Alfonso Munoz

List of Publications by Citations

276 papers	7,700 citations	46 h-index	73 g-index
296 ext. papers	8,595 ext. citations	3.3 avg, IF	5.72 L-index

#	Paper	IF	Citations
276	High-pressure phases of group-IV, III-V, and II-VI compounds. *Reviews of Modern Physics*, **2003**, 75, 863-912	40.5	815
275	Theoretical study of the relative stability of structural phases in group-III nitrides at high pressures. *Physical Review B*, **2000**, 62, 16612-16623	3.3	183
274	High-pressure structural study of the scheelite tungstates CaWO4 and SrWO4. *Physical Review B*, **2005**, 72,	3.3	152
273	Optical properties and electronic structure of rock-salt ZnO under pressure. *Applied Physics Letters*, **2003**, 83, 278-280	3.4	138
272	The electronic structure of zircon-type orthovanadates: Effects of high-pressure and cation substitution. *Journal of Applied Physics*, **2011**, 110, 043723	2.5	132
271	Elastic constants and electronic structure of beryllium chalcogenides BeS, BeSe, and BeTefrom first-principles calculations. *Physical Review B*, **1997**, 55, 14043-14046	3.3	117
270	Structural and vibrational study of Bi2Se3 under high pressure. *Physical Review B*, **2011**, 84,	3.3	115
269	Comment on "High-pressure x-ray diffraction study of YBO3/Eu3+, GdBO3, and EuBO3: Pressure-induced amorphization in GdBO3" [J. Appl. Phys. 115, 043507 (2014)]. *Journal of Applied Physics*, **2014**, 115, 216101	2.5	113
268	Electronic and structural properties of cubic BN and BP. *Physical Review B*, **1995**, 51, 14705-14708	3.3	111
267	Pressure effects on the electronic and optical properties of AWO4 wolframites (A = Cd, Mg, Mn, and Zn): The distinctive behavior of multiferroic MnWO4. *Physical Review B*, **2012**, 86,	3.3	96
266	Temperature dependence of band gaps in semiconductors: Electron-phonon interaction. *Physical Review B*, **2012**, 86,	3.3	88
265	Determination of the high-pressure crystal structure of BaWO4 and PbWO4. *Physical Review B*, **2006**, 73,	3.3	88
264	Pressure and temperature dependence of the lattice dynamics of CuAlO2 investigated by Raman scattering experiments and ab initio calculations. *Physical Review B*, **2006**, 74,	3.3	87
263	High-pressure phase of gallium nitride. *Physical Review B*, **1991**, 44, 10372-10373	3.3	87
262	Lattice dynamics study of scheelite tungstates under high pressure I. BaWO4. *Physical Review B*, **2006**, 74,	3.3	85
261	High-pressure vibrational and optical study of Bi2Te3. *Physical Review B*, **2011**, 84,	3.3	83
260	Lattice dynamics of Sb2Te3 at high pressures. *Physical Review B*, **2011**, 84,	3.3	81

259	High-pressure x-ray diffraction and ab initio study of Ni2Mo3N, Pd2Mo3N, Pt2Mo3N, Co3Mo3N, and Fe3Mo3N: Two families of ultra-incompressible bimetallic interstitial nitrides. *Physical Review B* , **2010**, 82,	3.3	80
258	Combined Raman scattering and ab initio investigation of pressure-induced structural phase transitions in the scintillator ZnWO4. *Physical Review B*, **2008**, 78,	3.3	80
257	On the band gap of CuAlO2 delafossite. *Applied Physics Letters*, **2006**, 88, 181904	3.4	79
256	Theoretical and Experimental Study of the Crystal Structures, Lattice Vibrations, and Band Structures of Monazite-Type PbCrO4, PbSeO4, SrCrO4, and SrSeO4. *Inorganic Chemistry*, **2015**, 54, 7524-35	3.1	78
255	First-principles pseudopotential study of the phase stability of the III-V semiconductors GaAs and AlAs. *Physical Review B*, **1995**, 52, 8881-8892	3.3	78
254	Electronic, vibrational, and thermodynamic properties of metacinnabar HgS, HgSe, and HgTe. *Physical Review B*, **2009**, 80,	3.3	75
253	Zircon to monazite phase transition in CeVO4: X-ray diffraction and Raman-scattering measurements. *Physical Review B*, **2011**, 84,	3.3	71
252	A combined high-pressure experimental and theoretical study of the electronic band-structure of scheelite-type AWO4 (A = Ca, Sr, Ba, Pb) compounds. *Journal of Applied Physics*, **2011**, 110, 043703	2.5	68
251	Ground-state properties and high-pressure phase of beryllium chalcogenides BeSe, BeTe, and BeS. *Physical Review B*, **1996**, 54, 11861-11864	3.3	66
250	Structural evolution of the CuGaO2 delafossite under high pressure. *Physical Review B*, **2004**, 69,	3.3	63
249	Phase transitions in wolframite-type CdWO4 at high pressure studied by Raman spectroscopy and density-functional theory. *Physical Review B*, **2009**, 79,	3.3	62
248	High-pressure studies of topological insulators Bi2Se3, Bi2Te3, and Sb2Te3. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 669-676	1.3	61
247	High-pressure Raman spectroscopy and lattice-dynamics calculations on scintillating MgWO4: Comparison with isomorphic compounds. *Physical Review B*, **2011**, 83,	3.3	61
246	High-pressure structural phase transitions in CuWO4. *Physical Review B*, **2010**, 81,	3.3	60
245	Experimental and theoretical investigations on the polymorphism and metastability of BiPO4. *Dalton Transactions*, **2013**, 42, 14999-5015	4.3	56
244	High-pressure phase transitions and compressibility of wolframite-type tungstates. *Journal of Applied Physics*, **2010**, 107, 083506	2.5	54
243	Lattice dynamics of YVO4 at high pressures. *Physical Review B*, **2010**, 81,	3.3	52
242	Structural, Vibrational, and Electronic Study of Sb2S3 at High Pressure. *Journal of Physical Chemistry C*, **2016**, 120, 10547-10558	3.8	52

241	Isostructural Second-Order Phase Transition of Bi2O3 at High Pressures: An Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2014**, 118, 23189-23201	3.8	50
240	Structural and dielectric properties of AlN under pressure. *Physica B: Condensed Matter*, **2008**, 403, 4059-4062	1.8	50
239	Exploring the high-pressure behavior of the three known polymorphs of BiPO4: Discovery of a new polymorph. *Journal of Applied Physics*, **2015**, 117, 105902	2.5	49
238	High-pressure lattice dynamical study of bulk and nanocrystalline In2O3. *Journal of Applied Physics*, **2012**, 112, 123511	2.5	49
237	Synthesis, structure and luminescence of Er3+-doped Y3Ga5O12 nano-garnets. *Journal of Materials Chemistry*, **2012**, 22, 13788		49
236	High-pressure study of ScVO4 by Raman scattering and ab initio calculations. *Physical Review B*, **2011**, 83,	3.3	49
235	First-principles study of the high-pressure phase transition in ZnAl2O4 and ZnGa2O4: From cubic spinel to orthorhombic post-spinel structures. *Physical Review B*, **2009**, 79,	3.3	49
234	High-pressure structural behaviour of HoVO4: combined XRD experiments and ab initio calculations. *Journal of Physics Condensed Matter*, **2014**, 26, 265402	1.8	47
233	First-principles study of high-pressure phonon dispersions of wurtzite, zinc-blende, and rocksalt AlN. *Journal of Applied Physics*, **2008**, 103, 013506	2.5	47
232	Lattice dynamics study of scheelite tungstates under high pressure II. PbWO4. *Physical Review B*, **2006**, 74,	3.3	47
231	High-Pressure Crystal Structure, Lattice Vibrations, and Band Structure of BiSbO4. *Inorganic Chemistry*, **2016**, 55, 4958-69	5.1	47
230	Tuning the band gap of PbCrO4 through high-pressure: Evidence of wide-to-narrow semiconductor transitions. *Journal of Alloys and Compounds*, **2014**, 587, 14-20	5.7	46
229	Structural stability of Fe5Si3 and Ni2Si studied by high-pressure x-ray diffraction and ab initio total-energy calculations. *Physical Review B*, **2008**, 77,	3.3	46
228	Ab initio lattice dynamics and piezoelectric properties of MgS and MgSe alkaline earth chalcogenides. *European Physical Journal B*, **2010**, 73, 185-193	1.2	45
227	Theoretical Study of the Elastic Properties of IIIP Compounds. *Physica Status Solidi (B): Basic Research*, **2001**, 223, 411-415	1.3	45
226	Electronic and Structural Properties of BeSe, BeTe, and BeS: Comparison between ab-initio Theory and Experiments. *Physica Status Solidi (B): Basic Research*, **1996**, 198, 439-446	1.3	45
225	K/Si(100) 2 1: A Case Study for the Transfer of Charge between Alkali Metals and Semiconductor Surfaces. *Europhysics Letters*, **1988**, 5, 727-732	1.6	44
224	First-principles calculation of the elastic constants of AlAs. *Physical Review B*, **1989**, 40, 11934-11936	3.3	42

223	Theoretical and experimental study of the structural stability of TbPO4 at high pressures. *Physical Review B*, **2010**, 81,	3.3	40
222	Structure and static properties of indium nitride at low and moderate pressures. *Journal of Physics Condensed Matter*, **1993**, 5, 6015-6022	1.8	40
221	High-pressure polymorphs of TbVO4: A Raman and ab initio study. *Journal of Alloys and Compounds*, **2013**, 577, 327-335	5.7	39
220	Heterojunction valence-band-discontinuity dependence on face orientation. *Physical Review B*, **1987**, 35, 6468-6470	3.3	39
219	Crystal Chemistry of CdIn2S4, MgIn2S4, and MnIn2S4 Thiospinels under High Pressure. *Journal of Physical Chemistry C*, **2012**, 116, 14078-14087	3.8	38
218	Optical properties of wurtzite and rock-salt ZnO under pressure. *Microelectronics Journal*, **2005**, 36, 928-932	1.8	37
217	High-pressure optical and vibrational properties of CdGa2Se4: Order-disorder processes in adamantine compounds. *Journal of Applied Physics*, **2012**, 111, 013518	2.5	36
216	Lattice dynamics of ZnAl2O4 and ZnGa2O4 under high pressure. *Annalen Der Physik*, **2011**, 523, 157-167	2.6	36
215	Experimental and theoretical study of structural properties and phase transitions in YAsO4 and YCrO4. *Physical Review B*, **2011**, 83,	3.3	36
214	Phase Stability of Lanthanum Orthovanadate at High Pressure. *Journal of Physical Chemistry C*, **2016**, 120, 13749-13762	3.8	36
213	Electronic structure of CuAlO2 and CuScO2 delafossites under pressure. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 309-314	1.3	33
212	Experimental and Theoretical Study of Bi2O2Se Under Compression. *Journal of Physical Chemistry C* , **2018**, 122, 8853-8867	3.8	32
211	First-principles study of electronic, vibrational, elastic, and magnetic properties of FeF2 as a function of pressure. *Physical Review B*, **2012**, 85,	3.3	32
210	High-pressure phase transformations, pressure-induced amorphization, and polyamorphic transition of the clathrate Rb6.15Si46. *Physical Review B*, **2009**, 79,	3.3	32
209	AlX (X = As, P, Sb) Compounds under Pressure. *Physica Status Solidi (B): Basic Research*, **1999**, 211, 39-43	1.3	32
208	Semiconductor interface formation: The role of the induced density of interface states. *Applied Surface Science*, **1990**, 41-42, 144-150	6.7	32
207	High-pressure structural, elastic, and thermodynamic properties of zircon-type HoPO and TmPO. *Journal of Physics Condensed Matter*, **2017**, 29, 095401	1.8	31
206	Theoretical study of the cinnabar phases in GaAs and GaP. *Physical Review B*, **1998**, 57, 1344-1347	3.3	31

205	Ab initio calculations of electronic structure and elastic constants in AlP. *Semiconductor Science and Technology*, **1992**, 7, 1437-1440	1.8	31
204	Lattice Dynamics Study of Nanocrystalline Yttrium Gallium Garnet at High Pressure. *Journal of Physical Chemistry C*, **2014**, 118, 13177-13185	3.8	30
203	First-principles study of lithium-doped carbon clathrates under pressure. *Journal of Physics Condensed Matter*, **2008**, 20, 215218	1.8	30
202	Crystal stability and pressure-induced phase transitions in scheelite AWO4 (A = Ca, Sr, Ba, Pb, Eu) binary oxides. II: Towards a systematic understanding. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 295-302	1.3	30
201	Electronic, vibrational, and thermodynamic properties of ZnS with zinc-blende and rocksalt structure. *Physical Review B*, **2010**, 81,	3.3	28
200	Crystal stability and pressure-induced phase transitions in scheelite AWO4 (A = Ca, Sr, Ba, Pb, Eu) binary oxides. I: A review of recent ab initio calculations, ADXRD, XANES, and Raman studies. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 325-330	1.3	28
199	Theoretical study of the pressure-induced structural phase transition of ScSb and YSb. *International Journal of Quantum Chemistry*, **2005**, 101, 770-773	2.1	28
198	High-pressure characterization of the optical and electronic properties of InVO4, InNbO4, and InTaO4. *SN Applied Sciences*, **2019**, 1, 1	1.8	27
197	Pressure-induced phase transition and band-gap collapse in the wide-band-gap semiconductor InTaO4. *Physical Review B*, **2016**, 93,	3.3	27
196	Structural study of □Bi2O3 under pressure. *Journal of Physics Condensed Matter*, **2013**, 25, 475402	1.8	27
195	Polymorphs of CaSeO4 under pressure: a first-principles study of structural, electronic, and vibrational properties. *Inorganic Chemistry*, **2015**, 54, 1765-77	5.1	27
194	Effects of pressure on the structure and lattice dynamics of TmPO4: Experiments and calculations. *Physical Review B*, **2012**, 85,	3.3	27
193	Trapping of three-dimensional electrons and transition to two-dimensional transport in the three-dimensional topological insulator Bi2Se3 under high pressure. *Physical Review B*, **2012**, 85,	3.3	27
192	Early Stages of GaAs-Ge(110) Interface Formation. *Europhysics Letters*, **1986**, 2, 385-391	1.6	27
191	Chemical pressure effects on the spectroscopic properties of Nd^3+-doped gallium nano-garnets. *Optical Materials Express*, **2015**, 5, 1661	2.6	26
190	Monazite-type SrCrO4 under compression. *Physical Review B*, **2016**, 94,	3.3	26
189	High-pressure Raman scattering of CaWO□up to 46.3 GPa: evidence of a new high-pressure phase. *Inorganic Chemistry*, **2014**, 53, 9729-38	5.1	26
188	Ab initiostudy of the phase transformations of ZnSe under high pressure: stability of the cinnabar and SC16 phases. *Journal of Physics Condensed Matter*, **2000**, 12, 1705-1713	1.8	26

187	Structural and elastic properties of defect chalcopyrite HgGa2S4 under high pressure. *Journal of Alloys and Compounds*, **2014**, 583, 70-78	5.7	25
186	Pressure-Driven Isostructural Phase Transition in InNbO: In Situ Experimental and Theoretical Investigations. *Inorganic Chemistry*, **2017**, 56, 5420-5430	5.1	24
185	Pbca-Type In2O3: The High-Pressure Post-Corundum phase at Room Temperature.. *Journal of Physical Chemistry C*, **2014**, 118, 20545-20552	3.8	24
184	High-pressure study of the structural and elastic properties of defect-chalcopyrite HgGa2Se4. *Journal of Applied Physics*, **2013**, 113, 073510	2.5	24
183	Nonlinear pressure dependence of the direct band gap in adamantine ordered-vacancy compounds. *Physical Review B*, **2010**, 81,	3.3	24
182	Theoretical and experimental study of CaWO4 and SrWO4 under pressure. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 2164-2171	3.9	24
181	Ordered helium trapping and bonding in compressed arsenolite: Synthesis of As4O6□2He. *Physical Review B*, **2016**, 93,	3.3	23
180	Pressure-induced phase-transition sequence in CoF2: An experimental and first-principles study on the crystal, vibrational, and electronic properties. *Physical Review B*, **2013**, 88,	3.3	23
179	Relative Stability of Calcium Chalcogenides from Ab initio Theory. *High Pressure Research*, **2002**, 22, 459-463	1.6	23
178	Polymorphism in Strontium Tungstate SrWO under Quasi-Hydrostatic Compression. *Inorganic Chemistry*, **2016**, 55, 10406-10414	5.1	22
177	Experimental and Theoretical Studies on □nSe at High Pressure. *Inorganic Chemistry*, **2018**, 57, 8241-8252	5.1	22
176	Broadband, site selective and time resolved photoluminescence spectroscopic studies of finely size-modulated Y2O3:Eu3+ phosphors synthesized by a complex based precursor solution method. *Current Applied Physics*, **2014**, 14, 72-81	2.6	21
175	Optical nanothermometer based on the calibration of the Stokes and upconverted green emissions of Er3+ ions in Y3Ga5O12 nano-garnets. *RSC Advances*, **2014**, 4, 57691-57701	3.7	21
174	Phase Behavior of Ag2CrO4 under Compression: Structural, Vibrational, and Optical Properties. *Journal of Physical Chemistry C*, **2013**, 117, 12239-12248	3.8	21
173	Electronic and phononic properties of cinnabar: Ab initio calculations and some experimental results. *Physical Review B*, **2010**, 82,	3.3	21
172	First-principles calculations of electronic, vibrational, and structural properties of scheelite EuWO4 under pressure. *Physical Review B*, **2011**, 84,	3.3	21
171	Ab initiolattice dynamics of zinc-blende GaxIn1□N alloys. *Journal of Physics Condensed Matter*, **2007**, 19, 486209	1.8	21
170	High-pressure lattice-dynamics of NdVO4. *Journal of Physics and Chemistry of Solids*, **2017**, 100, 126-133	3.9	20

169	Lattice dynamics properties of zinc-blende and Nickel arsenide phases of AlP. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 5340-5345	2.3	20
168	Experimental and theoretical study on the optical properties of LaVO crystals under pressure. *Physical Chemistry Chemical Physics*, **2018**, 20, 27314-27328	3.6	20
167	ScVO under non-hydrostatic compression: a new metastable polymorph. *Journal of Physics Condensed Matter*, **2017**, 29, 055401	1.8	19
166	Structural, vibrational, and electrical study of compressed BiTeBr. *Physical Review B*, **2016**, 93,	3.3	19
165	Structural and electrical study of the topological insulator SnBi2Te4 at high pressure. *Journal of Alloys and Compounds*, **2016**, 685, 962-970	5.7	19
164	Compressibility Systematics of Calcite-Type Borates: An Experimental and Theoretical Structural Study on ABO3 (A = Al, Sc, Fe, and In). *Journal of Physical Chemistry C*, **2014**, 118, 4354-4361	3.8	19
163	Lattice Dynamics Study of HgGa2Se4 at High Pressures. *Journal of Physical Chemistry C*, **2013**, 117, 15773-15781	3.8	19
162	Experimental and theoretical investigation of the stability of the monoclinic BaWO4-II phase at high pressure and high temperature. *Physical Review B*, **2010**, 81,	3.3	19
161	Comparative Study of Novel Structures in Silicon and Germanium. *Physica Status Solidi (B): Basic Research*, **2001**, 223, 379-384	1.3	19
160	Correspondence: Strongly-driven Re+CO redox reaction at high-pressure and high-temperature. *Nature Communications*, **2016**, 7, 13647	17.4	19
159	Stability and nature of the volume collapse of ε-FeO under extreme conditions. *Nature Communications*, **2018**, 9, 4554	17.4	19
158	First-Principles Study of InVO under Pressure: Phase Transitions from CrVO- to AgMnO-Type Structure. *Inorganic Chemistry*, **2017**, 56, 2697-2711	5.1	18
157	High pressure luminescence of Nd in YAlO perovskite nanocrystals: A crystal-field analysis. *Journal of Chemical Physics*, **2018**, 148, 044201	3.9	18
156	Pressure-induced phase transformation in zircon-type orthovanadate SmVO4 from experiment and theory. *Journal of Physics Condensed Matter*, **2016**, 28, 035402	1.8	18
155	Vibrational study of HgGa2S4 under high pressure. *Journal of Applied Physics*, **2013**, 113, 093512	2.5	18
154	High-pressure transition to the post-barite phase in BaCrO4 hashemite. *Physical Review B*, **2012**, 86,	3.3	18
153	The simultaneous low state spectral energy distribution of 1ES 2344+514 from radio to very high energies. *Astronomy and Astrophysics*, **2013**, 556, A67	5.1	18
152	Experimental and Theoretical Investigations on Structural and Vibrational Properties of Melilite-Type Sr2ZnGe2O7 at High Pressure and Delineation of a High-Pressure Monoclinic Phase. *Inorganic Chemistry*, **2015**, 54, 6594-605	5.1	17

151	Experimental and ab Initio Study of Catena(bis(μ2-iodo)-6-methylquinoline-copper(I)) under Pressure: Synthesis, Crystal Structure, Electronic, and Luminescence Properties. *Inorganic Chemistry* , **2016**, 55, 7476-84	5.1	17
150	Exploring the Chemical Reactivity between Carbon Dioxide and Three Transition Metals (Au, Pt, and Re) at High-Pressure, High-Temperature Conditions. *Inorganic Chemistry*, **2016**, 55, 10793-10799	5.1	17
149	Stability of FeVO under Pressure: An X-ray Diffraction and First-Principles Study. *Inorganic Chemistry*, **2018**, 57, 7860-7876	5.1	17
148	Pressure effects on the vibrational properties of β-Bi(2)O(3): an experimental and theoretical study. *Journal of Physics Condensed Matter*, **2014**, 26, 225401	1.8	17
147	Crystal structure of HgGa2Se4 under compression. *Materials Research Bulletin*, **2013**, 48, 2128-2133	5.1	17
146	Optical and structural study of the pressure-induced phase transition of CdWO4. *Physical Review B*, **2017**, 95,	3.3	17
145	Raman scattering study of bulk and nanocrystalline PbMoO4 at high pressures. *Journal of Applied Physics*, **2012**, 112, 103510	2.5	17
144	Electronic and phononic properties of the chalcopyrite CuGaS2. *Physical Review B*, **2011**, 83,	3.3	17
143	First-principles description of atomic gold chains on Ge(001). *Physical Review B*, **2010**, 81,	3.3	17
142	Theoretical calculation for a ZnSe-Ge(110) heterojunction with an ultrathin intralayer. *Physical Review B*, **1987**, 35, 7721-7724	3.3	17
141	Synthesis and High-Pressure Study of Corundum-Type In2O3. *Journal of Physical Chemistry C*, **2015**, 119, 29076-29087	3.8	16
140	Electronic structure of p-type ultraviolet-transparent conducting CuScO2 films. *Thin Solid Films*, **2008**, 516, 1431-1433	2.2	16
139	On the interaction of compounds of chromium(VI) with hydrogen peroxide. A study of chromium(VI) and (V) peroxides in the acidBasic pH range. *Inorganica Chimica Acta*, **2002**, 331, 16-24	2.7	16
138	Stability and Structural Properties of ZnS and ZnSe under High Pressure. *Physica Status Solidi (B): Basic Research*, **2001**, 223, 417-422	1.3	16
137	Electronic Structure of Interfaces. *Physica Scripta*, **1987**, T19A, 102-108	2.6	16
136	Equation of state and electronic properties of EuVO4: A high-pressure experimental and computational study. *Journal of Alloys and Compounds*, **2015**, 648, 1005-1016	5.7	15
135	High-pressure structural and vibrational properties of monazite-type BiPO, LaPO, CePO, and PrPO. *Journal of Physics Condensed Matter*, **2018**, 30, 065401	1.8	15
134	Bi2O3 under compression: Optical and elastic properties and electron density topology analysis. *Physical Review B*, **2016**, 93,	3.3	15

133	Effect of High Pressure on the Crystal Structure and Vibrational Properties of Olivine-Type LiNiPO. *Inorganic Chemistry*, **2018**, 57, 10265-10276	5.1	15
132	High-pressure structural and elastic properties of Tl2O3. *Journal of Applied Physics*, **2014**, 116, 133521	2.5	15
131	Bond length compressibility in hard ReB2 investigated by x-ray absorption under high pressure. *Journal of Physics Condensed Matter*, **2010**, 22, 045701	1.8	15
130	Super-orbital variability of LS I +61□303 at TeV energies. *Astronomy and Astrophysics*, **2016**, 591, A76	5.1	15
129	Phase transition systematics in BiVO4 by means of high-pressure□high-temperature Raman experiments. *Physical Review B*, **2018**, 98,	3.3	15
128	Pressure-induced amorphization of YVO□Eu□+ nanoboxes. *Nanotechnology*, **2016**, 27, 025701	3.4	14
127	Characterization of the spin-12 linear-chain ferromagnet CuAs2O4. *Physical Review B*, **2014**, 89,	3.3	14
126	High-pressure Raman scattering study of defect chalcopyrite and defect stannite ZnGa2Se4. *Journal of Applied Physics*, **2013**, 113, 233501	2.5	14
125	Elastic modulus and thermal properties of InN in the rocksalt phase. *Computational Materials Science*, **2014**, 81, 374-377	3.2	14
124	Composition-dependent elastic modulus, vibration frequency and polaron properties of ZnSexTe1□ system. *Optical Materials*, **2013**, 35, 2303-2308	3.3	14
123	Band discontinuities for the (110)-interfaces of semiconductor heterojunctions. *Surface Science*, **1987**, 181, L200-L204	1.8	14
122	Orpiment under compression: metavalent bonding at high pressure. *Physical Chemistry Chemical Physics*, **2020**, 22, 3352-3369	3.6	14
121	First-principles study of pressure-induced structural phase transitions in MnF. *Physical Chemistry Chemical Physics*, **2016**, 18, 33250-33263	3.6	13
120	An Ultrahigh CO-Loaded Silicalite-1 Zeolite: Structural Stability and Physical Properties at High Pressures and Temperatures. *Inorganic Chemistry*, **2018**, 57, 6447-6455	5.1	13
119	A combined study of the equation of state of monazite-type lanthanum orthovanadate using in situ high-pressure diffraction and ab initio calculations. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2014**, 70, 533-8	1.8	13
118	Electronic and elastic properties of yttrium gallium garnet under pressure from ab initio studies. *Journal of Applied Physics*, **2013**, 113, 183505	2.5	13
117	Negative pressures in CaWO4 nanocrystals. *Journal of Applied Physics*, **2009**, 105, 094321	2.5	13
116	Theoretical study of the YLiF4 phase transitions under pressure. *Physical Review B*, **2006**, 73,	3.3	13

115	Resonant tunnelling of electrons through parabolic quantum wells: an analytical calculation of the transmission coefficient. *Semiconductor Science and Technology*, **1991**, 6, 218-222	1.8	13
114	A theoretical analysis of the heterojunction band offsets as controlled by intralayer deposition. *Surface Science*, **1989**, 211-212, 503-510	1.8	13
113	Heterojunction band offsets and the interface dielectric function. *Physical Review B*, **1987**, 36, 5920-5924	3.3	13
112	High-pressure behavior of CaMoO4. *Physical Review Materials*, **2017**, 1,	3.2	13
111	Structural, elastic and vibrational properties of nanocrystalline lutetium gallium garnet under high pressure. *Physical Chemistry Chemical Physics*, **2015**, 17, 9454-64	3.6	12
110	Equation of state of zircon- and scheelite-type dysprosium orthovanadates: a combined experimental and theoretical study. *Journal of Physics Condensed Matter*, **2014**, 26, 025401	1.8	12
109	On the thermodynamic stability of alpha,omega-alkanedithiols self-assembled monolayers on unreconstructed and reconstructed Au(111). *Langmuir*, **2010**, 26, 9589-95	4	12
108	Lattice dynamics of CuAlO2 under high pressure from ab initio calculations. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 342-346	1.3	12
107	Theoretical study of graphitic analogues of simple semiconductors. *Modelling and Simulation in Materials Science and Engineering*, **1999**, 7, 929-938	2	12
106	New phases and physical properties of the semiconducting nitrides: AlN, GaN, InN. *Computational Materials Science*, **1994**, 2, 400-412	3.2	12
105	Post-tilleyite, a dense calcium silicate-carbonate phase. *Scientific Reports*, **2019**, 9, 7898	4.9	11
104	High-Pressure Single-Crystal X-ray Diffraction of Lead Chromate: Structural Determination and Reinterpretation of Electronic and Vibrational Properties. *Inorganic Chemistry*, **2019**, 58, 5966-5979	5.1	11
103	Characterization and Decomposition of the Natural van der Waals SnSbTe under Compression. *Inorganic Chemistry*, **2020**, 59, 9900-9918	5.1	11
102	First-Order Isostructural Phase Transition Induced by High Pressure in Fe(IO3)3. *Journal of Physical Chemistry C*, **2020**, 124, 8669-8679	3.8	11
101	On the Control Parameters of the Quasi-One Dimensional Superconductivity in Sc3CoC4. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2013**, 639, 1985-1995	1.3	11
100	High-pressure structural and lattice dynamical study of HgWO4. *Physical Review B*, **2010**, 82,	3.3	11
99	Ab initio calculations of the wolframite MnWO4 under high pressure. *High Pressure Research*, **2009**, 29, 578-581	1.6	11
98	Lattice vibration spectrum of GaN from first-principle calculations. *Semiconductor Science and Technology*, **2009**, 24, 025007	1.8	11

97	Ab initio study of high-pressure structural properties of the LuVO4 and ScVO4 zircon-type orthovanadates. *High Pressure Research*, **2009**, 29, 582-586	1.6	11
96	High Pressure Stability in III-V and II-VI Binary Compounds and the Cmcm Phase A Theoretical Study. *Physica Status Solidi (B): Basic Research*, **1996**, 198, 461-467	1.3	11
95	First-principles elastic properties of BAs. *International Journal of Quantum Chemistry*, **2003**, 91, 191-196	2.1	10
94	Ab Initio Study of the Mechanical Stability Criteria in BeSe and BeTe under Hydrostatic Pressure. *Physica Status Solidi (B): Basic Research*, **1999**, 211, 23-28	1.3	10
93	High-pressure structural phase transition and electronic properties of the group-III nitrides. *Physica B: Condensed Matter*, **1993**, 185, 422-425	2.8	10
92	High-Pressure Raman Study of Fe(IO3)3: Soft-Mode Behavior Driven by Coordination Changes of Iodine Atoms. *Journal of Physical Chemistry C*, **2020**, 124, 21329-21337	3.8	10
91	Lattice dynamics study of cubic Tb2O3. *Journal of Raman Spectroscopy*, **2018**, 49, 2021-2027	2.3	10
90	High-pressure polymorphs of gadolinium orthovanadate: X-ray diffraction, Raman spectroscopy, and ab initio calculations. *Physical Review B*, **2019**, 100,	3.3	9
89	Structural and Lattice-Dynamical Properties of TbO under Compression: A Comparative Study with Rare Earth and Related Sesquioxides. *Inorganic Chemistry*, **2020**, 59, 9648-9666	5.1	9
88	Yttrium aluminium garnet under pressure: Structural, elastic, and vibrational properties from ab initio studies. *Journal of Applied Physics*, **2015**, 118, 245902	2.5	9
87	HgGa2Se4 under high pressure: An optical absorption study. *Physica Status Solidi (B): Basic Research* , **2015**, 252, 2043-2051	1.3	9
86	High Pressure Phases of AlSb from ab-initio Theory. *Physica Status Solidi (B): Basic Research*, **1996**, 198, 455-459	1.3	9
85	The effect of a metal intralayer on the heterojunction band offset: Extrinsic and intrinsic charge neutrality levels. *Surface Science*, **1990**, 226, 371-380	1.8	9
84	Experimental and Theoretical Study of SbPO under Compression. *Inorganic Chemistry*, **2020**, 59, 287-307	5.1	9
83	Structural and vibrational properties of corundum-type InO nanocrystals under compression. *Nanotechnology*, **2017**, 28, 205701	3.4	8
82	Gold(i) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. *Chemical Science*, **2019**, 10, 6467-6475	9.4	8
81	High pressure theoretical and experimental analysis of the bandgap of BaMoO4, PbMoO4, and CdMoO4. *Applied Physics Letters*, **2019**, 115, 012102	3.4	8
80	Thermally activated cation ordering in ZnGa2Se4 single crystals studied by Raman scattering, optical absorption, and ab initio calculations. *Journal of Physics Condensed Matter*, **2013**, 25, 165802	1.8	8

79	Structural, Vibrational, and Elastic Properties of Yttrium Orthoaluminate Nanoperovskite at High Pressures. *Journal of Physical Chemistry C*, **2017**, 121, 15353-15367	3.8	8
78	High pressure phase transitions in NdVO4 **2015**,		8
77	Ab initio study of the high-pressure phases and dynamical properties of ZnAl2O4 and ZnGa2O4. *High Pressure Research*, **2009**, 29, 573-577	1.6	8
76	Theoretical study of ZnS under high pressure. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 452-455	1.3	8
75	Electronic structure and optical properties of CdTe rock-salt high pressure phase. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 509-513	1.3	8
74	High-Pressure Cinnabar-Like Phases in III□V Compounds. *Physica Status Solidi (B): Basic Research*, **1999**, 211, 345-350	1.3	8
73	Elastic and thermodynamic properties of □Bi2O3 at high pressures: Study of mechanical and dynamical stability. *Journal of Physics and Chemistry of Solids*, **2019**, 124, 111-120	3.9	8
72	Structural and Vibrational Study of Pseudocubic CdIn2Se4under Compression. *Journal of Physical Chemistry C*, **2014**, 118, 26987-26999	3.8	7
71	Structural properties of zinc-blende GaxIn1-xN: ab initio calculations. *European Physical Journal B*, **2007**, 60, 435-438	1.2	7
70	Optical Properties of High Pressure Phases in ZnTe 1□x Se x. *High Pressure Research*, **2002**, 22, 315-318	1.6	7
69	Vibrational and elastic properties of As4O6 and As4O6□2He at high pressures: Study of dynamical and mechanical stability. *Journal of Applied Physics*, **2016**, 120, 155901	2.5	7
68	Structural and Vibrational Properties of CdAl2S4 under High Pressure: Experimental and Theoretical Approach. *Journal of Physical Chemistry C*, **2014**, 118, 15363-15374	3.8	6
67	Structural phases of InAs under pressure. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 274-278	1.3	6
66	High-pressure phases of germanium. *Journal of Physics Condensed Matter*, **2001**, 13, 35-42	1.8	6
65	Selfconsistent tight-binding calculations of band offsets in GaAs/AlxGa1□As-(110) and GaSb/AlxGa1□Sb-(110) heterojunctions theoretical evidence for a new common-anion rule. *Solid State Communications*, **1992**, 81, 961-963	1.6	6
64	InBO3 and ScBO3 at high pressures: An ab initio study of elastic and thermodynamic properties. *Journal of Physics and Chemistry of Solids*, **2016**, 98, 198-208	3.9	6
63	Phase Behavior of TmVO under Hydrostatic Compression: An Experimental and Theoretical Study. *Inorganic Chemistry*, **2020**, 59, 4882-4894	5.1	5
62	High-Pressure Elastic, Vibrational and Structural Study of Monazite-Type GdPO4 from Ab Initio Simulations. *Crystals*, **2018**, 8, 209	2.3	5

61	Putting the Squeeze on Lead Chromate Nanorods. *Journal of Physical Chemistry Letters*, **2019**, 10, 4744-4751	6.4	5
60	Effect of pressure on La2(WO4)3 with a modulated scheelite-type structure. *Physical Review B*, **2014**, 89,	3.3	5
59	Very high energy gamma-ray observation of the peculiar transient event Swift J1644+57 with the MAGIC telescopes and AGILE. *Astronomy and Astrophysics*, **2013**, 552, A112	5.1	5
58	A High-Pressure Investigation of the Synthetic Analogue of Chalcomenite, CuSeO3·H2O. *Crystals*, **2019**, 9, 643	2.3	5
57	Anomalous Raman modes in tellurides. *Journal of Materials Chemistry C*,	7.1	5
56	Structural and vibrational study of Zn(IO3)2 combining high-pressure experiments and density-functional theory. *Physical Review B*, **2021**, 103,	3.3	5
55	Electronic properties and high-pressure behavior of wolframite-type CoWO4. *Materials Advances*, **2021**, 2, 5955-5966	3.3	5
54	Vibrational properties of CdGa2S4 at high pressure. *Journal of Applied Physics*, **2019**, 125, 115901	2.5	4
53	Dense Post-Barite-type Polymorph of PbSO Anglesite at High Pressures. *Inorganic Chemistry*, **2019**, 58, 2708-2716	5.1	4
52	Crystal Structure of Sinhalite MgAlBO4 under High Pressure. *Journal of Physical Chemistry C*, **2015**, 119, 6777-6784	3.8	4
51	Experimental and theoretical study of Eu2(MoO4)3 under compression. *Journal of Physics Condensed Matter*, **2015**, 27, 465401	1.8	4
50	Ab initio study of BAs under pressure. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 446-451	1.3	4
49	TUNNELING ESCAPE TIME OF ELECTRONS FROM A PARABOLIC QUANTUM WELL IN DOUBLE BARRIER HETEROSTRUCTURES. *Modern Physics Letters B*, **1991**, 05, 293-300	1.6	4
48	Heterojunction band offsets for polar interfaces: From a thin to a thick covalent intralayer. *Physical Review B*, **1992**, 46, 9641-9647	3.3	4
47	Correlation effects in the Si(111) surface. *Surface Science*, **1985**, 152-153, 1027-1034	1.8	4
46	Anion-induced surface states for the ideal (100) faces of GaAs, AlAs and GaSb. *Surface Science*, **1986**, 172, 47-56	1.8	4
45	High-pressure monoclinic-monoclinic transition in fergusonite-type HoNbO. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	4
44	Giant conductivity enhancement: Pressure-induced semiconductor-metal phase transition in Cd0.90Zn0.1Te. *Physical Review B*, **2019**, 99,	3.3	3

43	Arsenolite: a quasi-hydrostatic solid pressure-transmitting medium. *Journal of Physics Condensed Matter*, **2016**, 28, 475403	1.8	3
42	Study of the orpiment and anorpiment phases of As2S3 under pressure. *Journal of Physics: Conference Series*, **2017**, 950, 042018	0.3	3
41	Lattice and electronic contributions to the refractive index of CuWO4. *Journal of Applied Physics*, **2014**, 116, 103706	2.5	3
40	Theoretical study of the scheelite-to-fergusonite phase transition in YLiF4 under pressure. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 2077-2082	3.9	3
39	Relativistic corrections to resonant quantum tunnelling through heterostructures. *Semiconductor Science and Technology*, **1992**, 7, 66-70	1.8	3
38	Dynamics of coherent electron tunnelling in asymmetric coupled quantum wells under longitudinal magnetic fields. *Semiconductor Science and Technology*, **1992**, 7, 332-336	1.8	3
37	On the problem of the core level shifts at (110) surfaces of 111-v semiconductor compounds. *Journal of Electron Spectroscopy and Related Phenomena*, **1990**, 52, 155-160	1.7	3
36	Theoretical Ab Initio Calculations in Ordered-Vacancy Compounds at High Pressures. *Springer Series in Materials Science*, **2014**, 185-210	0.9	3
35	The structural phase transition of ammonia borane under high pressure. *International Journal of Hydrogen Energy*, **2020**, 45, 33047-33058	6.7	3
34	Structural, vibrational and electronic properties of □GaS under compression. *Physical Chemistry Chemical Physics*, **2021**, 23, 6841-6862	3.6	3
33	Crystal behavior of potassium bromate under compression. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2015**, 71, 798-804	1.8	2
32	Chemical vapor transport of chalcopyrite semiconductors: CuGaS2 and AgGaS2. *Journal of Crystal Growth*, **2014**, 401, 708-711	1.6	2
31	Phonons and electrons in chalcopyrite semiconductors **2012**,		2
30	First principles calculations of the band offset of the ZnSe/BeTe heterojunctions. *Applied Surface Science*, **1998**, 123-124, 445-448	6.7	2
29	Interdiffusion effects in the band offset modification by intralayer deposition at semiconductor homojunctions. *Physica B: Condensed Matter*, **1993**, 185, 546-550	2.8	2
28	Many-body effects in the paramagnetic and antiferromagnetic states of the (111) silicon face. *Physical Review B*, **1986**, 33, 537-543	3.3	2
27	Band offsets in Si?Si1□Gex and Ge?Si1□Gex strained heterojunctions. *Solid State Communications*, **1988**, 67, 445-447	1.6	2
26	Electronic properties of Si(111) semiconductor surfaces. *Surface Science*, **1985**, 162, 156-162	1.8	2

25	Experimental and Theoretical Study of Zircon and Scheelite Phases of DyVO4. *Acta Physica Polonica A*, **2012**, 121, 920-927	0.6	2
24	Combined Experimental and Theoretical Studies: Lattice-Dynamical Studies at High Pressures with the Help of Ab Initio Calculations. *Minerals (Basel, Switzerland)*, **2021**, 11, 1283	2.4	2
23	Unveiling the role of the lone electron pair in sesquioxides at high pressure: compressibility of □SbO. *Dalton Transactions*, **2021**, 50, 5493-5505	4.3	2
22	Pressure-Induced Phase Transition and Band Gap Decrease in Semiconducting □CuVO.. *Inorganic Chemistry*, **2022**,	5.1	2
21	High-Pressure Properties of Wolframite-Type ScNbO4. *Journal of Physical Chemistry C*, **2022**, 126, 4664-4676	3.7	2
20	Pressure-structure relationships in the 10 K layered carbide halide superconductor Y2C2I2. *Journal of Physics Condensed Matter*, **2016**, 28, 375703	1.8	1
19	High-pressure theoretical and experimental study of HgWO4. *High Pressure Research*, **2011**, 31, 58-63	1.6	1
18	Theoretical study of the role of natural intralayers in the band offsets of InAs/GaSb heterojunction. *Applied Surface Science*, **1998**, 123-124, 571-574	6.7	1
17	Phase diagram studies on iron and nickel silicides: high-pressure experiments andab initiocalculations. *Journal of Physics: Conference Series*, **2008**, 121, 022013	0.3	1
16	Preface: phys. stat. sol. (b) 1/2007. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 13-16	1.3	1
15	High-Pressure Behaviour of Si AND Ge: A Theoretical Study. *High Pressure Research*, **2002**, 22, 455-458	1.6	1
14	Band lineup modification by Ge interlayer deposition at II□VI/III□V semiconductor heterojunctions. *Applied Surface Science*, **1996**, 92, 408-411	6.7	1
13	Dynamics of resonant and non-resonant tunneling in asymmetric coupled quantum wells. *Applied Physics A: Solids and Surfaces*, **1993**, 56, 40-42		1
12	Dangling bond states for a buckled Si(111)2 □1 surface. *Surface Science*, **1987**, 182, 606-612	1.8	1
11	High pressure study of structural, electronic, elastic, and vibrational properties of NaNb3O8. *Journal of Alloys and Compounds*, **2017**, 725, 773-782	5.7	1
10	Theoretical Ab Initio Calculations in Spinels at High Pressures. *Springer Series in Materials Science*, **2014**, 103-129	0.9	1
9	Equation of state and structural characterization of Cu4I4{PPh2(CH2CH = CH2)}4 under pressure. *High Pressure Research*, **2019**, 39, 69-80	1.6	1
8	Pressure-driven configurational crossover between 4f7 and 4f65d1 States □Giant enhancement of narrow Eu2+ UV-Emission lines in SrB4O7 for luminescence manometry. *Acta Materialia*, **2022**, 231, 117886	8.4	1

7	Pressure-induced order-disorder transitions in □nS: an experimental and theoretical study of structural and vibrational properties. *Physical Chemistry Chemical Physics*, **2021**, 23, 23625-23642	3.6	0
6	A Pseudopotential Study of Structural, Mechanical, and Lattice Dynamics Behavior of the Binary Intermetallic Yttrium Tristannide YSn3. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2100219	1.3	0
5	Pressure-Driven Symmetry-Preserving Phase Transitions in Co(IO3)2. *Journal of Physical Chemistry C* , **2021**, 125, 17448-17461	3.8	0
4	Lattice dynamics study of (Gd1□Ybx)2O3(x=0.11) at high pressure. *Journal of Alloys and Compounds*, **2021**, 871, 159525	5.7	0
3	Electronic and Structural High Pressure Properties of CuGaS 2 Chalcopyrite Semiconductor. *High Pressure Research*, **2002**, 22, 361-364	1.6	
2	Quantum magnetotunneling time of electrons in Ga1□AlxA?GaAs superlattices. *Solid State Communications*, **1991**, 79, 749-754	1.6	
1	Auger linewidths for LILII,IIIV processes in Al, Mg and Na. *Journal of Physics C: Solid State Physics*, **1982**, 15, L1109-L1112		