Artem Oganov

List of Publications by Year in Descending Order

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	Ultrahigh-Pressure Magnesium Hydrosilicates as Reservoirs of Water in Early Earth.. *Physical Review Letters*, **2022**, 128, 035703	7.4	3
309	Electronegativity and chemical hardness of elements under pressure.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2117416119	11.5	3
308	Sr-Doped Superionic Hydrogen Glass: Synthesis and Properties of SrH.. *Advanced Materials*, **2022**, e2200924	24	2
307	Novel two-dimensional boron oxynitride predicted using the USPEX evolutionary algorithm. *Physical Chemistry Chemical Physics*, **2021**, 23, 26178-26184	3.6	1
306	Ethane and methane at high pressures: Structure and stability. *Journal of Chemical Physics*, **2021**, 155, 184503	3.9	0
305	Prediction of Novel van der Waals Boron Oxides with Superior Deep-Ultraviolet Nonlinear Optical Performance. *Angewandte Chemie*, **2021**, 133, 10886-10892	3.6	6
304	Prediction of Novel van der Waals Boron Oxides with Superior Deep-Ultraviolet Nonlinear Optical Performance. *Angewandte Chemie - International Edition*, **2021**, 60, 10791-10797	16.4	10
303	Anomalous High-Temperature Superconductivity in YH. *Advanced Materials*, **2021**, 33, e2006832	24	60
302	Thermochemical electronegativities of the elements. *Nature Communications*, **2021**, 12, 2087	17.4	29
301	Crystal and electronic structure engineering of tin monoxide by external pressure. *Journal of Advanced Ceramics*, **2021**, 10, 565-577	10.7	7
300	Unusual Chemistry of the C-H-N-O System under Pressure and Implications for Giant Planets. *Journal of Physical Chemistry A*, **2021**, 125, 3936-3942	2.8	3
299	Strong electronic correlations in interstitial magnetic centers of zero-dimensional electride Yb5Sb3. *Physical Review B*, **2021**, 103,	3.3	3
298	High-Pressure Phase Diagram of the Ti-O System. *Journal of Physical Chemistry Letters*, **2021**, 12, 5486-5493	6.4	2
297	Superconductivity at 253 K in lanthanum–yttrium ternary hydrides. *Materials Today*, **2021**, 48, 18-18	21.8	29
296	Novel Strongly Correlated Europium Superhydrides. *Journal of Physical Chemistry Letters*, **2021**, 12, 32-40	6.4	11
295	Synthesis of molecular metallic barium superhydride: pseudocubic BaH. *Nature Communications*, **2021**, 12, 273	17.4	29
294	Influence of the Pd : Bi ratio on Pd-Bi/AlO catalysts: structure, surface and activity in glucose oxidation. *Physical Chemistry Chemical Physics*, **2021**, 23, 14889-14897	3.6	0

293	Novel copper fluoride analogs of cuprates. *Physical Chemistry Chemical Physics*, **2021**, 23, 15989-15993	3.6	2
292	Helium-nitrogen mixtures at high pressure. *Physical Review B*, **2021**, 103,	3.3	3
291	Formation of copper boride on Cu(111). *Fundamental Research*, **2021**, 1, 482-487		2
290	Interacting Electrons in Two-Dimensional Electride Ca2N. *Journal of Physical Chemistry C*, **2021**, 125, 15724-15729	3.6	2
289	AICON2: A program for calculating transport properties quickly and accurately. *Computer Physics Communications*, **2021**, 266, 108027	4.2	2
288	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9
287	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
286	COPEX: co-evolutionary crystal structure prediction algorithm for complex systems. *Npj Computational Materials*, **2021**, 7,	10.9	3
285	Coevolutionary search for optimal materials in the space of all possible compounds. *Npj Computational Materials*, **2020**, 6,	10.9	11
284	Search for stable cocrystals of energetic materials using the evolutionary algorithm USPEX. *Physical Chemistry Chemical Physics*, **2020**, 22, 16822-16830	3.6	8
283	Discovery of new boron-rich chalcogenides: orthorhombic BX (X=S, Se). *Scientific Reports*, **2020**, 10, 9277	4.9	12
282	Weak Coulomb correlations stabilize the electride high-pressure phase of elemental calcium. *Journal of Physics Condensed Matter*, **2020**, 32, 445501	1.8	4
281	Prediction and Synthesis of Dysprosium Hydride Phases at High Pressure. *Inorganic Chemistry*, **2020**, 59, 5303-5312	5.1	5
280	Structure, Stability, and Mechanical Properties of Boron-Rich Mo-B Phases: A Computational Study. *Journal of Physical Chemistry Letters*, **2020**, 11, 2393-2401	6.4	12
279	WB : Synthesis, Properties, and Crystal Structure-New Insights into the Long-Debated Compound. *Advanced Science*, **2020**, 7, 2000775	13.6	9
278	A Revisited Mechanism of the Graphite-to-Diamond Transition at High Temperature. *Matter*, **2020**, 3, 864-878	12.7	8
277	Electronic correlations in uranium hydride UH under pressure. *Journal of Physics Condensed Matter*, **2020**, 32, 385602	1.8	2
276	Superconductivity of LaH10 and LaH16 polyhydrides. *Physical Review B*, **2020**, 101,	3.3	38

275	Superconducting praseodymium superhydrides. *Science Advances*, **2020**, 6, eaax6849	14.3	49
274	High-Pressure Synthesis of Magnetic Neodymium Polyhydrides. *Journal of the American Chemical Society*, **2020**, 142, 2803-2811	16.4	28
273	Exotic Two-Dimensional Structure: The First Case of Hexagonal NaCl. *Journal of Physical Chemistry Letters*, **2020**, 11, 3821-3827	6.4	19
272	Multi-objective Optimization as a Tool for Material Design **2020**, 2777-2790		1
271	Superconductivity at 161 K in thorium hydride ThH10: Synthesis and properties. *Materials Today*, **2020**, 33, 36-44	21.8	102
270	AICON: A program for calculating thermal conductivity quickly and accurately. *Computer Physics Communications*, **2020**, 251, 107074	4.2	7
269	Computational Search for New W-Mo-B Compounds. *Chemistry of Materials*, **2020**, 32, 7028-7035	9.6	6
268	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. *Chemistry of Materials*, **2020**, 32, 6947-6957	9.6	34
267	Nonempirical Definition of the Mendeleev Numbers: Organizing the Chemical Space. *Journal of Physical Chemistry C*, **2020**, 124, 23867-23878	3.8	7
266	Superconductivity and equation of state of lanthanum at megabar pressures. *Physical Review B*, **2020**, 102,	3.3	7
265	Collapse modes in simple cubic and body-centered cubic arrangements of elastic beads. *Physical Review E*, **2020**, 102, 032901	2.4	
264	Application of machine learning methods for predicting new superhard materials. *Journal of Applied Physics*, **2020**, 128, 075102	2.5	14
263	Imaging Domain Reversal in an Ultrathin Van der Waals Ferromagnet. *Advanced Materials*, **2020**, 32, e2003314	24	18
262	Novel Hydrogen Clathrate Hydrate. *Physical Review Letters*, **2020**, 125, 255702	7.4	4
261	On Distribution of Superconductivity in Metal Hydrides. *Current Opinion in Solid State and Materials Science*, **2020**, 24, 100808	12	43
260	High-temperature superconductivity in the Ti-H system at high pressures. *Physical Review B*, **2020**, 101,	3.3	6
259	Machine Learning Interatomic Potentials for Global Optimization and Molecular Dynamics Simulation **2019**, 253-288		2
258	Synthesis of clathrate cerium superhydride CeH at 80-100 GPa with atomic hydrogen sublattice. *Nature Communications*, **2019**, 10, 4453	17.4	64

257	A model of hardness and fracture toughness of solids. *Journal of Applied Physics*, **2019**, 126, 125109	2.5	51
256	Novel Unexpected Reconstructions of (100) and (111) Surfaces of NaCl: Theoretical Prediction. *Scientific Reports*, **2019**, 9, 14267	4.9	12
255	Multi-Objective Optimization as a Tool for Material Design **2019**, 1-15		3
254	Stable and hard hafnium borides: A first-principles study. *Journal of Applied Physics*, **2019**, 125, 205109	2.5	7
253	Magnetic borophenes from an evolutionary search. *Physical Review B*, **2019**, 99,	3.3	15
252	Interplay between the Coulomb Interaction and Hybridization in Ca and Anomalous Pressure Dependence of the Resistivity. *JETP Letters*, **2019**, 109, 387-391	1.2	4
251	Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning. *Physical Review B*, **2019**, 99,	3.3	125
250	Structure prediction drives materials discovery. *Nature Reviews Materials*, **2019**, 4, 331-348	73.3	242
249	Hydrocarbons under Pressure: Phase Diagrams and Surprising New Compounds in the C□H System. *Journal of Physical Chemistry C*, **2019**, 123, 20497-20501	3.8	10
248	Computational discovery of hard and superhard materials. *Journal of Applied Physics*, **2019**, 126, 040901	2.5	21
247	Measuring the Meissner effect at megabar pressures. *National Science Review*, **2019**, 6, 856	10.8	1
246	Predicted lithium oxide compounds and superconducting low-pressure LiO4. *Physical Review B*, **2019**, 100,	3.3	2
245	Phase diagram of uranium from ab initio calculations and machine learning. *Physical Review B*, **2019**, 100,	3.3	8
244	New two-dimensional phase of tin chalcogenides: Candidates for high-performance thermoelectric materials. *Physical Review Materials*, **2019**, 3,	3.2	26
243	Simple and accurate model of fracture toughness of solids. *Journal of Applied Physics*, **2019**, 125, 065105	2.5	56
242	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
241	Topology-based crystal structure generator. *Computer Physics Communications*, **2019**, 236, 1-7	4.2	41
240	Atomic-scale observation and analysis of chemical ordering in M3B2 and M5B3 borides. *Acta Materialia*, **2018**, 149, 274-284	8.4	21

239	Grain boundary phases in bcc metals. *Nanoscale*, **2018**, 10, 8253-8268	7.7	37
238	Boron monosulfide: Equation of state and pressure-induced phase transition. *Journal of Applied Physics*, **2018**, 123, 135903	2.5	8
237	Iron Superhydrides FeH5 and FeH6: Stability, Electronic Properties, and Superconductivity. *Journal of Physical Chemistry C*, **2018**, 122, 4731-4736	3.8	33
236	Predicting the ground-state structure of sodium boride. *Physical Review B*, **2018**, 97,	3.3	16
235	Actinium Hydrides AcH, AcH, and AcH as High-Temperature Conventional Superconductors. *Journal of Physical Chemistry Letters*, **2018**, 9, 1920-1926	6.4	70
234	Two-dimensional boron on Pb (1 1 0) surface. *FlatChem*, **2018**, 7, 34-41	5.1	5
233	Efficient technique for computational design of thermoelectric materials. *Computer Physics Communications*, **2018**, 222, 152-157	4.2	20
232	Theoretical and Experimental Investigations into Novel Oxynitride Discovery in the GaN-TiO2 System at High Pressure. *Crystals*, **2018**, 8, 15	2.3	1
231	Novel high-pressure calcium carbonates. *Physical Review B*, **2018**, 98,	3.3	21
230	Using virtualization to protect the proprietary material science applications in volunteer computing. *Open Engineering*, **2018**, 8, 57-60	1.7	1
229	First-principles study of thermoelectric properties of MgSi-MgPb semiconductor materials.. *RSC Advances*, **2018**, 8, 17168-17175	3.7	8
228	Titanium-hydrogen interaction at high pressure. *Journal of Applied Physics*, **2018**, 123, 235901	2.5	2
227	2D materials worth their salt. *Nature Chemistry*, **2018**, 10, 694-695	17.6	2
226	Chapter 1:Computational Materials Discovery: Dream or Reality? **2018**, 1-14		2
225	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. *Chemical Science*, **2018**, 9, 1022-1030	9.4	35
224	Applications of crystal structure prediction - inorganic and network structures: general discussion. *Faraday Discussions*, **2018**, 211, 613-642	3.6	4
223	The stability and unexpected chemistry of oxide clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 30437-30444	3.6	7
222	Boron oxides under pressure: Prediction of the hardest oxides. *Physical Review B*, **2018**, 98,	3.3	13

221	High-Temperature Superconductivity in a Th-H System under Pressure Conditions. *ACS Applied Materials & Interfaces*, **2018**, 10, 43809-43816	9.5	55
220	Role of temperature and Coulomb correlation in the stabilization of the CsCl-type phase in FeS under pressure. *Physical Review B*, **2018**, 98,	3.3	5
219	Structure searching methods: general discussion. *Faraday Discussions*, **2018**, 211, 133-180	3.6	3
218	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. *Faraday Discussions*, **2018**, 211, 325-381	3.6	6
217	Applications of crystal structure prediction - organic molecular structures: general discussion. *Faraday Discussions*, **2018**, 211, 493-539	3.6	6
216	Crystal structure prediction: reflections on present status and challenges. *Faraday Discussions*, **2018**, 211, 643-660	3.6	29
215	Uranium polyhydrides at moderate pressures: Prediction, synthesis, and expected superconductivity. *Science Advances*, **2018**, 4, eaat9776	14.3	52
214	Unexpected stable phases of tungsten borides. *Physical Chemistry Chemical Physics*, **2018**, 20, 24665-24670	3.6	20
213	Old puzzle of incommensurate crystal structure of calaverite AuTe and predicted stability of novel AuTe compound. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 9945-9950	11.5	8
212	Tetrahedral honeycomb surface reconstructions of quartz, cristobalite and stishovite. *Scientific Reports*, **2018**, 8, 11947	4.9	7
211	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. *Journal of Physical Chemistry Letters*, **2018**, 9, 3470-3477	6.4	40
210	Computational Search for Novel Hard Chromium-Based Materials. *Journal of Physical Chemistry Letters*, **2017**, 8, 755-764	6.4	50
209	First-principles study of ZrN crystalline phases: phase stability, electronic and mechanical properties. *RSC Advances*, **2017**, 7, 4697-4703	3.7	31
208	Prediction of thermodynamically stable Li-B compounds at ambient pressure. *Physical Chemistry Chemical Physics*, **2017**, 19, 8471-8477	3.6	5
207	Pressure-stabilized hafnium nitrides and their properties. *Physical Review B*, **2017**, 95,	3.3	53
206	Emergence of novel hydrogen chlorides under high pressure. *Physical Chemistry Chemical Physics*, **2017**, 19, 8236-8242	3.6	13
205	A stable compound of helium and sodium at high pressure. *Nature Chemistry*, **2017**, 9, 440-445	17.6	199
204	First-principles investigation of Zr-O compounds, their crystal structures, and mechanical properties. *Journal of Applied Physics*, **2017**, 121, 155104	2.5	11

203	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
202	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. *Chemical Science*, **2017**, 8, 4926-4940	9.4	70
201	Novel magnesium borides and their superconductivity. *Physical Chemistry Chemical Physics*, **2017**, 19, 14486-14494	3.6	6
200	Mechanism of the fcc-to-hcp phase transformation in solid Ar. *Journal of Chemical Physics*, **2017**, 146, 214502	3.9	10
199	Electrides and Their High-Pressure Chemistry **2017**, 69-84		1
198	Volunteer computing for computational materials design. *Lobachevskii Journal of Mathematics*, **2017**, 38, 926-930	0.9	2
197	Raman spectroscopy and x-ray diffraction of sp3CaCO3 at lower mantle pressures. *Physical Review B*, **2017**, 96,	3.3	41
196	Predicting the Structure and Chemistry of Low-Dimensional Materials **2017**, 527-570		
195	Energy-free machine learning force field for aluminum. *Scientific Reports*, **2017**, 7, 8512	4.9	36
194	Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO. *Scientific Reports*, **2017**, 7, 10357	4.9	19
193	From Linear Molecular Chains to Extended Polycyclic Networks: Polymerization of Dicyanoacetylene. *Chemistry of Materials*, **2017**, 29, 6706-6718	9.6	7
192	Superconductivity and unexpected chemistry of germanium hydrides under pressure. *Physical Review B*, **2017**, 95,	3.3	15
191	High-pressure behavior of the FeS system and composition of the Earth's inner core. *Physics-Uspekhi*, **2017**, 60, 1025-1032	2.8	8
190	Reactivity of elements and compounds: results of sructure-prediction algorithm USPEX. *Acta Crystallographica Section A: Foundations and Advances*, **2017**, 73, C863-C863	1.7	
189	Refined phase diagram of the H-S system with high-Tc superconductivity. *Physical Review B*, **2017**, 96,	3.3	21
188	Synthesis of Ultra-incompressible sp3-Hybridized Carbon Nitride with 1:1 Stoichiometry. *Chemistry of Materials*, **2016**, 28, 6925-6933	9.6	29
187	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
186	Two-dimensional magnetic boron. *Physical Review B*, **2016**, 93,	3.3	75

185	Hydrogen sulfide at high pressure: Change in stoichiometry. *Physical Review B*, **2016**, 93,	3.3	77
184	Super-oxidation of silicon nanoclusters: magnetism and reactive oxygen species at the surface. *Nanoscale*, **2016**, 8, 18616-18620	7.7	13
183	Diverse Chemistry of Stable Hydronitrogens, and Implications for Planetary and Materials Sciences. *Scientific Reports*, **2016**, 6, 25947	4.9	25
182	Stability of numerous novel potassium chlorides at high pressure. *Scientific Reports*, **2016**, 6, 26265	4.9	16
181	Superconductivity of novel tin hydrides (Sn(n)H(m)) under pressure. *Scientific Reports*, **2016**, 6, 22873	4.9	29
180	Prediction of a new ground state of superhard compound B6O at ambient conditions. *Scientific Reports*, **2016**, 6, 31288	4.9	26
179	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. *Nano Letters*, **2016**, 16, 4236-42	11.5	35
178	Antiferromagnetic Stabilization in the Ti8O12 Cluster. *Angewandte Chemie*, **2016**, 128, 1731-1735	3.6	2
177	Alkali subhalides: high-pressure stability and interplay between metallic and ionic bonds. *Physical Chemistry Chemical Physics*, **2016**, 18, 2840-9	3.6	15
176	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
175	Combined Theoretical and in Situ Scattering Strategies for Optimized Discovery and Recovery of High-Pressure Phases: A Case Study of the GaN-Nb2O5 System. *Inorganic Chemistry*, **2016**, 55, 3384-92	5.1	3
174	Explaining stability of transition metal carbides and why TcC does not exist. *RSC Advances*, **2016**, 6, 16197-16202	3.7	30
173	Novel superhard B-C-O phases predicted from first principles. *Physical Chemistry Chemical Physics*, **2016**, 18, 1859-63	3.6	36
172	Pressure induced Ag2Te polymorphs in conjunction with topological non trivial to metal transition. *AIP Advances*, **2016**, 6, 085003	1.5	4
171	Antiferromagnetic Stabilization in the Ti8O12 Cluster. *Angewandte Chemie - International Edition*, **2016**, 55, 1699-703	16.4	19
170	Machine learning scheme for fast extraction of chemically interpretable interatomic potentials. *AIP Advances*, **2016**, 6, 085318	1.5	41
169	Novel Stable Compounds in the C-H-O Ternary System at High Pressure. *Scientific Reports*, **2016**, 6, 32486	4.9	19
168	The impact of electron correlations on the energetics and stability of silicon nanoclusters. *Journal of Chemical Physics*, **2016**, 145, 074313	3.9	7

167	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
166	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
165	d-AO spherical aromaticity in Ce6O8. *Journal of Computational Chemistry*, **2016**, 37, 103-9	3.5	25
164	Exploring the Real Ground-State Structures of Molybdenum Dinitride. *Journal of Physical Chemistry C*, **2016**, 120, 11060-11067	3.8	31
163	Prediction of a stable post-post-perovskite structure from first principles. *Physical Review B*, **2015**, 91,	3.3	20
162	Backbone NxH compounds at high pressures. *Journal of Chemical Physics*, **2015**, 142, 214308	3.9	35
161	Generalized evolutionary metadynamics for sampling the energy landscapes and its applications. *Physical Review B*, **2015**, 92,	3.3	26
160	A Novel Phase of Li15Si4 Synthesized under Pressure. *Advanced Energy Materials*, **2015**, 5, 1500214	21.8	12
159	Prediction of new thermodynamically stable aluminum oxides. *Scientific Reports*, **2015**, 5, 9518	4.9	14
158	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
157	A novel phase of beryllium fluoride at high pressure. *Physical Chemistry Chemical Physics*, **2015**, 17, 26283-8	3.8	10
156	Prediction of novel stable compounds in the Mg-Si-O system under exoplanet pressures. *Scientific Reports*, **2015**, 5, 18347	4.9	26
155	Pressure-induced novel compounds in the Hf-O system from first-principles calculations. *Physical Review B*, **2015**, 92,	3.3	31
154	Stable magnesium peroxide at high pressure. *Scientific Reports*, **2015**, 5, 13582	4.9	25
153	Effects of ferroelectric polarization on surface phase diagram: Evolutionary algorithm study of the BaTiO3(001) surface. *Physical Review B*, **2015**, 92,	3.3	12
152	Novel lithium-nitrogen compounds at ambient and high pressures. *Scientific Reports*, **2015**, 5, 14204	4.9	48
151	Nitrogen oxides under pressure: stability, ionization, polymerization, and superconductivity. *Scientific Reports*, **2015**, 5, 16311	4.9	8
150	Pressure-driven formation and stabilization of superconductive chromium hydrides. *Scientific Reports*, **2015**, 5, 17764	4.9	25

149	Rational design of inorganic dielectric materials with expected permittivity. *Scientific Reports*, **2015**, 5, 16769	4.9	7
148	Investigation of exotic stable calcium carbides using theory and experiment. *Nature Communications*, **2015**, 6, 6974	17.4	61
147	The phase diagram and hardness of carbon nitrides. *Scientific Reports*, **2015**, 5, 9870	4.9	66
146	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
145	Novel compounds in the Zr-O system, their crystal structures and mechanical properties. *Physical Chemistry Chemical Physics*, **2015**, 17, 17301-10	3.6	13
144	Formation of As-As Interlayer Bonding in the collapsed tetragonal phase of NaFe2As2 under pressure. *Scientific Reports*, **2015**, 5, 9868	4.9	13
143	Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. *Science*, **2015**, 350, 1513-6	33.3	1479
142	Formation of stoichiometric CsFn compounds. *Scientific Reports*, **2015**, 5, 7875	4.9	17
141	Structure prediction and its applications in computational materials design. *Chemical Modelling*, **2015**, 219-248	2	3
140	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
139	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. *Physical Review Letters*, **2014**, 112,	7.4	397
138	Boron phosphide under pressure: In situ study by Raman scattering and X-ray diffraction. *Journal of Applied Physics*, **2014**, 116, 033501	2.5	22
137	Unexpected reconstruction of the □boron (111) surface. *Physical Review Letters*, **2014**, 113, 176101	7.4	26
136	Predicting polymeric crystal structures by evolutionary algorithms. *Journal of Chemical Physics*, **2014**, 141, 154102	3.9	36
135	Variable-composition structural optimization and experimental verification of MnB3 and MnB4. *Physical Chemistry Chemical Physics*, **2014**, 16, 15866-73	3.6	43
134	High throughput exploration of ZrxSi1□xO2 dielectrics by evolutionary first-principles approaches. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 3549-3553	2.3	7
133	Prediction of the atomic structure and stability for the ensemble of silicon nanoclusters passivated by hydrogen. *Europhysics Letters*, **2014**, 106, 37002	1.6	11
132	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

131	BaC: a thermodynamically stable layered superconductor. *Physical Chemistry Chemical Physics*, **2014**, 16, 20780-4	3.6	7
130	Metastable host-guest structure of carbon. *Journal of Superhard Materials*, **2014**, 36, 246-256	0.9	2
129	Rational design of all organic polymer dielectrics. *Nature Communications*, **2014**, 5, 4845	17.4	206
128	Tuning the crystal structure and electronic states of Ag2Se: Structural transitions and metallization under pressure. *Physical Review B*, **2014**, 89,	3.3	19
127	Superconductivity of lithium-doped hydrogen under high pressure. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 104-11	0.8	43
126	Synthesis of Mg(2)C(3): a monoclinic high-pressure polymorph of magnesium sesquicarbide. *Inorganic Chemistry*, **2014**, 53, 7020-7	5.1	38
125	Crystal structure prediction and its application in Earth and materials sciences. *Topics in Current Chemistry*, **2014**, 345, 223-56		10
124	First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric BaAl2O4. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 1867-1870	2.3	12
123	Novel hydrogen hydrate structures under pressure. *Scientific Reports*, **2014**, 4, 5606	4.9	36
122	Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations. *Scientific Reports*, **2014**, 4, 5889	4.9	22
121	Theory of Superhard Materials **2014**, 59-79		3
120	Discovering low-permittivity materials: Evolutionary search for MgAl2O4 polymorphs. *Applied Physics Letters*, **2014**, 105, 022907	3.4	3
119	Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system. *AIP Advances*, **2014**, 4, 107118	1.5	15
118	New reconstructions of the (110) surface of rutile TiO2 predicted by an evolutionary method. *Physical Review Letters*, **2014**, 113, 266101	7.4	50
117	Variable cell nudged elastic band method for studying solid–solid structural phase transitions. *Computer Physics Communications*, **2013**, 184, 2111-2118	4.2	56
116	Compressed carbon nanotubes: a family of new multifunctional carbon allotropes. *Scientific Reports*, **2013**, 3, 1331	4.9	73
115	Unexpected stable stoichiometries of sodium chlorides. *Science*, **2013**, 342, 1502-5	33.3	329
114	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. *Physical Review B*, **2013**, 88,	3.3	41

113	Stability of xenon oxides at high pressures. *Nature Chemistry*, **2013**, 5, 61-5	17.6	101
112	Structure, Bonding, and Mineralogy of Carbon at Extreme Conditions. *Reviews in Mineralogy and Geochemistry*, **2013**, 75, 47-77	7.1	76
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