Victor Milman

List of Publications by Year
in descending order

172	6,902	81900 39	66911 78
papers	citations	h-index	g-index

174	174	174	6647
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis of calcium orthocarbonate, Ca2CO4-Pnma at P-T conditions of Earthâ€™s transition zone and lower mantle. American Mineralogist, 2022, 107, 336-342.	1.9	23
2	A Reentrant Phase Transition and a Novel Polymorph Revealed in High-Pressure Investigations of CF4 up to 46.5 GPa. Journal of Chemical Physics, 2022, 156, 044503.	3.0	2
3	Novel Calcium sp³ Carbonate CaC₂O₅-I4Ì…2d May Be a Carbon Host in Earthâ€™s Lower Mantle. ACS Earth and Space Chemistry, 2022, 6, 73-80.	2.7	13
4	Sr[C₂O₅] is an Inorganic Pyrocarbonate Salt with [C₂O₅]^{2â€“} Complex Anions. Journal of the American Chemical Society, 2022, 144, 2899-2904.	13.7	14
5	High pressure chemistry of xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mn>3</mml:mn></mml: <mml:math		

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19	High-Pressure Polymeric Nitrogen Allotrope with the Black Phosphorus Structure. Physical Review Letters, 2020, 124, 216001.	7.8	119
20	A chondrule formation experiment aboard the ISS: Experimental set-up and test experiments. Icarus, 2020, 350, 113898.	2.5	7
21	Phase stabilities of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgCO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> studied by Raman spectroscopy, x-ray diffraction, and density functional theory calculations. Physical Review Materials, 2020, 4, .	2.4	23
22	Pressure-induced Pbâ€“Pb bonding and phase transition in Pb₂SnO₄. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 979-991.	1.1	8
23	A new BaCa(CO₃)₂polymorph. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 291-300.	1.1	5
24	High-pressure compressibility and electronic properties of bismuth silicate Bi2SiO5 from synchrotron experiments and first-principles calculations. Physical Review B, 2019, 99, .	3.2	8
25	Phonon-driven phase transitions in calcite, dolomite, and magnesite. Physical Review B, 2019, 99, .	3.2	7
26	Structural, elastic and vibrational properties of celestite, SrSO₄, from synchrotron x-ray diffraction, thermal diffuse scattering and Raman scattering. Journal of Physics Condensed Matter, 2019, 31, 055703.	1.8	7
27	Pressure-induced changes of the structure and properties of monoclinic Î± -chalcocite Cu2S. Physical Review B, 2018, 97, .	3.2	9
28	Compressibility, microcalorimetry, elastic properties and EELS of rhenium borides. Solid State Sciences, 2018, 81, 71-81.	3.2	6
29	Synthesis of Hf8O7, a new binary hafnium oxide, at high pressures and high temperatures. High Pressure Research, 2017, 37, 147-158.	1.2	3
30	Lattice dynamics and Mg/Ti order in orthorhombic pseudobrookite-type MgTi2 O5. Journal of Alloys and Compounds, 2017, 699, 16-24.	5.5	12
31	Phase transition of tetragonal copper sulfide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:mrow><mml:mathvariant="normal">S</mml:mi></mml:mrow></mml:math> at low temperatures. Physical Review B, 2017, 96, .	3.2	15
32	High pressure elasticity of FeCO 3 -MgCO 3 carbonates. Physics of the Earth and Planetary Interiors, 2017, 271, 57-63.	1.9	22
33	Lattice dynamics and elasticity of SrCO₃. Journal of Applied Crystallography, 2016, 49, 1982-1990.	4.5	21
34	High-pressure phase of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaPO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> by x-ray diffraction and second harmonic generation. Physical Review B, 2016, 94, .	3.2	21
35	Ferroelectric soft mode of polarZnTiO3investigated by Raman spectroscopy at high pressure. Physical Review B, 2015, 91, .	3.2	15
36	Pressure-induced spin collapse of octahedrally coordinated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Mn</mml:mi></mml:mrow><mml:mrow><m the tetragonal hydrogarnet henritermierite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ca</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2015, 92, .	3.2	8

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37	Study of the reaction products of SF6 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
38	High-pressure phases of SF6 up to 32GPa from X-ray diffraction and Raman spectroscopy. Journal of Physics and Chemistry of Solids, 2015, 80, 11-21.	4.0	4
39	Density functional theory based calculations for high pressure research. Zeitschrift Fur Kristallographie - Crystalline Materials, 2014, 229, .	0.8	10
40	Compression behavior of Sm2Ti2O7-pyrochlore up to 50ÂGPa: single-crystal X-ray diffraction and density functional theory calculations. Science Bulletin, 2014, 59, 5278-5282.	1.7	7
41	Local structure of CuxZn2â^'xTiO4 inverse spinel. Applied Physics Letters, 2014, 105, 071911.	3.3	8
42	Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses. Physical Review Letters, 2014, 112, 025502.	7.8	125
43	The Local Atomic Structures of Liquid CO at 3.6â€...GPa and Polymerized CO at 0 to 30â€...GPa from Highâ€Pressure Pair Distribution Function Analysis. Chemistry - A European Journal, 2014, 20, 11531-11539.	3.3	17
44	High-Pressure Phase Transition of Coffinite, USiO₄. Journal of Physical Chemistry C, 2014, 118, 25141-25149.	3.1	14
45	Pressure-induced spin collapse of octahedrally coordinated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi mathvariant="normal">Fe</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math> in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">Ca</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">Fe</mml:mi></mml:mrow><mml:mn>2</mml:mn>. Physical Review B, 2014, 90, .	3.2	12
46	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
47	Oxygen K-edge electron energy loss spectra of hydrous and anhydrous compounds. Journal of Physics Condensed Matter, 2013, 25, 485401.	1.8	10
48	Amino-Acid Adsorption in MFI-Type Zeolites Enabled by the pH-Dependent Ability to Displace Water. Journal of Physical Chemistry C, 2013, 117, 18927-18935.	3.1	18
49	Implication of volume changes in uranium oxides: A density functional study. Solid State Sciences, 2013, 24, 44-53.	3.2	13
50	In situ study of the formation of rhenium borides from the elements atÂhigh-(p, T) conditions: Extreme incompressibility of Re7B3 and formation of new phases. Solid State Sciences, 2013, 25, 85-92.	3.2	6
51	Emergence of Crystal-like Atomic Dynamics in Glasses at the Nanometer Scale. Physical Review Letters, 2013, 110, 185503.	7.8	47
52	Structureâ€"property relations and thermodynamic properties of monoclinic petalite, LiAlSi₄O₁₀. Journal of Physics Condensed Matter, 2012, 24, 345402.	1.8	14
53	Experimental evidence for the structural models of Re <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>N and Re <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>C from micro-Raman spectroscopy. Physical Review B, 2012, 86, .	3.2	10
54	Structure, elasticity, thermodynamics and high pressure behavior of ZnB4O7 and CdB4O7. Solid State Sciences, 2012, 14, 1080-1085.	3.2	12

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55	Elastic stiffness coefficients of thenardite and their pressure and temperature dependence. Zeitschrift Fur Kristallographie - Crystalline Materials, 2012, 227, 503-513.	0.8	4
56	New insights into the lattice dynamics ofÎ±-quartz. Zeitschrift FÃ¼r Kristallographie, 2012, 227, 84-91.	1.1	20
57	Pressure dependence of the lattice dynamics of diaspore, Î±-AlO(OH), from Raman spectroscopy and density functional perturbation theory. Physics and Chemistry of Minerals, 2011, 38, 693-700.	0.8	15
58	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
59	Piezoelastic properties of retgersite determined by ultrasonic measurements. European Physical Journal B, 2010, 73, 167-175.	1.5	15
60	In situ synchrotron X-ray diffraction study of the formation of TaB2 from the elements in a laser heated diamond anvil cell. Solid State Sciences, 2010, 12, 2059-2064.	3.2	15
61	Formation of scandium carbides and scandium oxycarbide from the elements at high-(P, T) conditions. Journal of Solid State Chemistry, 2010, 183, 975-983.	2.9	15
62	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
63	Orientational ordering, tilting and lone-pair activity in the perovskite methylammonium tin bromide, CH₃NH₃SnBr₃. Acta Crystallographica Section B: Structural Science, 2010, 66, 422-429.	1.8	56
64	Vibrational properties ofRe3Nfrom experiment and theory. Physical Review B, 2010, 82, .	3.2	24
65	Electronic structure of oxide fuels from experiment and first principles calculations. Journal of Physics: Conference Series, 2010, 241, 012062.	0.4	5
66	Structural compression and vibrational properties of Bi₁₂SiO₂₀sillenite from experiment and theory. Journal of Physics Condensed Matter, 2010, 22, 505401.	1.8	33
67	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
68	Elastic Properties, Thermal Expansion, and Polymorphism of Acetylsalicylic Acid. Crystal Growth and Design, 2010, 10, 3132-3140.	3.0	47
69	Novel Rhenium Nitrides. Physical Review Letters, 2010, 105, 085504.	7.8	148
70	Core-level spectroscopy calculation and the plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104203.	1.8	78
71	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
72	3DÂImaging of the Fermi Surface by Thermal Diffuse Scattering. Physical Review Letters, 2009, 103, 076403.	7.8	14

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73	Stability field of the high-(P, T) Re2C phase and properties of an analogous osmium carbide phase. Journal of Alloys and Compounds, 2009, 481, 577-581.	5.5	50
74	Lattice dynamics of stishovite from powder inelastic Xâ€ray scattering. Geophysical Research Letters, 2009, 36, .	4.0	18
75	Structural, electronic and vibrational properties of tetragonal zirconia under pressure: a density functional theory study. Journal of Physics Condensed Matter, 2009, 21, 485404.	1.8	97
76	Defect properties of albite. Physics and Chemistry of Minerals, 2008, 35, 129-135.	0.8	9
77	Virtual crystal approximation study of nitridosilicates and oxonitridoaluminosilicates. Journal of Physics and Chemistry of Solids, 2008, 69, 1861-1868.	4.0	12
78	The influence of pressure on the structure and dynamics of hydrogen bonds in zoisite and clinozoisite. Physics and Chemistry of Minerals, 2008, 35, 25-35.	0.8	15
79	Dispersion Relation of an OH-Stretching Vibration from Inelastic X-Ray Scattering. Physical Review Letters, 2008, 101, 065501.	7.8	19
80	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
81	Correlation between composition and structure in boracites. Journal of Physics Condensed Matter, 2007, 19, 275207.	1.8	6
82	Pressure Response of an Organicâ"Inorganic Perovskite:Â Methylammonium Lead Bromide. Chemistry of Materials, 2007, 19, 2401-2405.	6.7	119
83	High-pressure properties of diaspore, AlO(OH). Physics and Chemistry of Minerals, 2007, 34, 145-157.	0.8	45
84	Structural and magnetic properties of betaine adducts with transition metals: I. ((CH3)3NCH2COO)3MnMCl4with M = Mn2+, Co2+, Zn2+. Journal of Physics Condensed Matter, 2006, 18, 11067-11079.	1.8	5
85	Thermodynamics of pyropeâ€"majorite, Mg3Al2Si3O12â€"Mg4Si4O12, solid solution from atomistic model calculations. Molecular Simulation, 2006, 32, 85-99.	2.0	31
86	Quantum technology in catalysis. Applied Catalysis A: General, 2005, 280, 105-113.	4.3	4
87	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
88	Theoretical investigation of moganite. European Journal of Mineralogy, 2005, 17, 21-30.	1.3	11
89	Stiffness and thermal expansion of ZrB2: anab initiostudy. Journal of Physics Condensed Matter, 2005, 17, 2233-2241.	1.8	85
90	Na3O(CN):â€ƒAb initiocalculations on a multidomain structure. Physical Review B, 2004, 70, .	3.2	1

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91	Quantum mechanical study of Al/Si disorder in leucite and bicchulite. Mineralogical Magazine, 2004, 68, 819-824.	1.4	9
92	Lattice dynamics and elastic properties of PbF$mathsf{_2}$ and BaF$mathsf{_2}$ from quantum mechanical calculations. European Physical Journal B, 2004, 39, 27-33.	1.5	14
93	Molybdenum Phosphide as ano-Propylaniline Hydrodenitrogenation Catalyst: A First Principles Study. Chemistry - A European Journal, 2004, 10, 6279-6284.	3.3	10
94	Systematic prediction of crystal structures: An application tosp3-hybridized carbon polymorphs. Physical Review B, 2004, 70, .	3.2	70
95	Prediction of the Structure of LaF3 at High Pressure.. ChemInform, 2003, 34, no.	0.0	0
96	The isotypism of BeH2 and SiO2: an ab initio study. Chemical Physics Letters, 2003, 378, 343-348.	2.6	14
97	Crystal chemistry of molybdenum phosphides from density functional theory calculations. Journal of Physics and Chemistry of Solids, 2003, 64, 405-411.	4.0	19
98	â€œErrata to the Journal of Physics and Chemistry of Solids 64(3) (2003)â€• Journal of Physics and Chemistry of Solids, 2003, 64, 1431.	4.0	1
99	Crystal structures of curium compounds: an ab initio study. Journal of Nuclear Materials, 2003, 322, 165-179.	2.7	37
100	Prediction of the structure of LaF3 at high pressures. Journal of Alloys and Compounds, 2003, 349, 111-113.	5.5	21
101	The crystal structure of CaSiO3-walstromite, a special isomorph of wollastonite-II. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, 811-818.	0.8	25
102	The Low-Temperature Structure of LiSH. Phase Transitions, 2003, 76, 187-195.	1.3	3
103	Theoretical investigation of Ca(OH)2-II. European Journal of Mineralogy, 2002, 14, 557-560.	1.3	2
104	Klockmannite, CuSe: structure, properties and phase stability from ab initio modeling. Acta Crystallographica Section B: Structural Science, 2002, 58, 437-447.	1.8	40
105	Density functional study of the polymorphism of Cs2C2 and Rb2C2. Solid State Communications, 2002, 121, 155-158.	1.9	4
106	Applicability of a quantum mechanical `virtual crystal approximation' to study Al/Si-disorder. Chemical Physics Letters, 2002, 362, 266-270.	2.6	72
107	An ab Initio Study of the Structure and Properties of Aluminum Hydroxide:Â Gibbsite and Bayerite. Journal of Physical Chemistry B, 2001, 105, 10236-10242.	2.6	86
108	Elasticity of hexagonal BeO. Journal of Physics Condensed Matter, 2001, 13, 241-251.	1.8	254

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109	Density-functional study of charge disordering inCs2Au(I)Au(III)Cl6under pressure. Physical Review B, 2001, 63, .	3.2	31
110	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
111	Elastic properties of TiB2and MgB2. Journal of Physics Condensed Matter, 2001, 13, 5585-5595.	1.8	122
112	Compression mechanism of cubic silica sodalite [Si12O24]: a first principles study of the Im3Ì…m to I4Ì…3m phase transition. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 495-500.	0.8	6
113	Prediction of hydrogen positions in complex structures. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 99-104.	0.8	18
114	Theoretical investigation of bonding in diaspore. European Journal of Mineralogy, 2001, 13, 343-349.	1.3	45
115	A theoretical investigation of the relative stabilities of Fe-free clinozoisite and orthozoisite. Physics and Chemistry of Minerals, 2001, 28, 471-474.	0.8	9
116	Systematic ab initio study of the compressibility of silicate garnets. Acta Crystallographica Section B: Structural Science, 2001, 57, 163-177.	1.8	33
117	Systematic prediction of crystal structures. Chemical Physics Letters, 2001, 337, 36-42.	2.6	52
118	Theoretical study of the structures and properties of SrSiAl2O3N2 and Ce4[Si4O4N6]O. Chemical Physics Letters, 2001, 343, 622-626.	2.6	7
119	Calculation of the elastic constants of the Al2SiO5 polymorphs andalusite, sillimanite and kyanite. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 67-70.	0.8	56
120	Bonding and dynamics of Mg in pyrope: a theoretical investigation. American Mineralogist, 2000, 85, 608-612.	1.9	16
121	Electronic structure, properties, and phase stability of inorganic crystals: A pseudopotential plane-wave study. International Journal of Quantum Chemistry, 2000, 77, 895-910.	2.0	1,566
122	Aplanarity of CO3 groups: a theoretical investigation. Acta Crystallographica Section B: Structural Science, 2000, 56, 648-653.	1.8	17
123	Structure of Cu6PbO8. Acta Crystallographica Section B: Structural Science, 2000, 56, 22-26.	1.8	12
124	Computational chemistry on Fujitsu vectorâ€“parallel processors: Development and performance of applications software. Parallel Computing, 2000, 26, 887-911.	2.1	7
125	Garnets: Structure, compressibility, dynamics, and disorder. Jom, 2000, 52, 22-25.	1.9	87
126	An ab initio study of hydrogarnets. American Mineralogist, 2000, 85, 1706-1715.	1.9	22

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127	First-principles study of impurity segregation in edge dislocations in Si. Physical Review B, 2000, 61, 1674-1676.	3.2	21
128	Structural Properties of Lanthanide and Actinide Compounds within the Plane Wave Pseudopotential Approach. Physical Review Letters, 2000, 85, 5122-5125.	7.8	92
129	Experimental and theoretical high pressure study of Î²-Cs2SO4. Zeitschrift Fur Kristallographie - Crystalline Materials, 2000, 215, 17-22.	0.8	0
130	Structure and properties of aluminosilicate garnets and katoite: an ab initio study. Computational Materials Science, 2000, 17, 141-145.	3.0	37
131	A computer simulation study of domain walls in NH4Cl. Journal of Physics Condensed Matter, 2000, 12, 2093-2101.	1.8	1
132	Density-functional study of bulk and surface properties of titanium nitride using different exchange-correlation functionals. Physical Review B, 2000, 62, 2899-2907.	3.2	386
133	Structural properties of garnets under pressure: An ab initio study. Zeitschrift Fur Kristallographie - Crystalline Materials, 1999, 214, 808-819.	0.8	19
134	Prediction of a nanoporous sp2-carbon framework structure by combining graph theory with quantum mechanics. Chemical Physics Letters, 1999, 312, 536-541.	2.6	25
135	Ab initio modeling in crystallography. Solid State Sciences, 1999, 1, 273-279.	0.7	11
136	Structure and properties of supercubane from density functional calculations. Chemical Physics Letters, 1998, 293, 284-288.	2.6	22
137	Pressure-induced change of the stereochemical activity of a lone electron pair. Journal of Chemical Physics, 1998, 108, 5506-5509.	3.0	19
138	Prediction of structural parameters and physical properties ofCsHSO3up to 60 GPa. Physical Review B, 1998, 57, 4321-4326.	3.2	5
139	Polymorphism of CsI. Journal of Physics Condensed Matter, 1997, 9, 9811-9817.	1.8	5
140	Ab initio study of epitaxial growth on stepped Si(100) surface. International Journal of Quantum Chemistry, 1997, 61, 719-724.	2.0	3
141	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
142	Ab initio total energy study of adsorption and diffusion on the Si(100) surface. Thin Solid Films, 1996, 272, 375-385.	1.8	23
143	Improved representation of metallic bonding in atomistic simulations. Philosophical Magazine Letters, 1996, 73, 39-44.	1.2	4
144	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

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145	Ab initiocalculation of the high-pressure behaviour of hydrogen cyanide. Journal of Physics Condensed Matter, 1996, 8, 9049-9057.	1.8	11
146	Ab initio total energy study of brucite, diaspore and hypothetical hydrous wadsleyite. Physics and Chemistry of Minerals, 1995, 22, 461.	0.8	44
147	Ab initio total energy studies of minerals using density functional theory and the local density approximation. Mineralogical Magazine, 1995, 59, 589-596.	1.4	18
148	Ab initioatomistic simulation of the strength of defective aluminum and tests of empirical force models. Physical Review B, 1995, 52, 15191-15207.	3.2	66
149	Ab initiototal-energy pseudopotential calculations for polymorphicB2O3crystals. Physical Review B, 1995, 51, 1447-1455.	3.2	35
150	Electronic and elastic properties of edge dislocations in Si. Physical Review B, 1995, 51, 17192-17195.	3.2	46
151	Water chemisorption and reconstruction of the MgO surface. Physical Review B, 1995, 52, 10823-10826.	3.2	232
152	Tetrahedral structures and phase transitions in III-V semiconductors. Physical Review B, 1994, 50, 8389-8401.	3.2	55
153	Theoretical study of high-density phases of covalent semiconductors. I.Ab initiotreatment. Physical Review B, 1994, 49, 5329-5340.	3.2	74
154	Ground-state properties ofCoSi2determined by a total-energy pseudopotential method. Physical Review B, 1994, 49, 16300-16308.	3.2	33
155	Large-scaleab initiostudy of the binding and diffusion of a Ge adatom on the Si(100) surface. Physical Review B, 1994, 50, 2663-2666.	3.2	50
156	Reflectance anisotropy of reconstructed GaAs(001) surfaces. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1994, 12, 2684.	1.6	26
157	Fracture surfaces: A critical review of fractal studies and a novel morphological analysis of scanning tunneling microscopy measurements. Progress in Materials Science, 1994, 38, 425-474.	32.8	104
158	First-Principles Calculations for Niobium Atoms on a Sapphire Surface. Journal of the American Ceramic Society, 1994, 77, 431-436.	3.8	64
159	Chemisorption and vibration of hydrogen on Cu(111). Surface Science, 1993, 285, 27-30.	1.9	43
160	Free energy and entropy of diffusion byab initiomolecular dynamics: Alkali ions in silicon. Physical Review Letters, 1993, 70, 2928-2931.	7.8	81
161	Electronic structure of the Si6/Ge6(111) superlattice strained to a Ge substrate. Semiconductor Science and Technology, 1993, 8, 2121-2124.	2.0	3
162	Crystals from metallic clusters: A first-principles calculation. Physical Review B, 1993, 48, 1981-1983.	3.2	39

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163	Comment on â€˜â€˜Experimental measurements of the roughness of brittle cracksâ€™â€™. Physical Review Letters, 1993, 71, 204-204.	7.8	58
164	Point-defect-induced crystal growth: Anab initiostudy. Physical Review B, 1993, 48, 11465-11468.	3.2	4
165	Stacking fault energies in aluminium. Journal of Physics Condensed Matter, 1992, 4, 10453-10460.	1.8	54
166	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
167	Point-contact spectroscopy of the electron-phonon interaction in palladium. Journal of Physics Condensed Matter, 1991, 3, 6523-6530.	1.8	3
168	Lattice dynamics of FCC transition metals: A pseudopotential approach. European Physical Journal B, 1990, 79, 223-232.	1.5	31
169	Equation of state and thermodynamics of fcc transition metals: A pseudopotential approach. European Physical Journal B, 1990, 79, 233-239.	1.5	16
170	Iow-teperature lattice properties of transtticn metals : pseudopotential model coupled with band structure calculation. Physica B: Condensed Matter, 1990, 165-166, 207-208.	2.7	0
171	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
172	Relativistic pseudopotentials for transition metals. I. Construction and application to atoms. Journal of Physics Condensed Matter, 1990, 2, 7101-7114.	1.8	0