio evolutionary techniques: principles and applications. *Journal of Chemical Physics*, **2006**, 124, 244704	3.9	1658
309	Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. *Science*, **2015**, 350, 1513-6	33.3	1479
308	Theoretical and experimental evidence for a post-perovskite phase of MgSiO3 in Earth's D" layer. *Nature*, **2004**, 430, 445-8	50.4	809
307	New developments in evolutionary structure prediction algorithm USPEX. *Computer Physics Communications*, **2013**, 184, 1172-1182	4.2	784
306	USPEXEvolutionary crystal structure prediction. *Computer Physics Communications*, **2006**, 175, 713-720	4.2	748
305	How evolutionary crystal structure prediction works--and why. *Accounts of Chemical Research*, **2011**, 44, 227-37	24.3	723
304	Ionic high-pressure form of elemental boron. *Nature*, **2009**, 457, 863-7	50.4	680
303	Transparent dense sodium. *Nature*, **2009**, 458, 182-5	50.4	584
302	Superhard monoclinic polymorph of carbon. *Physical Review Letters*, **2009**, 102, 175506	7.4	434
301	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. *Physical Review Letters*, **2014**, 112,	7.4	397
300	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
299	Unexpected stable stoichiometries of sodium chlorides. *Science*, **2013**, 342, 1502-5	33.3	329
298	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5-6-7 Carbon Rings with Distorted Dirac Cones. *Nano Letters*, **2015**, 15, 6182-6	11.5	325
297	High-pressure phases of CaCO3: Crystal structure prediction and experiment. *Earth and Planetary Science Letters*, **2006**, 241, 95-103	5.3	291
296	Structure prediction drives materials discovery. *Nature Reviews Materials*, **2019**, 4, 331-348	73.3	242
295	Rational design of all organic polymer dielectrics. *Nature Communications*, **2014**, 5, 4845	17.4	206
294	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, 17640-3	11.5	205

293	Superconducting high pressure phase of germane. *Physical Review Letters*, **2008**, 101, 107002	7.4	204
292	Anisotropy of Earth's D'' layer and stacking faults in the MgSiO3 post-perovskite phase. *Nature*, **2005**, 438, 1142-4	50.4	203
291	A stable compound of helium and sodium at high pressure. *Nature Chemistry*, **2017**, 9, 440-445	17.6	199
290	Evolutionary search for superhard materials: Methodology and applications to forms of carbon and TiO2. *Physical Review B*, **2011**, 84,	3.3	187
289	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	5.3	187
288	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. *Nature Materials*, **2006**, 5, 623-6	27	183
287	Novel high pressure structures of polymeric nitrogen. *Physical Review Letters*, **2009**, 102, 065501	7.4	181
286	Ruby, metals, and MgO as 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,	3.3	173
285	The elastic constants of MgSiO3 perovskite at pressures and temperatures of the Earth's mantle. *Nature*, **2001**, 411, 934-7	50.4	172
284	How to quantify energy landscapes of solids. *Journal of Chemical Physics*, **2009**, 130, 104504	3.9	157
283	High-pressure crystal structures and superconductivity of Stannane (SnH4). *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 1317-20	11.5	153
282	Evolutionary Crystal Structure Prediction as a Method for the Discovery of Minerals and Materials. *Reviews in Mineralogy and Geochemistry*, **2010**, 71, 271-298	7.1	143
281	How to predict very large and complex crystal structures. *Computer Physics Communications*, **2010**, 181, 1623-1632	4.2	142
280	Novel structures and superconductivity of silane under pressure. *Physical Review Letters*, **2009**, 102, 087005	7.4	137
279	All-electron and pseudopotential study of MgO: Equation of state, anharmonicity, and stability. *Physical Review B*, **2003**, 67,	3.3	135
278	Ab initio lattice dynamics and structural stability of MgO. *Journal of Chemical Physics*, **2003**, 118, 10174-10182	3.9	130
277	Constrained evolutionary algorithm for structure prediction of molecular crystals: methodology and applications. *Acta Crystallographica Section B: Structural Science*, **2012**, 68, 215-26		126
276	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	5.3	126

275	Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning. *Physical Review B*, **2019**, 99,	3.3	125
274	Ab initio elasticity and thermal equation of state of MgSiO3 perovskite. *Earth and Planetary Science Letters*, **2001**, 184, 555-560	5.3	125
273	Structural stability of silica at high pressures and temperatures. *Physical Review B*, **2005**, 71,	3.3	121
272	Boron: a hunt for superhard polymorphs. *Journal of Superhard Materials*, **2009**, 31, 285-291	0.9	113
271	Valence state and spin transitions of iron in Earth's mantle silicates. *Earth and Planetary Science Letters*, **2006**, 249, 436-443	5.3	110
270	Graphane sheets and crystals under pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6833-6837	11.5	108
269	High-pressure structures of lithium, potassium, and rubidium predicted by an ab initio evolutionary algorithm. *Physical Review B*, **2008**, 78,	3.3	108
268	On the hardness of a new boron phase, orthorhombic □B28. *Journal of Superhard Materials*, **2008**, 30, 428-429	0.9	108
267	Denser than diamond: Ab initio search for superdense carbon allotropes. *Physical Review B*, **2011**, 83,	3.3	103
266	Superconductivity at 161 K in thorium hydride ThH10: Synthesis and properties. *Materials Today*, **2020**, 33, 36-44	21.8	102
265	Stability of xenon oxides at high pressures. *Nature Chemistry*, **2013**, 5, 61-5	17.6	101
264	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, 10828-31	11.5	99
263	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	2.3	97
262	Structure of the metallic □phase of oxygen and isosymmetric nature of the □phase transition: Ab initio simulations. *Physical Review B*, **2007**, 76,	3.3	96
261	Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure. *Physical Review B*, **2008**, 77,	3.3	95
260	Phase stability, chemical bonding and mechanical properties of titanium nitrides: a first-principles study. *Physical Chemistry Chemical Physics*, **2015**, 17, 11763-9	3.6	87
259	Novel stable compounds in the Mg-O system under high pressure. *Physical Chemistry Chemical Physics*, **2013**, 15, 7696-700	3.6	86
258	Dissociation of methane under high pressure. *Journal of Chemical Physics*, **2010**, 133, 144508	3.9	86

257	Evolutionary method for predicting surface reconstructions with variable stoichiometry. *Physical Review B*, **2013**, 87,	3.3	82
256	Systematic search for low-enthalpy sp3 carbon allotropes using evolutionary metadynamics. *Physical Review B*, **2012**, 85,	3.3	78
255	Hydrogen sulfide at high pressure: Change in stoichiometry. *Physical Review B*, **2016**, 93,	3.3	77
254	Understanding the nature of "superhard graphite". *Scientific Reports*, **2012**, 2, 471	4.9	77
253	Structure, Bonding, and Mineralogy of Carbon at Extreme Conditions. *Reviews in Mineralogy and Geochemistry*, **2013**, 75, 47-77	7.1	76
252	Two-dimensional magnetic boron. *Physical Review B*, **2016**, 93,	3.3	75
251	Exotic behavior and crystal structures of calcium under pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 7646-51	11.5	74
250	The performance of minima hopping and evolutionary algorithms for cluster structure prediction. *Journal of Chemical Physics*, **2009**, 130, 144108	3.9	74
249	Compressed carbon nanotubes: a family of new multifunctional carbon allotropes. *Scientific Reports* , **2013**, 3, 1331	4.9	73
248	Evolutionary crystal structure prediction as a tool in materials design. *Journal of Physics Condensed Matter*, **2008**, 20, 064210	1.8	73
247	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	5.3	71
246	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. *Chemical Science*, **2017**, 8, 4926-4940	9.4	70
245	Actinium Hydrides AcH, AcH, and AcH as High-Temperature Conventional Superconductors. *Journal of Physical Chemistry Letters*, **2018**, 9, 1920-1926	6.4	70
244	The phase diagram and hardness of carbon nitrides. *Scientific Reports*, **2015**, 5, 9870	4.9	66
243	Synthesis of clathrate cerium superhydride CeH at 80-100 GPa with atomic hydrogen sublattice. *Nature Communications*, **2019**, 10, 4453	17.4	64
242	Investigation of exotic stable calcium carbides using theory and experiment. *Nature Communications*, **2015**, 6, 6974	17.4	61
241	Pressure-induced stabilization and insulator-superconductor transition of BH. *Physical Review Letters*, **2013**, 110, 165504	7.4	61
240	Towards the theory of hardness of materials. *Journal of Superhard Materials*, **2010**, 32, 143-147	0.9	60

239	Intrinsic anharmonicity in equations of state and thermodynamics of solids. *Journal of Physics Condensed Matter*, **2004**, 16, 1351-1360	1.8	60
238	Anomalous High-Temperature Superconductivity in YH. *Advanced Materials*, **2021**, 33, e2006832	24	60
237	Variable cell nudged elastic band method for studying solid□solid structural phase transitions. *Computer Physics Communications*, **2013**, 184, 2111-2118	4.2	56
236	Crystal fingerprint space--a novel paradigm for studying crystal-structure sets. *Acta Crystallographica Section A: Foundations and Advances*, **2010**, 66, 507-17		56
235	Ab initio study of the high-pressure behavior of CaSiO3 perovskite. *Physics and Chemistry of Minerals*, **2005**, 32, 146-153	1.6	56
234	Simple and accurate model of fracture toughness of solids. *Journal of Applied Physics*, **2019**, 125, 065105	2.5	56
233	Resorcinol Crystallization from the Melt: A New Ambient Phase and New "Riddles". *Journal of the American Chemical Society*, **2016**, 138, 4881-9	16.4	55
232	Ultra-incompressible phases of tungsten dinitride predicted from first principles. *Physical Review B*, **2009**, 79,	3.3	55
231	High-Temperature Superconductivity in a Th-H System under Pressure Conditions. *ACS Applied Materials & Interfaces*, **2018**, 10, 43809-43816	9.5	55
230	Novel high pressure structures and superconductivity of CaLi2. *Physical Review Letters*, **2010**, 104, 177005	7.4	54
229	Pressure-stabilized hafnium nitrides and their properties. *Physical Review B*, **2017**, 95,	3.3	53
228	Fe□ and Fe□ systems at pressures of the Earth's inner core. *Physics-Uspekhi*, **2012**, 55, 489-497	2.8	52
227	Rhombohedral superhard structure of BC2N. *Journal of Applied Physics*, **2009**, 105, 053514	2.5	52
226	Uranium polyhydrides at moderate pressures: Prediction, synthesis, and expected superconductivity. *Science Advances*, **2018**, 4, eaat9776	14.3	52
225	A model of hardness and fracture toughness of solids. *Journal of Applied Physics*, **2019**, 126, 125109	2.5	51
224	Evolutionary metadynamics: a novel method to predict crystal structures. *CrystEngComm*, **2012**, 14, 3596	3.3	51
223	Computational Search for Novel Hard Chromium-Based Materials. *Journal of Physical Chemistry Letters*, **2017**, 8, 755-764	6.4	50
222	New reconstructions of the (110) surface of rutile TiO2 predicted by an evolutionary method. *Physical Review Letters*, **2014**, 113, 266101	7.4	50

221	Superconducting praseodymium superhydrides. *Science Advances*, **2020**, 6, eaax6849	14.3	49
220	Emergence of Novel Polynitrogen Molecule-like Species, Covalent Chains, and Layers in Magnesium Nitrogen MgxNy Phases under High Pressure. *Journal of Physical Chemistry C*, **2017**, 121, 11037-11046	3.8	48
219	Novel lithium-nitrogen compounds at ambient and high pressures. *Scientific Reports*, **2015**, 5, 14204	4.9	48
218	High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores. *Earth and Planetary Science Letters*, **2008**, 272, 481-487	5.3	46
217	High-pressure phases in the Al2SiO5 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	1.6	45
216	Variable-composition structural optimization and experimental verification of MnB3 and MnB4. *Physical Chemistry Chemical Physics*, **2014**, 16, 15866-73	3.6	43
215	Superconductivity of lithium-doped hydrogen under high pressure. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 104-11	0.8	43
214	First-principles determination of the structure of magnesium borohydride. *Physical Review Letters*, **2012**, 109, 245503	7.4	43
213	Superconducting high-pressure phase of platinum hydride from first principles. *Physical Review B*, **2011**, 84,	3.3	43
212	On Distribution of Superconductivity in Metal Hydrides. *Current Opinion in Solid State and Materials Science*, **2020**, 24, 100808	12	43
211	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. *Physical Review B*, **2013**, 88,	3.3	41
210	Raman spectroscopy and x-ray diffraction of sp3CaCO3 at lower mantle pressures. *Physical Review B*, **2017**, 96,	3.3	41
209	Machine learning scheme for fast extraction of chemically interpretable interatomic potentials. *AIP Advances*, **2016**, 6, 085318	1.5	41
208	Topology-based crystal structure generator. *Computer Physics Communications*, **2019**, 236, 1-7	4.2	41
207	Periodic-Graph Approaches in Crystal Structure Prediction **2010**, 1-28		40
206	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. *Journal of Physical Chemistry Letters*, **2018**, 9, 3470-3477	6.4	40
205	Absence of superconductivity in the high-pressure polymorph of MgB2. *Physical Review B*, **2009**, 79,	3.3	39
204	From four- to six-coordinated silica: Transformation pathways from metadynamics. *Physical Review B*, **2007**, 76,	3.3	39

203	Superconductivity of LaH10 and LaH16 polyhydrides. *Physical Review B*, **2020**, 101,	3.3	38
202	Synthesis of Mg(2)C(3): a monoclinic high-pressure polymorph of magnesium sesquicarbide. *Inorganic Chemistry*, **2014**, 53, 7020-7	5.1	38
201	Grain boundary phases in bcc metals. *Nanoscale*, **2018**, 10, 8253-8268	7.7	37
200	Evolutionary search for new high-k dielectric materials: methodology and applications to hafnia-based oxides. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 76-84	0.8	37
199	Novel superhard B-C-O phases predicted from first principles. *Physical Chemistry Chemical Physics*, **2016**, 18, 1859-63	3.6	36
198	Predicting polymeric crystal structures by evolutionary algorithms. *Journal of Chemical Physics*, **2014**, 141, 154102	3.9	36
197	Energy-free machine learning force field for aluminum. *Scientific Reports*, **2017**, 7, 8512	4.9	36
196	Novel hydrogen hydrate structures under pressure. *Scientific Reports*, **2014**, 4, 5606	4.9	36
195	Backbone NxH compounds at high pressures. *Journal of Chemical Physics*, **2015**, 142, 214308	3.9	35
194	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. *Nano Letters*, **2016**, 16, 4236-42	11.5	35
193	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. *Chemical Science*, **2018**, 9, 1022-1030	9.4	35
192	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	2.9	34
191	Ab initio molecular dynamics study of CaSiO3 perovskite at P T conditions of Earth lower mantle. *Physical Review B*, **2006**, 73,	3.3	34
190	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. *Chemistry of Materials*, **2020**, 32, 6947-6957	9.6	34
189	Iron Superhydrides FeH5 and FeH6: Stability, Electronic Properties, and Superconductivity. *Journal of Physical Chemistry C*, **2018**, 122, 4731-4736	3.8	33
188	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, 12299-306	3.6	33
187	The high-pressure phase of boron, B28: Disputes and conclusions of 5 years after discovery. *Journal of Superhard Materials*, **2011**, 33, 363-379	0.9	32
186	Ab initio theory of planetary materials. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	32

185	First-principles study of ZrN crystalline phases: phase stability, electronic and mechanical properties. *RSC Advances*, **2017**, 7, 4697-4703	3.7	31
184	Pressure-induced novel compounds in the Hf-O system from first-principles calculations. *Physical Review B*, **2015**, 92,	3.3	31
183	Crystal structure prediction and simulations of structural transformations: metadynamics and evolutionary algorithms. *Phase Transitions*, **2007**, 80, 277-298	1.3	31
182	Exploring the Real Ground-State Structures of Molybdenum Dinitride. *Journal of Physical Chemistry C*, **2016**, 120, 11060-11067	3.8	31
181	Explaining stability of transition metal carbides and why TcC does not exist. *RSC Advances*, **2016**, 6, 16197-16202	3.7	30
180	Synthesis of Ultra-incompressible sp3-Hybridized Carbon Nitride with 1:1 Stoichiometry. *Chemistry of Materials*, **2016**, 28, 6925-6933	9.6	29
179	Superconductivity of novel tin hydrides (Sn(n)H(m)) under pressure. *Scientific Reports*, **2016**, 6, 22873	4.9	29
178	Ionic high-pressure form of elemental boron. *Nature*, **2009**, 460, 292	50.4	29
177	Mechanisms of Al3+ incorporation in MgSiO3 post-perovskite at high pressures. *Earth and Planetary Science Letters*, **2006**, 248, 69-76	5.3	29
176	Thermochemical electronegativities of the elements. *Nature Communications*, **2021**, 12, 2087	17.4	29
175	Superconductivity at 253 K in lanthanum–yttrium ternary hydrides. *Materials Today*, **2021**, 48, 18-18	21.8	29
174	Synthesis of molecular metallic barium superhydride: pseudocubic BaH. *Nature Communications*, **2021**, 12, 273	17.4	29
173	Crystal structure prediction: reflections on present status and challenges. *Faraday Discussions*, **2018**, 211, 643-660	3.6	29
172	High-Pressure Synthesis of Magnetic Neodymium Polyhydrides. *Journal of the American Chemical Society*, **2020**, 142, 2803-2811	16.4	28
171	Lattice dynamics of MgO at high pressure: theory and experiment. *Physical Review Letters*, **2006**, 96, 035507	7.4	28
170	Theoretical investigation of metastable Al2SiO5 polymorphs. *Acta Crystallographica Section A: Foundations and Advances*, **2001**, 57, 548-57		28
169	Generalized evolutionary metadynamics for sampling the energy landscapes and its applications. *Physical Review B*, **2015**, 92,	3.3	26
168	Prediction of novel stable compounds in the Mg-Si-O system under exoplanet pressures. *Scientific Reports*, **2015**, 5, 18347	4.9	26

167	Prediction of a new ground state of superhard compound B6O at ambient conditions. *Scientific Reports*, **2016**, 6, 31288	4.9	26
166	Unexpected reconstruction of the □boron (111) surface. *Physical Review Letters*, **2014**, 113, 176101	7.4	26
165	Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied using ab initio calculations. *Physical Review B*, **2007**, 75,	3.3	26
164	New two-dimensional phase of tin chalcogenides: Candidates for high-performance thermoelectric materials. *Physical Review Materials*, **2019**, 3,	3.2	26
163	Diverse Chemistry of Stable Hydronitrogens, and Implications for Planetary and Materials Sciences. *Scientific Reports*, **2016**, 6, 25947	4.9	25
162	Stable magnesium peroxide at high pressure. *Scientific Reports*, **2015**, 5, 13582	4.9	25
161	Pressure-driven formation and stabilization of superconductive chromium hydrides. *Scientific Reports*, **2015**, 5, 17764	4.9	25
160	d-AO spherical aromaticity in Ce6O8. *Journal of Computational Chemistry*, **2016**, 37, 103-9	3.5	25
159	Fermi surface nesting and phonon instabilities in simple cubic calcium. *High Pressure Research*, **2008** , 28, 443-448	1.6	24
158	Boron phosphide under pressure: In situ study by Raman scattering and X-ray diffraction. *Journal of Applied Physics*, **2014**, 116, 033501	2.5	22
157	Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations. *Scientific Reports*, **2014**, 4, 5889	4.9	22
156	Superconducting high-pressure phase of cesium iodide. *Physical Review B*, **2009**, 79,	3.3	22
155	Atomic-scale observation and analysis of chemical ordering in M3B2 and M5B3 borides. *Acta Materialia*, **2018**, 149, 274-284	8.4	21
154	Novel high-pressure calcium carbonates. *Physical Review B*, **2018**, 98,	3.3	21
153	Computational discovery of hard and superhard materials. *Journal of Applied Physics*, **2019**, 126, 040901	2.5	21
152	Refined phase diagram of the H-S system with high-Tc superconductivity. *Physical Review B*, **2017**, 96,	3.3	21
151	Prediction of a stable post-post-perovskite structure from first principles. *Physical Review B*, **2015**, 91,	3.3	20
150	Efficient technique for computational design of thermoelectric materials. *Computer Physics Communications*, **2018**, 222, 152-157	4.2	20

149	Unexpected stable phases of tungsten borides. *Physical Chemistry Chemical Physics*, **2018**, 20, 24665-24670	3.6	20
148	Exotic Two-Dimensional Structure: The First Case of Hexagonal NaCl. *Journal of Physical Chemistry Letters*, **2020**, 11, 3821-3827	6.4	19
147	Tuning the crystal structure and electronic states of Ag2Se: Structural transitions and metallization under pressure. *Physical Review B*, **2014**, 89,	3.3	19
146	Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO. *Scientific Reports*, **2017**, 7, 10357	4.9	19
145	Effect of hydrostatic pressure on the crystal structure of sodium oxalate: X-ray diffraction study and ab initio simulations. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2006**, 221,	1	19
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143	Antiferromagnetic Stabilization in the Ti8O12 Cluster. *Angewandte Chemie - International Edition*, **2016**, 55, 1699-703	16.4	19
142	Novel Stable Compounds in the C-H-O Ternary System at High Pressure. *Scientific Reports*, **2016**, 6, 32486	4.9	19
141	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	6.4	19
140	High-Temperature Superconducting Phases in Cerium Superhydride with a T_{c} up to 115 K below a Pressure of 1 Megabar. *Physical Review Letters*, **2021**, 127, 117001	7.4	19
139	Ab initio thermodynamics of MgSiO3 perovskite at high pressures and temperatures. *Journal of Chemical Physics*, **2005**, 122, 124501	3.9	18
138	Imaging Domain Reversal in an Ultrathin Van der Waals Ferromagnet. *Advanced Materials*, **2020**, 32, e2003314	24	18
137	Formation of stoichiometric CsFn compounds. *Scientific Reports*, **2015**, 5, 7875	4.9	17
136	Crystal Structure Prediction Using Evolutionary Approach **2010**, 147-180		17
135	Equations of state of Al, Au, Cu, Pt, Ta, and W and revised ruby pressure scale. *Doklady Earth Sciences*, **2006**, 410, 1091-1095	0.6	17
134	Crystal morphology and surface structures of orthorhombic MgSiO3 perovskite. *Physics and Chemistry of Minerals*, **2005**, 31, 671-682	1.6	17
133	The unexpectedly rich reconstructions of rutile TiO2(011)-(2 1) surface and the driving forces behind their formation: an ab initio evolutionary study. *Physical Chemistry Chemical Physics*, **2016**, 18, 19549-56	3.6	17
132	Predicting the ground-state structure of sodium boride. *Physical Review B*, **2018**, 97,	3.3	16

131	Stability of numerous novel potassium chlorides at high pressure. *Scientific Reports*, **2016**, 6, 26265	4.9	16
130	Crystal structure prediction of LiBeH3 using ab initio total-energy calculations and evolutionary simulations. *Journal of Chemical Physics*, **2008**, 129, 234105	3.9	16
129	The crystal structure and thermal expansion of the perovskite-type Nd0.75Sm0.25GaO3: powder diffraction and lattice dynamical studies. *Journal of Physics Condensed Matter*, **2004**, 16, 253-265	1.8	16
128	Magnetic borophenes from an evolutionary search. *Physical Review B*, **2019**, 99,	3.3	15
127	Alkali subhalides: high-pressure stability and interplay between metallic and ionic bonds. *Physical Chemistry Chemical Physics*, **2016**, 18, 2840-9	3.6	15
126	Superconductivity and unexpected chemistry of germanium hydrides under pressure. *Physical Review B*, **2017**, 95,	3.3	15
125	Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system. *AIP Advances*, **2014**, 4, 107118	1.5	15
124	Theoretical Studies of High-Pressure Phases, Electronic Structure, and Vibrational Properties of NaNH2. *Journal of Physical Chemistry C*, **2012**, 116, 8387-8393	3.8	15
123	Iron silicides at pressures of the Earth's inner core. *Geophysical Research Letters*, **2010**, 37, n/a-n/a	4.9	15
122	Prediction of new thermodynamically stable aluminum oxides. *Scientific Reports*, **2015**, 5, 9518	4.9	14
121	Novel sp3 forms of carbon predicted by evolutionary metadynamics and analysis of their synthesizability using transition path sampling. *Journal of Superhard Materials*, **2012**, 34, 350-359	0.9	14
120	Application of machine learning methods for predicting new superhard materials. *Journal of Applied Physics*, **2020**, 128, 075102	2.5	14
119	Emergence of novel hydrogen chlorides under high pressure. *Physical Chemistry Chemical Physics*, **2017**, 19, 8236-8242	3.6	13
118	Super-oxidation of silicon nanoclusters: magnetism and reactive oxygen species at the surface. *Nanoscale*, **2016**, 8, 18616-18620	7.7	13
117	Novel compounds in the Zr-O system, their crystal structures and mechanical properties. *Physical Chemistry Chemical Physics*, **2015**, 17, 17301-10	3.6	13
116	Formation of As-As Interlayer Bonding in the collapsed tetragonal phase of NaFe2As2 under pressure. *Scientific Reports*, **2015**, 5, 9868	4.9	13
115	Structural transformations of minerals in deep geospheres: A review. *Crystallography Reports*, **2006**, 51, 767-777	0.6	13
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