

Victor Milman

List of Publications by Year in descending order

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172
papers

6,902
citations

81900

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174
docs citations

174
times ranked

6647
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic structure, properties, and phase stability of inorganic crystals: A pseudopotential plane-wave study. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 895-910.	2.0	1,566
2	Density-functional study of bulk and surface properties of titanium nitride using different exchange-correlation functionals. <i>Physical Review B</i> , 2000, 62, 2899-2907.	3.2	386
3	Elasticity of hexagonal BeO. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 241-251.	1.8	254
4	Water chemisorption and reconstruction of the MgO surface. <i>Physical Review B</i> , 1995, 52, 10823-10826.	3.2	232
5	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. <i>Computational and Theoretical Chemistry</i> , 2010, 954, 22-35.	1.5	205
6	Novel Rhenium Nitrides. <i>Physical Review Letters</i> , 2010, 105, 085504.	7.8	148
7	Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses. <i>Physical Review Letters</i> , 2014, 112, 025502.	7.8	125
8	Elastic properties of TiB ₂ and MgB ₂ . <i>Journal of Physics Condensed Matter</i> , 2001, 13, 5585-5595.	1.8	122
9	Pressure Response of an Organic-Inorganic Perovskite: Methylammonium Lead Bromide. <i>Chemistry of Materials</i> , 2007, 19, 2401-2405.	6.7	119
10	High-Pressure Polymeric Nitrogen Allotrope with the Black Phosphorus Structure. <i>Physical Review Letters</i> , 2020, 124, 216001.	7.8	119
11	Fracture surfaces: A critical review of fractal studies and a novel morphological analysis of scanning tunneling microscopy measurements. <i>Progress in Materials Science</i> , 1994, 38, 425-474.	32.8	104
12	Structural, electronic and vibrational properties of tetragonal zirconia under pressure: a density functional theory study. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 485404.	1.8	97
13	Structural Properties of Lanthanide and Actinide Compounds within the Plane Wave Pseudopotential Approach. <i>Physical Review Letters</i> , 2000, 85, 5122-5125.	7.8	92
14	Garnets: Structure, compressibility, dynamics, and disorder. <i>Jom</i> , 2000, 52, 22-25.	1.9	87
15	An ab Initio Study of the Structure and Properties of Aluminum Hydroxide: Gibbsite and Bayerite. <i>Journal of Physical Chemistry B</i> , 2001, 105, 10236-10242.	2.6	86
16	Stiffness and thermal expansion of ZrB ₂ : an ab initio study. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 2233-2241.	1.8	85
17	Free energy and entropy of diffusion by ab initio molecular dynamics: Alkali ions in silicon. <i>Physical Review Letters</i> , 1993, 70, 2928-2931.	7.8	81
18	Core-level spectroscopy calculation and the plane wave pseudopotential method. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 104203.	1.8	78

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19	Theoretical study of high-density phases of covalent semiconductors. I.Ab initio treatment. Physical Review B, 1994, 49, 5329-5340.	3.2	74
20	Applicability of a quantum mechanical 'virtual crystal approximation' to study Al/Si-disorder. Chemical Physics Letters, 2002, 362, 266-270.	2.6	72
21	Systematic prediction of crystal structures: An application to sp ³ -hybridized carbon polymorphs. Physical Review B, 2004, 70, .	3.2	70
22	Ab initio atomistic simulation of the strength of defective aluminum and tests of empirical force models. Physical Review B, 1995, 52, 15191-15207.	3.2	66
23	First-Principles Calculations for Niobium Atoms on a Sapphire Surface. Journal of the American Ceramic Society, 1994, 77, 431-436.	3.8	64
24	Comment on "Experimental measurements of the roughness of brittle cracks". Physical Review Letters, 1993, 71, 204-204.	7.8	58
25	Calculation of the elastic constants of the Al ₂ SiO ₅ polymorphs andalusite, sillimanite and kyanite. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 67-70.	0.8	56
26	Orientalional ordering, tilting and lone-pair activity in the perovskite methylammonium tin bromide, CH ₃ NH ₃ SnBr ₃ . Acta Crystallographica Section B: Structural Science, 2010, 66, 422-429.	1.8	56
27	Tetrahedral structures and phase transitions in III-V semiconductors. Physical Review B, 1994, 50, 8389-8401.	3.2	55
28	Stacking fault energies in aluminium. Journal of Physics Condensed Matter, 1992, 4, 10453-10460.	1.8	54
29	First-principles study of the atomistic and electronic structure of the niobium-alumina (0001) interface. Philosophical Magazine Letters, 1996, 73, 377-384.	1.2	53
30	Systematic prediction of crystal structures. Chemical Physics Letters, 2001, 337, 36-42.	2.6	52
31	Large-scale ab initio study of the binding and diffusion of a Ge adatom on the Si(100) surface. Physical Review B, 1994, 50, 2663-2666.	3.2	50
32	Stability field of the high-(P, T) Re ₂ C phase and properties of an analogous osmium carbide phase. Journal of Alloys and Compounds, 2009, 481, 577-581.	5.5	50
33	Elastic Properties, Thermal Expansion, and Polymorphism of Acetylsalicylic Acid. Crystal Growth and Design, 2010, 10, 3132-3140.	3.0	47
34	Emergence of Crystal-like Atomic Dynamics in Glasses at the Nanometer Scale. Physical Review Letters, 2013, 110, 185503.	7.8	47
35	Electronic and elastic properties of edge dislocations in Si. Physical Review B, 1995, 51, 17192-17195.	3.2	46
36	Theoretical investigation of bonding in diasporite. European Journal of Mineralogy, 2001, 13, 343-349.	1.3	45

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37	High-pressure properties of diaspore, AlO(OH). <i>Physics and Chemistry of Minerals</i> , 2007, 34, 145-157.	0.8	45
38	Ab initio total energy study of brucite, diaspore and hypothetical hydrous wadsleyite. <i>Physics and Chemistry of Minerals</i> , 1995, 22, 461.	0.8	44
39	Chemisorption and vibration of hydrogen on Cu(111). <i>Surface Science</i> , 1993, 285, 27-30.	1.9	43
40	Klockmannite, CuSe: structure, properties and phase stability from ab initio modeling. <i>Acta Crystallographica Section B: Structural Science</i> , 2002, 58, 437-447.	1.8	40
41	Crystals from metallic clusters: A first-principles calculation. <i>Physical Review B</i> , 1993, 48, 1981-1983.	3.2	39
42	Structure and properties of aluminosilicate garnets and katoite: an ab initio study. <i>Computational Materials Science</i> , 2000, 17, 141-145.	3.0	37
43	Crystal structures of curium compounds: an ab initio study. <i>Journal of Nuclear Materials</i> , 2003, 322, 165-179.	2.7	37
44	Ab initio total-energy pseudopotential calculations for polymorphic B ₂ O ₃ crystals. <i>Physical Review B</i> , 1995, 51, 1447-1455.	3.2	35
45	Ground-state properties of CoSi ₂ determined by a total-energy pseudopotential method. <i>Physical Review B</i> , 1994, 49, 16300-16308.	3.2	33
46	Systematic ab initio study of the compressibility of silicate garnets. <i>Acta Crystallographica Section B: Structural Science</i> , 2001, 57, 163-177.	1.8	33
47	Structural compression and vibrational properties of Bi ₁₂ Si ₂₀ sillenite from experiment and theory. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 505401.	1.8	33
48	Lattice dynamics of FCC transition metals: A pseudopotential approach. <i>European Physical Journal B</i> , 1990, 79, 223-232.	1.5	31
49	Density-functional study of charge disordering in Cs ₂ Au(I)Au(III)Cl ₆ under pressure. <i>Physical Review B</i> , 2001, 63, .	3.2	31
50	Thermodynamics of pyrope-majorite, Mg ₃ Al ₂ Si ₃ O ₁₂ –Mg ₄ Si ₄ O ₁₂ , solid solution from atomistic model calculations. <i>Molecular Simulation</i> , 2006, 32, 85-99.	2.0	31
51	Tetrahedrally Coordinated sp ³ -Hybridized Carbon in Sr ₂ CO ₄ Orthocarbonate at Ambient Conditions. <i>Inorganic Chemistry</i> , 2021, 60, 5419-5422.	4.0	27
52	Reflectance anisotropy of reconstructed GaAs(001) surfaces. <i>Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena</i> , 1994, 12, 2684.	1.6	26
53	Novel sulfur hydrides synthesized at extreme conditions. <i>Physical Review B</i> , 2020, 102, .	3.2	26
54	Prediction of a nanoporous sp ² -carbon framework structure by combining graph theory with quantum mechanics. <i>Chemical Physics Letters</i> , 1999, 312, 536-541.	2.6	25

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55	The crystal structure of CaSiO ₃ -wastromite, a special isomorph of wollastonite-II. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, 811-818.	0.8	25
56	Is there theoretical evidence for a metallic carbon polymorph with space group symmetry at ambient conditions?. Diamond and Related Materials, 2001, 10, 2225-2227.	3.9	24
57	Vibrational properties of Re ₃ N from experiment and theory. Physical Review B, 2010, 82, .	3.2	24
58	Ab initio total energy study of adsorption and diffusion on the Si(100) surface. Thin Solid Films, 1996, 272, 375-385.	1.8	23
59	Synthesis of calcium orthocarbonate, Ca ₂ CO ₄ at P-T conditions of Earth's transition zone and lower mantle. American Mineralogist, 2022, 107, 336-342.	1.9	23
60	Phase stabilities of MgCO ₃ studied by Raman spectroscopy, x-ray diffraction, and density functional theory calculations. Physical Review Materials, 2020, 4, .	2.1	23
61	Structure and properties of supercubane from density functional calculations. Chemical Physics Letters, 1998, 293, 284-288.	2.6	22
62	An ab initio study of hydrogarnets. American Mineralogist, 2000, 85, 1706-1715.	1.9	22
63	In situ observation of the formation of TiC from the elements by neutron diffraction. Journal of Alloys and Compounds, 2007, 441, 374-380.	5.5	22
64	High pressure elasticity of FeCO ₃ -MgCO ₃ carbonates. Physics of the Earth and Planetary Interiors, 2017, 271, 57-63.	1.9	22
65	First-principles study of impurity segregation in edge dislocations in Si. Physical Review B, 2000, 61, 1674-1676.	3.2	21
66	Prediction of the structure of LaF ₃ at high pressures. Journal of Alloys and Compounds, 2003, 349, 111-113.	5.5	21
67	Lattice dynamics and elasticity of SrCO ₃ . Journal of Applied Crystallography, 2016, 49, 1982-1990.	4.5	21
68	High-pressure phase of LaPO ₄ by x-ray diffraction and second harmonic generation. Physical Review B, 2016, 94, .	4.2	21
69	New insights into the lattice dynamics of α -quartz. Zeitschrift Fur Kristallographie, 2012, 227, 84-91.	1.1	20
70	On the Accuracy of the Total Energy Pseudopotential Scheme Applied to Small Molecules. The Journal of Physical Chemistry, 1996, 100, 6093-6096.	2.9	19
71	Pressure-induced change of the stereochemical activity of a lone electron pair. Journal of Chemical Physics, 1998, 108, 5506-5509.	3.0	19
72	Structural properties of garnets under pressure: An ab initio study. Zeitschrift Fur Kristallographie - Crystalline Materials, 1999, 214, 808-819.	0.8	19

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73	Crystal chemistry of molybdenum phosphides from density functional theory calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2003, 64, 405-411.	4.0	19
74	Dispersion Relation of an OH-Stretching Vibration from Inelastic X-Ray Scattering. <i>Physical Review Letters</i> , 2008, 101, 065501.	7.8	19
75	Ab initio total energy studies of minerals using density functional theory and the local density approximation. <i>Mineralogical Magazine</i> , 1995, 59, 589-596.	1.4	18
76	Prediction of hydrogen positions in complex structures. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2001, 216, 99-104.	0.8	18
77	Lattice dynamics of stishovite from powder inelastic X-ray scattering. <i>Geophysical Research Letters</i> , 2009, 36, .	4.0	18
78	Amino-Acid Adsorption in MFI-Type Zeolites Enabled by the pH-Dependent Ability to Displace Water. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18927-18935.	3.1	18
79	Aplanarity of CO ₃ groups: a theoretical investigation. <i>Acta Crystallographica Section B: Structural Science</i> , 2000, 56, 648-653.	1.8	17
80	The Local Atomic Structures of Liquid CO at 3.6â€¦GPa and Polymerized CO at 0 to 30â€¦GPa from High-Pressure Pair Distribution Function Analysis. <i>Chemistry - A European Journal</i> , 2014, 20, 11531-11539.	3.3	17
81	Sr ₃ [CO ₄]O Antiperovskite with Tetrahedrally Coordinated sp ³ -Hybridized Carbon and OSr ₆ Octahedra. <i>Inorganic Chemistry</i> , 2021, 60, 14504-14508.	4.0	17
82	Equation of state and thermodynamics of fcc transition metals: A pseudopotential approach. <i>European Physical Journal B</i> , 1990, 79, 233-239.	1.5	16
83	Bonding and dynamics of Mg in pyrope: a theoretical investigation. <i>American Mineralogist</i> , 2000, 85, 608-612.	1.9	16
84	High-pressure, high-temperature phase stability of iron-poor dolomite and the structures of dolomite-IIIc and dolomite-V. <i>Physics of the Earth and Planetary Interiors</i> , 2020, 299, 106403.	1.9	16
85	Synthesis, crystal structure and structure-property relations of strontium orthocarbonate, Sr ₂ CO ₄ . <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 131-137.	1.1	16
86	The influence of pressure on the structure and dynamics of hydrogen bonds in zoisite and clinozoisite. <i>Physics and Chemistry of Minerals</i> , 2008, 35, 25-35.	0.8	15
87	Piezoelastic properties of retgersite determined by ultrasonic measurements. <i>European Physical Journal B</i> , 2010, 73, 167-175.	1.5	15
88	In situ synchrotron X-ray diffraction study of the formation of TaB ₂ from the elements in a laser heated diamond anvil cell. <i>Solid State Sciences</i> , 2010, 12, 2059-2064.	3.2	15
89	Formation of scandium carbides and scandium oxycarbide from the elements at high-(P, T) conditions. <i>Journal of Solid State Chemistry</i> , 2010, 183, 975-983.	2.9	15
90	Pressure dependence of the lattice dynamics of diaspore, $\hat{1}\pm$ -AlO(OH), from Raman spectroscopy and density functional perturbation theory. <i>Physics and Chemistry of Minerals</i> , 2011, 38, 693-700.	0.8	15

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91	Ferroelectric soft mode of polar ZnTiO ₃ investigated by Raman spectroscopy at high pressure. Physical Review B, 2015, 91, .	3.2	15
92	Phase transition of tetragonal copper sulfide Cu_2S at low temperatures. Physical Review B, 2017, 96, .	3.2	15
93	The isotypism of BeH ₂ and SiO ₂ : an ab initio study. Chemical Physics Letters, 2003, 378, 343-348.	2.6	14
94	Lattice dynamics and elastic properties of PbF ₂ and BaF ₂ from quantum mechanical calculations. European Physical Journal B, 2004, 39, 27-33.	1.5	14
95	3D Å Imaging of the Fermi Surface by Thermal Diffuse Scattering. Physical Review Letters, 2009, 103, 076403.	7.8	14
96	Structure-property relations and thermodynamic properties of monoclinic petalite, LiAlSi ₄ O ₁₀ . Journal of Physics Condensed Matter, 2012, 24, 345402.	1.8	14
97	High-Pressure Phase Transition of Coffinite, USiO ₄ . Journal of Physical Chemistry C, 2014, 118, 25141-25149.	3.1	14
98	Sr[C ₂ O ₅] is an Inorganic Pyrocarbonate Salt with [C ₂ O ₅] ²⁻ Complex Anions. Journal of the American Chemical Society, 2022, 144, 2899-2904.	13.7	14
99	Implication of volume changes in uranium oxides: A density functional study. Solid State Sciences, 2013, 24, 44-53.	3.2	13
100	Novel Calcium sp ³ Carbonate CaC ₂ O ₅ ·4H ₂ O May Be a Carbon Host in Earth's Lower Mantle. ACS Earth and Space Chemistry, 2022, 6, 73-80.	2.7	13
101	Structure of Cu ₆ PbO ₈ . Acta Crystallographica Section B: Structural Science, 2000, 56, 22-26.	1.8	12
102	Virtual crystal approximation study of nitridosilicates and oxonitridoaluminosilicates. Journal of Physics and Chemistry of Solids, 2008, 69, 1861-1868.	4.0	12
103	Structure, elasticity, thermodynamics and high pressure behavior of ZnB ₄ O ₇ and CdB ₄ O ₇ . Solid State Sciences, 2012, 14, 1080-1085.	3.2	12
104	Pressure-induced spin collapse of octahedrally coordinated Fe ₃ Ca ₃ Fe ₂	3.2	12
105	Lattice dynamics and Mg/Ti order in orthorhombic pseudobrookite-type MgTi ₂ O ₅ . Journal of Alloys and Compounds, 2017, 699, 16-24.	5.5	12
106	Ab initio calculation of the high-pressure behaviour of hydrogen cyanide. Journal of Physics Condensed Matter, 1996, 8, 9049-9057.	1.8	11
107	Ab initio modeling in crystallography. Solid State Sciences, 1999, 1, 273-279.	0.7	11
108	Theoretical investigation of moganite. European Journal of Mineralogy, 2005, 17, 21-30.	1.3	11

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109	Accuracy of Dispersion-Corrected Density Functional Theory Calculations of Elastic Tensors of Organic Molecular Structures. <i>Crystal Growth and Design</i> , 2020, 20, 206-213.	3.0	11
110	GaSeCl ₅ O: A Molecular Compound with Very Strong SHG Effect. <i>Inorganic Chemistry</i> , 2021, 60, 15653-15658. High pressure γ-irradiation	4.0	11
111	$\langle \text{mml:math} \rangle$		

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127	Theoretical study of the structures and properties of SrSiAl ₂ O ₃ N ₂ and Ce ₄ [Si ₄ O ₄ N ₆]O. Chemical Physics Letters, 2001, 343, 622-626.	2.6	7
128	Compression behaviour of nitridocarbidosilicates studied with X-ray diffraction and ab initio calculations. Journal of Physics and Chemistry of Solids, 2009, 70, 97-106.	4.0	7
129	Compression behavior of Sm ₂ Ti ₂ O ₇ -pyrochlore up to 50 GPa: single-crystal X-ray diffraction and density functional theory calculations. Science Bulletin, 2014, 59, 5278-5282.	1.7	7
130	Determination of the Crystal Structure of Hexaphenyldisilane from Powder Diffraction Data and Its Thermodynamic Properties. Crystal Growth and Design, 2014, 14, 2937-2944.	3.0	7
131	Phonon-driven phase transitions in calcite, dolomite, and magnesite. Physical Review B, 2019, 99, .	3.2	7
132	Structural, elastic and vibrational properties of celestite, SrSO ₄ , from synchrotron x-ray diffraction, thermal diffuse scattering and Raman scattering. Journal of Physics Condensed Matter, 2019, 31, 055703.	1.8	7
133	A chondrule formation experiment aboard the ISS: Experimental set-up and test experiments. Icarus, 2020, 350, 113898.	2.5	7
134	Compression mechanism of cubic silica sodalite [Si ₁₂ O ₂₄]: a first principles study of the Im $\bar{3}$ m to I $\bar{4}$ m phase transition. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 495-500.	0.8	6
135	Correlation between composition and structure in boracites. Journal of Physics Condensed Matter, 2007, 19, 275207.	1.8	6
136	In situ study of the formation of rhenium borides from the elements at high-(p, T) conditions: Extreme incompressibility of Re ₇ B ₃ and formation of new phases. Solid State Sciences, 2013, 25, 85-92.	3.2	6
137	Compressibility, microcalorimetry, elastic properties and EELS of rhenium borides. Solid State Sciences, 2018, 81, 71-81.	3.2	6
138	Polymorphism of CsI. Journal of Physics Condensed Matter, 1997, 9, 9811-9817.	1.8	5
139	Prediction of structural parameters and physical properties of CsHSO ₃ up to 60 GPa. Physical Review B, 1998, 57, 4321-4326.	3.2	5
140	Structural and magnetic properties of betaine adducts with transition metals: I. ((CH ₃) ₃ NCH ₂ COO) ₃ MnMCl ₄ with M = Mn ²⁺ , Co ²⁺ , Zn ²⁺ . Journal of Physics Condensed Matter, 2006, 18, 11067-11079.	1.8	5
141	Electronic structure of oxide fuels from experiment and first principles calculations. Journal of Physics: Conference Series, 2010, 241, 012062.	0.4	5
142	A new BaCa(CO ₃) ₂ polymorph. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 291-300.	1.1	5
143	Nitrosonium nitrate (NO ⁺ NO ₃ ⁻) structure solution using <i>in situ</i> single-crystal X-ray diffraction in a diamond anvil cell. IUCr, 2021, 8, 208-214.	2.2	5
144	Point-defect-induced crystal growth: An ab initio study. Physical Review B, 1993, 48, 11465-11468.	3.2	4

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145	Improved representation of metallic bonding in atomistic simulations. Philosophical Magazine Letters, 1996, 73, 39-44.	1.2	4
146	Density functional study of the polymorphism of Cs ₂ C ₂ and Rb ₂ C ₂ . Solid State Communications, 2002, 121, 155-158.	1.9	4
147	Quantum technology in catalysis. Applied Catalysis A: General, 2005, 280, 105-113.	4.3	4
148	Revised prediction of B1 to B2 phase transition pressures in YbN, YbP and YbAs. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, 700-703.	0.8	4
149	A Service-Oriented Framework for Running Quantum Mechanical Simulations of Material Properties in a Grid Environment. IEEE Transactions on Systems, Man and Cybernetics, Part C: Applications and Reviews, 2010, 40, 485-490.	2.9	4
150	Elastic stiffness coefficients of thenardite and their pressure and temperature dependence. Zeitschrift Fur Kristallographie - Crystalline Materials, 2012, 227, 503-513.	0.8	4
151	Study of the reaction products of SF ₆ and C in the laser heated diamond anvil cell by pair distribution function analysis and micro-Raman spectroscopy. Journal of Solid State Chemistry, 2015, 225, 141-148.	2.9	4
152	High-pressure phases of SF ₆ up to 32GPa from X-ray diffraction and Raman spectroscopy. Journal of Physics and Chemistry of Solids, 2015, 80, 11-21.	4.0	4
153	Structural, Physical, and Thermodynamic Properties of Aragonitic Ca _x Sr _{1-x} CO ₃ Solid Solutions. Journal of Physical Chemistry C, 2021, 125, 17474-17481.	3.1	4
154	Electronic, Structural, and Mechanical Properties of SiO_2 Glass at High Pressure Inferred from its Refractive Index. Physical Review Letters, 2022, 128, 077403.	7.8	4
155	Pseudopotential model calculation of the off-symmetry phonon frequencies and of the equation of state of copper. Solid State Communications, 1990, 76, 1247-1249.	1.9	3
156	Point-contact spectroscopy of the electron-phonon interaction in palladium. Journal of Physics Condensed Matter, 1991, 3, 6523-6530.	1.8	3
157	Electronic structure of the Si ₆ /Ge ₆ (111) superlattice strained to a Ge substrate. Semiconductor Science and Technology, 1993, 8, 2121-2124.	2.0	3
158	Ab initio study of epitaxial growth on stepped Si(100) surface. International Journal of Quantum Chemistry, 1997, 61, 719-724.	2.0	3
159	The Low-Temperature Structure of LiSH. Phase Transitions, 2003, 76, 187-195.	1.3	3
160	Influence of deuteration on lithium acetate dihydrate studied by inelastic X-ray scattering, density functional theory, thermal expansion, elastic and thermodynamic measurements. Dalton Transactions, 2011, 40, 1737.	3.3	3
161	Synthesis of Hf ₈ O ₇ , a new binary hafnium oxide, at high pressures and high temperatures. High Pressure Research, 2017, 37, 147-158.	1.2	3
162	Elastic stiffness coefficients of thiourea from thermal diffuse scattering. Journal of Applied Crystallography, 2021, 54, 287-294.	4.5	3

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163	Theoretical study of lattice heat capacity, thermal expansion and phonon-limited resistivity of transition metals. Journal of Physics and Chemistry of Solids, 1992, 53, 565-575.	4.0	2
164	Theoretical investigation of Ca(OH) ₂ -II. European Journal of Mineralogy, 2002, 14, 557-560.	1.3	2
165	A Reentrant Phase Transition and a Novel Polymorph Revealed in High-Pressure Investigations of CF ₄ up to 46.5 GPa. Journal of Chemical Physics, 2022, 156, 044503.	3.0	2
166	A computer simulation study of domain walls in NH ₄ Cl. Journal of Physics Condensed Matter, 2000, 12, 2093-2101.	1.8	1
167	“Errata to the Journal of Physics and Chemistry of Solids 64(3) (2003)” Journal of Physics and Chemistry of Solids, 2003, 64, 1431.	4.0	1
168	Na ₃ O(CN): <i>Ab</i> initio calculations on a multidomain structure. Physical Review B, 2004, 70, .	3.2	1
169	low-temperature lattice properties of transition metals : pseudopotential model coupled with band structure calculation. Physica B: Condensed Matter, 1990, 165-166, 207-208.	2.7	0
170	Relativistic pseudopotentials for transition metals. I. Construction and application to atoms. Journal of Physics Condensed Matter, 1990, 2, 7101-7114.	1.8	0
171	Experimental and theoretical high pressure study of ¹²⁵ Cs ₂ SO ₄ . Zeitschrift Fur Kristallographie - Crystalline Materials, 2000, 215, 17-22.	0.8	0
172	Prediction of the Structure of LaF ₃ at High Pressure.. ChemInform, 2003, 34, no.	0.0	0