Yanming

List of Publications by Year in Descending Order

287 papers	20,535 citations	67 h-index	136 g-index
294 ext. papers	23,542 ext. citations	6.4 avg, IF	6.96 L-index

#	Paper	IF	Citations
287	A symmetry-orientated divide-and-conquer method for crystal structure prediction.. *Journal of Chemical Physics*, **2022**, 156, 014105	3.9	8
286	Materials by design at high pressures.. *Chemical Science*, **2022**, 13, 329-344	9.4	3
285	Low-Pressure Electrochemical Synthesis of Complex High-Pressure Superconducting Superhydrides.. *Physical Review Letters*, **2022**, 128, 186001	7.4	0
284	Experimental clathrate superhydrides EuH6 and EuH9 at extreme pressure conditions. *Physical Review Research*, **2021**, 3,	3.9	2
283	High-temperature superconductivity on the verge of a structural instability in lanthanum superhydride. *Nature Communications*, **2021**, 12, 6863	17.4	6
282	Metastable 1TRphase group VIB transition metal dichalcogenide crystals. *Nature Materials*, **2021**, 20, 1113-1120	27	36
281	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9
280	Superconductivity in Compression-Shear Deformed Diamond. *Physical Review Letters*, **2020**, 124, 147001	7.4	33
279	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. *Matter and Radiation at Extremes*, **2020**, 5, 068101	4.7	17
278	Xenon iron oxides predicted as potential Xe hosts in Earthℝ lower mantle. *Nature Communications*, **2020**, 11, 5227	17.4	6
277	Pressure-stabilized divalent ozonide CaO and its impact on Earthℝ oxygen cycles. *Nature Communications*, **2020**, 11, 4702	17.4	3
276	Computational discovery and characterization of new BO phases. *Physical Chemistry Chemical Physics*, **2019**, 21, 2499-2506	3.6	6
275	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. *Physical Review Letters*, **2019**, 123, 195504	7.4	27
274	First-principles study of high-pressure phase stability and superconductivity of Bi4I4. *Physical Review B*, **2019**, 100,	3.3	4
273	Superconductivity in Pristine 2H_{a}-MoS_{2} at Ultrahigh Pressure. *Physical Review Letters*, **2018**, 120, 037002	7.4	62
272	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. *Faraday Discussions*, **2018**, 211, 31-43	3.6	40
271	Hydrogen-rich superconductors at high pressures. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1330	7.9	41

270	Novel phases in ammonia-water mixtures under pressure. *Journal of Chemical Physics*, **2018**, 149, 234501	3.9	18
269	Two-Dimensional C4N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. *Journal of Physical Chemistry C*, **2017**, 121, 2669-2674	3.8	37
268	Structural metatransition of energetically tangled crystalline phases. *Physical Chemistry Chemical Physics*, **2017**, 19, 4560-4566	3.6	20
267	Materials discovery at high pressures. *Nature Reviews Materials*, **2017**, 2,	73.3	266
266	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO(011) Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 7891-7896	9.5	22
265	Structural evolution of FeH4 under high pressure. *RSC Advances*, **2017**, 7, 12570-12575	3.7	13
264	Computer-Assisted Inverse Design of Inorganic Electrides. *Physical Review X*, **2017**, 7,	9.1	51
263	Effects of manganese doping on the structure evolution of small-sized boron clusters. *Journal of Physics Condensed Matter*, **2017**, 29, 265401	1.8	14
262	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. *Inorganic Chemistry*, **2017**, 56, 7545-7549	5.1	3
261	Construction of crystal structure prototype database: methods and applications. *Journal of Physics Condensed Matter*, **2017**, 29, 165901	1.8	17
260	Nb-H system at high pressures and temperatures. *Physical Review B*, **2017**, 95,	3.3	27
259	X-ray diffraction data-assisted structure searches. *Computer Physics Communications*, **2017**, 213, 40-45	4.2	21
258	A two-dimensional TiB monolayer exhibits planar octacoordinate Ti. *Nanoscale*, **2017**, 9, 17983-17990	7.7	28
257	A database assisted protein structure prediction method via a swarm intelligence algorithm. *RSC Advances*, **2017**, 7, 39869-39876	3.7	2
256	Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity. *Physical Review Letters*, **2017**, 119, 107001	7.4	352
255	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. *Physical Review Letters*, **2017**, 119, 115503	7.4	108
254	Stabilization of ammonia-rich hydrate inside icy planets. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 9003-9008	11.5	26
253	Investigations on structural determination of semi-transition-metal borides. *Physical Chemistry Chemical Physics*, **2017**, 19, 31592-31598	3.6	14

252	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. *Applied Surface Science*, **2017**, 393, 422-427	6.7	10
251	Ultrastrong Boron Frameworks in ZrB : A Highway for Electron Conducting. *Advanced Materials*, **2017**, 29, 1604003	24	50
250	Sn(II)-Containing Phosphates as Optoelectronic Materials. *Chemistry of Materials*, **2017**, 29, 2459-2465	9.6	16
249	The diverse electronic properties of C4N3monolayer under biaxial compressive strain: a theoretical study. *Journal Physics D: Applied Physics*, **2016**, 49, 295301	3	7
248	Calculated high-pressure structural properties, lattice dynamics and quasi particle band structures of perovskite fluorides KZnF3, CsCaF3 and BaLiF3. *Journal of Physics Condensed Matter*, **2016**, 28, 315403	1.8	5
247	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
246	Dissociation products and structures of solid H2S at strong compression. *Physical Review B*, **2016**, 93,	3.3	96
245	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. *Physical Review Letters*, **2016**, 116, 057002	7.4	104
244	Unexpected Trend in Stability of Xe-F Compounds under Pressure Driven by Xe-Xe Covalent Bonds. *Journal of Physical Chemistry Letters*, **2016**, 7, 4562-4567	6.4	33
243	Silicon Framework-Based Lithium Silicides at High Pressures. *ACS Applied Materials & Interfaces* , **2016**, 8, 16761-7	9.5	11
242	Globally stable structures of LixZn (x = 1-4) compounds at high pressures. *Physical Chemistry Chemical Physics*, **2016**, 18, 4437-43	3.6	6
241	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. *Nature*, **2016**, 532, 81-4	50.4	165
240	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. *Chemistry of Materials*, **2016**, 28, 1746-1755	9.6	57
239	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications*, **2016**, 200, 87-95	4.2	29
238	Gold as a 6p-Element in Dense Lithium Aurides. *Journal of the American Chemical Society*, **2016**, 138, 4046-52	13.4	70
237	CALYPSO structure prediction method and its wide application. *Computational Materials Science*, **2016**, 112, 406-415	3.2	102
236	Prediction of Host-Guest Na-Fe Intermetallics at High Pressures. *Inorganic Chemistry*, **2016**, 55, 7026-32	5.1	8
235	O(NlogN) scaling method to evaluate the ion-electron potential of crystalline solids. *Journal of Chemical Physics*, **2016**, 145, 184110	3.9	6

234	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. *Physical Review B*, **2016**, 94,	3.3	9
233	First-principle optimal local pseudopotentials construction via optimized effective potential method. *Journal of Chemical Physics*, **2016**, 144, 134108	3.9	15
232	Design of ternary alkaline-earth metal Sn(II) oxides with potential good p-type conductivity. *Journal of Materials Chemistry C*, **2016**, 4, 4592-4599	7.1	23
231	Catenation of carbon in LaC2 predicted under high pressure. *Physical Chemistry Chemical Physics*, **2016**, 18, 14286-91	3.6	5
230	Theoretical realization of half-metallicity in two-dimensional monolayered molybdenum dinitride by Mo vacancy tuning. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2016**, 380, 2669-2673	2.3	3
229	Two-dimensional boron-nitrogen-carbon monolayers with tunable direct band gaps. *Nanoscale*, **2015**, 7, 12023-9	7.7	63
228	Structure Prediction of Atoms Adsorbed on Two-Dimensional Layer Materials: Method and Applications. *Journal of Physical Chemistry C*, **2015**, 119, 20111-20118	3.8	28
227	A Protocol to Fabricate Nanostructured New Phase: B31-Type MnS Synthesized under High Pressure. *Journal of the American Chemical Society*, **2015**, 137, 10297-303	16.4	55
226	Gluing together metallic and covalent layers to form Ru2C under ambient conditions. *Physical Chemistry Chemical Physics*, **2015**, 17, 9730-6	3.6	8
225	Structural morphologies of high-pressure polymorphs of strontium hydrides. *Physical Chemistry Chemical Physics*, **2015**, 17, 19379-85	3.6	29
224	Materials discovery via CALYPSO methodology. *Journal of Physics Condensed Matter*, **2015**, 27, 203203	1.8	63
223	High-pressure hydrogen sulfide from first principles: a strongly anharmonic phonon-mediated superconductor. *Physical Review Letters*, **2015**, 114, 157004	7.4	299
222	Insight into the role of Li2S2 in Li–S batteries: a first-principles study. *Journal of Materials Chemistry A*, **2015**, 3, 8865-8869	13	57
221	Metallic icosahedron phase of sodium at terapascal pressures. *Physical Review Letters*, **2015**, 114, 125501	7.4	56
220	Stabilization of fullerene-like boron cages by transition metal encapsulation. *Nanoscale*, **2015**, 7, 10482-9	7.7	59
219	Superhard-driven search of the covalent network in the B3NO system. *RSC Advances*, **2015**, 5, 35882-35887	3.7	17
218	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. *Journal of Physical Chemistry C*, **2015**, 119, 24996-25002	3.8	12
217	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. *RSC Advances*, **2015**, 5, 104426-104432	3.7	4

216	Stabilization of H in the high pressure crystalline structure of H Cl (= 2-7). *Chemical Science*, **2015**, 6, 522-526	9.4	25
215	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. *Scientific Reports*, **2015**, 5, 15433	4.9	56
214	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. *Scientific Reports*, **2015**, 5, 13039	4.9	14
213	Stable xenon nitride at high pressures. *Physical Review B*, **2015**, 92,	3.3	39
212	Anomalous Stress Response of Ultrahard WB_{n} Compounds. *Physical Review Letters*, **2015**, 115, 185502	7.4	85
211	Stable Lithium Argon compounds under high pressure. *Scientific Reports*, **2015**, 5, 16675	4.9	26
210	Magnetism in Na-filled Fe-based skutterudites. *Scientific Reports*, **2015**, 5, 10782	4.9	9
209	High pressure–low temperature phase diagram of barium: Simplicity versus complexity. *Applied Physics Letters*, **2015**, 107, 221908	3.4	7
208	Nitrogen Backbone Oligomers. *Scientific Reports*, **2015**, 5, 13239	4.9	27
207	Mercury under Pressure acts as a Transition Metal: Calculated from First Principles. *Angewandte Chemie - International Edition*, **2015**, 54, 9280-3	16.4	34
206	Two-dimensional silicon monolayers generated on c-BN(111) substrate. *Physical Chemistry Chemical Physics*, **2015**, 17, 15694-700	3.6	9
205	Pressure-stabilized superconductive yttrium hydrides. *Scientific Reports*, **2015**, 5, 9948	4.9	184
204	Crystalline LiN5 Predicted from First-Principles as a Possible High-Energy Material. *Journal of Physical Chemistry Letters*, **2015**, 6, 2363-6	6.4	98
203	Room-temperature ferromagnetism of 2H-SiC–Al2O3 solid solution nanowires and the physical origin. *Nanoscale*, **2015**, 7, 4912-9	7.7	6
202	Pressure-Induced Reversible Phase Transformation in Nanostructured Bi2Te3 with Reduced Transition Pressure. *Journal of Physical Chemistry C*, **2015**, 119, 3843-3848	3.8	25
201	Insights into Enhanced Visible-Light Photocatalytic Hydrogen Evolution of g-C3N4 and Highly Reduced Graphene Oxide Composite: The Role of Oxygen. *Chemistry of Materials*, **2015**, 27, 1612-1621	9.6	219
200	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. *APL Materials*, **2015**, 3, 011102	5.7	27
199	Superhard BC(3) in cubic diamond structure. *Physical Review Letters*, **2015**, 114, 015502	7.4	147

198	Metallization and superconductivity of BeH2 under high pressure. *Journal of Chemical Physics*, **2014**, 140, 124707	3.9	39
197	Perspective: crystal structure prediction at high pressures. *Journal of Chemical Physics*, **2014**, 140, 040901	3.9	116
196	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. *Nature Chemistry*, **2014**, 6, 644-8	17.6	314
195	Self-assembled ultrathin nanotubes on diamond (100) surface. *Nature Communications*, **2014**, 5, 3666	17.4	133
194	Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen. *Journal of Physical Chemistry C*, **2014**, 118, 11902-11905	3.8	7
193	Exploring the high pressure behavior of 2D and quasi-3D boron layers in MoB2. *RSC Advances*, **2014**, 4, 52878-52882	3.7	3
192	Pressure-induced isostructural phase transition in CaB4. *RSC Advances*, **2014**, 4, 42523-42529	3.7	3
191	Carbon coated face-centered cubic Ru-C nanoalloys. *Nanoscale*, **2014**, 6, 10370-6	7.7	16
190	Prediction of silicon-based layered structures for optoelectronic applications. *Journal of the American Chemical Society*, **2014**, 136, 15992-7	16.4	36
189	Two dimensional Dirac carbon allotropes from graphene. *Nanoscale*, **2014**, 6, 1113-8	7.7	147
188	B38: an all-boron fullerene analogue. *Nanoscale*, **2014**, 6, 11692-6	7.7	127
187	The metallization and superconductivity of dense hydrogen sulfide. *Journal of Chemical Physics*, **2014**, 140, 174712	3.9	481
186	High-pressure phase transition of cesium chloride and cesium bromide. *Physical Chemistry Chemical Physics*, **2014**, 16, 17924-9	3.6	11
185	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. *Chemical Science*, **2014**, 5, 3936-3940	9.4	19
184	Structural and mechanical properties of platinum carbide. *Inorganic Chemistry*, **2014**, 53, 5797-802	5.1	16
183	A Stable, Magnetic, and Metallic Li3O4 Compound as a Discharge Product in a Li-Air Battery. *Journal of Physical Chemistry Letters*, **2014**, 5, 2516-21	6.4	48
182	Acoustic waves and phonon focus in Li crystal: the first principle study. *European Physical Journal B*, **2014**, 87, 1	1.2	3
181	Exploring Hardness and the Distorted sp2 Hybridization of B–B Bonds in WB3. *Chemistry of Materials*, **2014**, 26, 5297-5302	9.6	59

180	The effect of oxygen vacancy on the half-metallic nature of double perovskite Sr2FeMoO6: A theoretical study. *Solid State Communications*, **2014**, 177, 57-60	1.6	20
179	Nanotwinned diamond with unprecedented hardness and stability. *Nature*, **2014**, 510, 250-3	50.4	440
178	Oxygen-doped boron nitride nanosheets with excellent performance in hydrogen storage. *Nano Energy*, **2014**, 6, 219-224	17.1	170
177	Unexpected room-temperature ferromagnetism in nanostructured Bi2Te3. *Angewandte Chemie - International Edition*, **2014**, 53, 729-33	16.4	31
176	Spectroscopic and Computational Characterizations of Alkaline-Earth- and Heavy-Metal-Exchanged Natrolites. *ChemPlusChem*, **2014**, 79, 1096-1102	2.8	3
175	Inter- and Intralayer Compression of Germanane. *Journal of Physical Chemistry C*, **2014**, 118, 28196-28201	3.8	7
174	Orientation dependence of elastic constants and electronic properties of rhenium nitrides first-principle calculations. *Journal of Materials Science*, **2013**, 48, 4284-4296	4.3	6
173	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. *Journal of Physical Chemistry C*, **2013**, 117, 5352-5357	3.8	35
172	Elastic anisotropy and phonon focusing in NiAl: Atomic study. *Intermetallics*, **2013**, 42, 156-164	3.5	5
171	Nanocrystalline tungsten hydrides at high pressures. *Physical Review B*, **2013**, 87,	3.3	28
170	Structural evolution of carbon dioxide under high pressure. *Journal of the American Chemical Society*, **2013**, 135, 14167-71	16.4	101
169	Exploring High-Pressure Lithium Beryllium Hydrides: A New Chemical Perspective. *Journal of Physical Chemistry C*, **2013**, 117, 13879-13886	3.8	22
168	Proton or deuteron transfer in phase IV of solid hydrogen and deuterium. *Physical Review Letters*, **2013**, 110, 025903	7.4	57
167	Enhanced Vickers hardness by quasi-3D boron network in MoB2. *RSC Advances*, **2013**, 3, 18317	3.7	42
166	Ultrahard nanotwinned cubic boron nitride. *Nature*, **2013**, 493, 385-8	50.4	519
165	Magnetism and thermodynamic properties of a spin-1/2 ferrimagnetic diamond XY chain in magnetic fields at finite temperatures. *Journal of the Korean Physical Society*, **2013**, 62, 104-115	0.6	1
164	Global structural optimization of tungsten borides. *Physical Review Letters*, **2013**, 110, 136403	7.4	216
163	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. *Journal of Physical Chemistry C* , **2013**, 117, 12266-12271	3.8	24

162	Anomalous Melting Behavior of Solid Hydrogen at High Pressures. *Journal of Physical Chemistry C*, **2013**, 117, 11873-11877	3.8	10
161	First-principles structural design of superhard materials. *Journal of Chemical Physics*, **2013**, 138, 114101	3.9	151
160	Stabilization of 9/10-Fold Structure in Bismuth Selenide at High Pressures. *Journal of Physical Chemistry C*, **2013**, 117, 10045-10050	3.8	38
159	Pressure induced phase transitions in TiH2. *Journal of Applied Physics*, **2013**, 113, 103512	2.5	14
158	One-Dimensional Al4O4C Ceramics: A New Type of Blue Light Emitter. *Scientific Reports*, **2013**, 3,	4.9	17
157	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. *Physical Review B*, **2013**, 88,	3.3	52
156	Tian et al. reply. *Nature*, **2013**, 502, E2-3	50.4	10
155	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. *Journal of Physical Chemistry C*, **2013**, 117, 8437-8442	3.8	15
154	Dynamic nano-pulling effect of the boron-functionalized graphene monovacancy for molecule dissociation. *Journal Physics D: Applied Physics*, **2013**, 46, 385302	3	7
153	Pressure-Induced Formation of Noble Metal Hydrides. *Journal of Physical Chemistry C*, **2012**, 116, 1995-2000	3.8	42
152	Modulated structure and molecular dissociation of solid chlorine at high pressures. *Journal of Chemical Physics*, **2012**, 137, 064502	3.9	16
151	Size-dependent phase transition of graphite to superhard graphite under high pressure at room temperature. *Journal of Applied Physics*, **2012**, 112, 103707	2.5	4
150	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. *Journal of Chemical Physics*, **2012**, 137, 224108	3.9	223
149	High pressure structures of "111" type iron-based superconductors predicted from first-principles. *Physical Chemistry Chemical Physics*, **2012**, 14, 15029-35	3.6	15
148	Lattice instability and martensitic transformation in LaAg predicted from first-principles theory. *Journal of Physics Condensed Matter*, **2012**, 24, 075402	1.8	5
147	Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures. *Journal of Chemical Physics*, **2012**, 137, 184502	3.9	13
146	A novel low compressible and superhard carbon nitride: body-centered tetragonal CN2. *Physical Chemistry Chemical Physics*, **2012**, 14, 13081-7	3.6	91
145	Cagelike diamondoid nitrogen at high pressures. *Physical Review Letters*, **2012**, 109, 175502	7.4	139

144	Superconductive sodalite-like clathrate calcium hydride at high pressures. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 6463-6	11.5	449
143	Spiral chain O form of dense oxygen. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 751-3	11.5	104
142	High-pressure and high-temperature phase transitions in FeTiO3 and a new dense FeTi3O7 structure. *American Mineralogist*, **2012**, 97, 568-572	2.9	36
141	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. *Journal of Physical Chemistry C*, **2012**, 116, 9221-9226	3.8	67
140	Crystal structures, stability, electronic and elastic properties of 4d and 5d transition metal monoborides: First-principles calculations. *Journal of Alloys and Compounds*, **2012**, 538, 115-124	5.7	15
139	Predicted lithium-boron compounds under high pressure. *Journal of the American Chemical Society*, **2012**, 134, 18599-605	16.4	93
138	Synthesis and high-pressure transformation of metastable wurtzite-structured CuGaS2 nanocrystals. *Nanoscale*, **2012**, 4, 7443-7	7.7	32
137	Particle-swarm structure prediction on clusters. *Journal of Chemical Physics*, **2012**, 137, 084104	3.9	340
136	Determinations of the high-pressure crystal structures of Sb2Te3. *Journal of Physics Condensed Matter*, **2012**, 24, 475403	1.8	33
135	Polymorphism and Formation Mechanism of Nanobipods in Manganese Sulfide Nanocrystals Induced by Temperature or Pressure. *Journal of Physical Chemistry C*, **2012**, 116, 3292-3297	3.8	39
134	High-pressure structures and metallization of sodium chloride. *Europhysics Letters*, **2012**, 100, 26005	1.6	12
133	Tetragonal allotrope of group 14 elements. *Journal of the American Chemical Society*, **2012**, 134, 12362-5	16.4	146
132	CALYPSO: A method for crystal structure prediction. *Computer Physics Communications*, **2012**, 183, 2063-2070	4.2	1464
131	Room-temperature structures of solid hydrogen at high pressures. *Journal of Chemical Physics*, **2012**, 137, 074501	3.9	64
130	Ab initio study revealing a layered structure in hydrogen-rich KH6 under high pressure. *Physical Review B*, **2012**, 86,	3.3	63
129	Properties and order-disorder competition of spin-1/2 XY model in the ferrimagnetic diamond chain. *Wuli Xuebao/Acta Physica Sinica*, **2012**, 61, 187502	0.6	
128	Predicting two-dimensional boron-carbon compounds by the global optimization method. *Journal of the American Chemical Society*, **2011**, 133, 16285-90	16.4	209
127	Substitutional alloy of Bi and Te at high pressure. *Physical Review Letters*, **2011**, 106, 145501	7.4	318

126	Electronic and dynamical properties of NiAl studied from first principles. *Intermetallics*, **2011**, 19, 1959-1967	3.5	45
125	First-principles study of phase transitions in antiferromagnetic □(, Co and Ni). *Solid State Communications*, **2011**, 151, 1475-1478	1.6	8
124	Phase transition of cadmium fluoride under high pressure. *Solid State Communications*, **2011**, 151, 1899-1902	1.6	11
123	Lattice dynamics and elastic properties of the 4f electron system: CeN. *Physical Review B*, **2011**, 84,	3.3	29
122	Exotic high pressure behavior of light alkali metals, lithium and sodium. *European Physical Journal B* , **2011**, 81, 1-14	1.2	56
121	High pressure partially ionic phase of water ice. *Nature Communications*, **2011**, 2, 563	17.4	201
120	Predicted novel high-pressure phases of lithium. *Physical Review Letters*, **2011**, 106, 015503	7.4	429
119	B 2 CO: A potential superhard material in the B-C-O system. *Europhysics Letters*, **2011**, 95, 66006	1.6	34
118	Carbon-in-Al4C3 nanowire superstructures for field emitters. *ACS Nano*, **2011**, 5, 932-41	16.7	38
117	Atomistic Design of High Thermoelectricity on Si/Ge Superlattice Nanowires. *Journal of Physical Chemistry C*, **2011**, 115, 20696-20702	3.8	25
116	Determination of structures, stabilities, and electronic properties for bimetallic cesium-doped gold clusters: a density functional theory study. *Journal of Physical Chemistry A*, **2011**, 115, 9273-81	2.8	40
115	Superhard phases of B2O: An isoelectronic compound of diamond. *Diamond and Related Materials*, **2011**, 20, 501-504	3.5	14
114	Superhard and superconductive polymorphs of diamond-like BC3. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2011**, 375, 771-774	2.3	53
113	Crystal structures of under high pressure. *Solid State Communications*, **2011**, 151, 388-391	1.6	10
112	Superhard polymorphs of diamond-like BC7. *Solid State Communications*, **2011**, 151, 716-719	1.6	34
111	Metallic and superconducting gallane under high pressure. *Physical Review B*, **2011**, 84,	3.3	58
110	Pressure-induced amorphization in mayenite (12CaO□7Al2O3). *Journal of Chemical Physics*, **2011**, 135, 094506	3.9	9
109	Comment on "Pressure-dependent metallic and superconducting phases in a germanium artificial metal". *Physical Review Letters*, **2010**, 104, 139701; author reply 139702	7.4	1

108	Order-disorder phase transition and dissociation of hydrogen sulfide under high pressure: ab initio molecular dynamics study. *Journal of Chemical Physics*, **2010**, 132, 164506	3.9	16
107	Novel high pressure structures and superconductivity of CaLi2. *Physical Review Letters*, **2010**, 104, 177005	7.4	54
106	High-pressure phase transitions in NiAs-type compounds from first-principles calculations. *Physical Review B*, **2010**, 81,	3.3	17
105	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
104	Superhard and superconducting structures of BC5. *Journal of Applied Physics*, **2010**, 108, 023507	2.5	60
103	Structural Modifications and Mechanical Properties of Molybdenum Borides from First Principles. *Journal of Physical Chemistry C*, **2010**, 114, 6722-6725	3.8	125
102	Structural Investigation of Solid Methane at High Pressure. *Chinese Physics Letters*, **2010**, 27, 066101	1.8	1
101	Orientationally disordered H2 in the high-pressure van der Waals compound SiH4(H2)2. *Physical Review B*, **2010**, 82,	3.3	20
100	High Thermoelectric Performance of Ge/Si Core−Shell Nanowires: First-Principles Prediction. *Journal of Physical Chemistry C*, **2010**, 114, 9096-9100	3.8	34
99	Raman Scattering Study of AlN Nanowires under High Pressure. *Journal of Physical Chemistry C*, **2010**, 114, 8241-8244	3.8	7
98	Superconductivity at approximately 100 K in dense SiH4(H2)2 predicted by first principles. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 15708-11	11.5	121
97	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
96	Superconducting high-pressure phases of disilane. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 9969-73	11.5	91
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