Wai-Yim Ching

List of Publications by Year
in descending order

193 papers	13,411 citations	16451 64 h-index	24258 110 g-index
207 all docs	207 docs citations	207 times ranked	11471 citing authors

#	Article	IF	Citations
1	Electronic and optical properties of three phases of titanium dioxide: Rutile, anatase, and brookite. Physical Review B, 1995, 51, 13023-13032.	3.2	891
2	Electronic, optical, and structural properties of some wurtzite crystals. Physical Review B, 1993, 48, 4335-4351.	3.2	642
3	Experimental and theoretical determination of the electronic structure and optical properties of three phases ofZrO2. Physical Review B, 1994, 49, 5133-5142.	3.2	476
4	Calculation of ground-state and optical properties of boron nitrides in the hexagonal, cubic, and wurtzite structures. Physical Review B, 1991, 44, 7787-7798.	3.2	433
5	Grain Boundary Strengthening in Alumina by Rare Earth Impurities. Science, 2006, 311, 212-215.	12.6	391
6	Long range interactions in nanoscale science. Reviews of Modern Physics, 2010, 82, 1887-1944.	45.6	359
7	A minimal basis semi-ab initio approach to the band structures of semiconductors. Journal of Physics and Chemistry of Solids, 1985, 46, 977-995.	4.0	297
8	Ab Initio Calculation of Elastic Constants of Ceramic Crystals. Journal of the American Ceramic Society, 2007, 90, 3194-3204.	3.8	281
9	Theoretical Studies of the Electronic Properties of Ceramic Materials. Journal of the American Ceramic Society, 1990, 73, 3135-3160.	3.8	253
10	Ground-state and optical properties ofCu2O and CuO crystals. Physical Review B, 1989, 40, 7684-7695.	3.2	244
11	Analytic solution of a two-dimensional hydrogen atom. I. Nonrelativistic theory. Physical Review A, 1991, 43, 1186-1196.	2.5	236
12	Self-consistent band structures, charge distributions, and optical-absorption spectra in MgO, Î±-Al2O3, andMgAl2O4. Physical Review B, 1991, 43, 4461-4472.	3.2	226
13	Interesting Physical Properties of the New Spinel Phase ofSi3N4andC3N4. Physical Review Letters, 1999, 83, 5046-5049.	7.8	205
14	Electronic structure and optical properties of Î± and Î² phases of silicon nitride, silicon oxynitride, and with comparison to silicon dioxide. Physical Review B, 1995, 51, 17379-17389.	3.2	194
15	Calculation of optical excitations in cubic semiconductors. I. Electronic structure and linear response. Physical Review B, 1993, 47, 9449-9463.	3.2	186
16	First-principles calculation of optical properties of C_{60} in the fcc lattice. Physical Review Letters, 1991, 67, 2045-2048.	7.8	177
17	Electronic structure of yttrium aluminum garnet(Y3Al5O12). Physical Review B, 1999, 59, 10530-10535.	3.2	158
18	Electronic and optical properties of all polymorphic forms of silicon dioxide. Physical Review B, 1991, 44, 11048-11059.	3.2	153

#	Article	IF	Citations
19	First-Principles Calculation of Electronic, Optical, and Structural Properties of alpha-Al2O3. Journal of the American Ceramic Society, 1994, 77, 404-411.	3.8	139
20	Electronic, structural, and optical properties of crystalline yttria. Physical Review B, 1997, 56, 14993-15000.	3.2	139
21	Ab initiocalculation of the core-hole effect in the electron energy-loss near-edge structure. Physical Review B, 2000, 62, 7901-7907.	3.2	139
22	Electronic Structure and Electrical Conductivity of Undoped LiFePO[sub 4]. Electrochemical and Solid-State Letters, 2004, 7, A131.	2.2	131
23	Band theory of linear and nonlinear susceptibilities of some binary ionic insulators. Physical Review B, 1995, 52, 1596-1611.	3.2	127
24	Recent Advances in New Hard High-Pressure Nitrides. Advanced Materials, 2006, 18, 2933-2948.	21.0	127
25	A genomic approach to the stability, elastic, and electronic properties of the MAX phases. Physica Status Solidi (B): Basic Research, 2014, 251, 1480-1497.	1.5	126
26	Electronic structure of AlN. Physical Review B, 1986, 34, 5305-5308.	3.2	123
27	Electronic structures ofÎ²- andÎ±-silicon nitride. Physical Review B, 1981, 23, 5454-5463.	3.2	122
28	Ab initio elastic properties and tensile strength of crystalline hydroxyapatite. Acta Biomaterialia, 2009, 5, 3067-3075.	8.3	121
29	Electronic structure and excitonic-enhanced superconducting mechanism inYBa2Cu3O7â^'Î´. Physical Review Letters, 1987, 59, 1333-1336.	7.8	115
30	Nonscalability and nontransferability in the electronic properties of the Y-Al-O system. Physical Review B, 1999, 59, 12815-12821.	3.2	112
31	Band structure, cohesive energy, optical conductivity, and Compton profile of lithium. Physical Review B, 1974, 9, 5115-5121.	3.2	111
32	Electronic and optical properties ofÎ¸â^'Al2O3and comparison toÎ±â^'Al2O3. Physical Review B, 1998, 57, 15219-15228.	3.2	105
33	Calculation of optical excitations in cubic semiconductors. II. Second-harmonic generation. Physical Review B, 1993, 47, 9464-9478.	3.2	104
34	Key Interacting Residues between RBD of SARS-CoV-2 and ACE2 Receptor: Combination of Molecular Dynamics Simulation and Density Functional Calculation. Journal of Chemical Information and Modeling, 2021, 61, 4425-4441.	5.4	100
35	Theory of amorphous SiO2andSiOx. I. Atomic structural models. Physical Review B, 1982, 26, 6610-6621.	3.2	99
36	Band structures of all polycrystalline forms of silicon dioxide. Physical Review B, 1985, 31, 2172-2179.	3.2	98

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37	Intrinsic Mechanical Properties of 20 MAXâ€Phase Compounds. Journal of the American Ceramic Society, 2013, 96, 2292-2297.	3.8	95
38	Higher-Order Continuum Theory Applied to Fracture Simulation of Nanoscale Intergranular Glassy Film. Journal of Nanomechanics & Micromechanics, 2011, 1, 60-71.	1.4	91
39	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. Journal of the American Ceramic Society, 2002, 85, 75-80.	3.8	90
40	Electronic states and bonding configurations in hydrogenated amorphous silicon. Physical Review B, 1980, 21, 2378-2387.	3.2	89
41	Electronic structure of a grain-boundary model inSrTiO3. Physical Review B, 1999, 60, 2416-2424.	3.2	86
42	Electronic structure and bonding in garnet crystalsGd3Sc2Ga3O12,Gd3Sc2Al3O12,andGd3Ga3O12compared toY3Al3O12. Physical Review B, 2000, 61, 1817-1824.	3.2	85
43	First-principles calculation of the electronic and optical properties ofLiNbO3. Physical Review B, 1994, 50, 1992-1995.	3.2	84
44	Accurate Redetermination of the X-ray Structure and Electronic Bonding in Adenosylcobalamin. Inorganic Chemistry, 2004, 43, 1235-1241.	4.0	83
45	Mechanical properties, electronic structure and bonding of Î±- and Î²-tricalcium phosphates with surface characterization. Acta Biomaterialia, 2010, 6, 3763-3771.	8.3	83
46	Order-disorder transformations in chemisorbed layers: Oxygen on W(110). Surface Science, 1978, 77, 550-560.	1.9	82
47	Fullab initiogeometry optimization of all known crystalline phases ofSi3N4. Physical Review B, 2000, 61, 8696-8700.	3.2	82
48	Electronic structure of aluminum nitride: Theory and experiment. Applied Physics Letters, 1993, 63, 1182-1184.	3.3	81
49	Abâ€Initio Total Energy Calculation of Î±â€•and Î²â€Silicon Nitride and the Derivation of Effective Pair Potentials with Application to Lattice Dynamics. Journal of the American Ceramic Society, 1998, 81, 3189-3196.	3.8	81
50	Fundamental electronic structure and multiatomic bonding in 13 biocompatible high-entropy alloys. Npj Computational Materials, 2020, 6, .	8.7	79
51	Identification of ultradilute dopants in ceramics. Nature Materials, 2003, 2, 541-545.	27.5	78
52	Approximate lattice thermal conductivity of MAX phases at high temperature. Journal of the European Ceramic Society, 2015, 35, 3203-3212.	5.7	78
53	Structural disorder and electronic properties of amorphous silicon. Physical Review B, 1977, 16, 5488-5498.	3.2	75
54	Quantum Mechanical Metric for Internal Cohesion in Cement Crystals. Scientific Reports, 2014, 4, 7332.	3.3	74

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55	Electronic and Structural Properties of Bulk Î³â€Al₂O₃. Journal of the American Ceramic Society, 1997, 80, 1193-1197.	3.8	73
56	X-ray absorption near-edge structure in alpha-quartz and stishovite: Ab initio calculation with coreâ€“hole interaction. Applied Physics Letters, 2001, 78, 3809-3811.	3.3	72
57	Orthogonalized linear combinations of atomic orbitals: Application to the calculation of energy bands of Si III. Physical Review B, 1975, 12, 5536-5544.	3.2	71
58	Role of interatomic bonding in the mechanical anisotropy and interlayer cohesion of CSH crystals. Cement and Concrete Research, 2013, 52, 123-130.	11.0	71
59	Molecular mechanism and binding free energy of doxorubicin intercalation in DNA. Physical Chemistry Chemical Physics, 2019, 21, 3877-3893.	2.8	70
60	Electronic structure of normal, inverse, and partially inverse spinels in theMgAl2O4system. Physical Review B, 1996, 54, 16555-16561.	3.2	69
61	Optical properties of vanadium pentoxide determined from ellipsometry and band-structure calculations. Physical Review B, 1990, 42, 5289-5293.	3.2	68
62	Theory of amorphous SiO2andSiOx. II. Electron states in an intrinsic glass. Physical Review B, 1982, 26, 6622-6632.	3.2	66
63	Optical properties of superconductingK3C60and insulatingK6C60. Physical Review B, 1991, 44, 13171-13174.	3.2	66
64	Critical point analysis of the interband transition strength of electrons. Journal Physics D: Applied Physics, 1996, 29, 1740-1750.	2.8	66
65	Comparative studies of electronic and magnetic structures inY2Fe14B,Nd2Fe14B,Y2Co14B, andNd2Co14B. Physical Review B, 1987, 36, 8530-8546.	3.2	65
66	Electronic- and vibrational-structure calculations in models of the compressedSiO2glass system. Physical Review B, 1989, 39, 1320-1331.	3.2	64
67	Optical properties of aCaF2crystal. Physical Review B, 1992, 45, 8248-8255.	3.2	63
68	Theoretical calculation of optical properties of Y-Ba-Cu-O superconductors. Physical Review B, 1987, 36, 7203-7206.	3.2	62
69	Microscopic Calculation of Localized Electron States in an Intrinsic Glass. Physical Review Letters, 1981, 46, 607-610.	7.8	61
70	Selfconsistent band structures and optical calculations in cubic ferroelectric perovskites. Ferroelectrics, 1990, 111, 23-32.	0.6	61
71	Theoretical Studies of Electronic States Produced by Hydrogenation of Amorphous Silicon. Physical Review Letters, 1979, 42, 805-808.	7.8	60
72	The electronic structure and spectroscopic properties of 3C, 2H, 4H, 6H, 15R and 21R polymorphs of SiC. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 422, 147-156.	5.6	60

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73	Structure and Electronic Properties of a Continuous Random Network Model of an Amorphous Zeolitic Imidazolate Framework (a-ZIF). Journal of Physical Chemistry C, 2016, 120, 15362-15368.	3.1	60
74	Calculation of optical excitations in cubic semiconductors. III. Third-harmonic generation. Physical Review B, 1993, 47, 9479-9491.	3.2	59
75	Comprehending the occupying preference of manganese substitution in crystalline cement clinker phases: A theoretical study. Cement and Concrete Research, 2018, 109, 19-29.	11.0	59
76	Energy bands, optical conductivity, and Compton profile of sodium. Physical Review B, 1975, 11, 1324-1329.	3.2	58
77	Electronic properties of negative-curvature periodic graphitic carbon surfaces. Physical Review B, 1993, 47, 1593-1606.	3.2	58
78	Comparative studies of the electronic structure of LiFePO4, FePO4, Li3PO4, LiMnPO4, LiCoPO4, and LiNiPO4. Journal of Applied Physics, 2004, 95, 6583-6585.	2.5	58
79	Charge-Density Variation in a Model of Amorphous Silicon. Physical Review Letters, 1980, 44, 1513-1516.	7.8	57
80	Calculation of XANES/ELNES Spectra of All Edges in Si₃N₄ and Si₂N₂O. Journal of the American Ceramic Society, 2002, 85, 11-15.	3.8	57
81	Structural, electronic and optical properties of a large random network model of amorphous SiO2 glass. Journal of Non-Crystalline Solids, 2014, 383, 28-32.	3.1	56
82	Densification of a continuous random network model of amorphous SiO₂glass. Physical Chemistry Chemical Physics, 2014, 16, 1500-1514.	2.8	56
83	Monte Carlo studies of the critical behavior of site-dilute two-dimensional Ising models. Physical Review B, 1976, 13, 2962-2964.	3.2	55
84	Complex Nonlinear Deformation of Nanometer Intergranular Glassy Films inÎ²âˆ’Si3N4. Physical Review Letters, 2005, 95, 256103.	7.8	54
85	Intra- and intermolecular atomic-scale interactions in the receptor binding domain of SARS-CoV-2 spike protein: implication for ACE2 receptor binding. Physical Chemistry Chemical Physics, 2020, 22, 18272-18283.	2.8	53
86	Optical properties of Î²-C3N4and its pressure dependence. Physical Review B, 1994, 50, 11231-11234.	3.2	52
87	Electronic structures, total energies, and optical properties of Î±-rhombohedralB12and Î±-tetragonalB50crystals. Physical Review B, 1992, 45, 5895-5905.	3.2	50
88	Electronic structures and optical properties of low- and high-pressure phases of crystallineB2O3. Physical Review B, 1996, 54, 13616-13622.	3.2	50
89	Ab initiocalculations for the neutral and charged O vacancy in sapphire. Physical Review B, 1997, 56, 7277-7284.	3.2	50
90	Prediction of the new spinel phase ofTi3N4andSiTi2N4and the metal-insulator transition. Physical Review B, 2000, 61, 10609-10614.	3.2	50

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91	Electron energy loss near-edge structures of cubic Si3N4. Applied Physics Letters, 2001, 78, 2134-2136.	3.3	49
92	Ab initio simulation of elastic and mechanical properties of Zn- and Mg-doped hydroxyapatite (HAP). Journal of the Mechanical Behavior of Biomedical Materials, 2015, 47, 135-146.	3.1	49
93	Binding Interactions between Receptor-Binding Domain of Spike Protein and Human Angiotensin Converting Enzyme-2 in Omicron Variant. Journal of Physical Chemistry Letters, 2022, 13, 3915-3921.	4.6	49
94	Electronic and optical properties of Â-Al2O3fromab initiotheory. Journal of Physics Condensed Matter, 2004, 16, 2891-2900.	1.8	47
95	Mechanical Properties and Electronic Structure of Mullite Phases Using Firstâ€Principles Modeling. Journal of the American Ceramic Society, 2012, 95, 2075-2088.	3.8	46
96	Electronic Structure and Bonding of All Crystalline Phases in the Silicaâ€“Yttriaâ€“Silicon Nitride Phase Equilibrium Diagram. Journal of the American Ceramic Society, 2004, 87, 1996-2013.	3.8	44
97	Ab Initio Modeling of Structure and Properties of Single and Mixed Alkali Silicate Glasses. Journal of Physical Chemistry A, 2017, 121, 7697-7708.	2.5	44
98	Observation of reduced phase transition temperature in N-doped thermochromic film of monoclinic VO2. Applied Surface Science, 2017, 410, 363-372.	6.1	43
99	Disentangling the Effects of Shape and Dielectric Response in van der Waals Interactions between Anisotropic Bodies. Journal of Physical Chemistry C, 2015, 119, 19083-19094.	3.1	41
100	Nature of Interatomic Bonding in Controlling the Mechanical Properties of Calcium Silicate Hydrates. Journal of the American Ceramic Society, 2016, 99, 2120-2130.	3.8	41
101	Implication of the solvent effect, metal ions and topology in the electronic structure and hydrogen bonding of human telomeric G-quadruplex DNA. Physical Chemistry Chemical Physics, 2016, 18, 21573-21585.	2.8	41
102	Ab initio theoretical tensile test on Y-doped Î£=3 grain boundary in Î±-Al2O3. Acta Materialia, 2005, 53, 403-410.	7.9	40
103	Electronic Structure and Bonding of Î²â€SiAlON. Journal of the American Ceramic Society, 2000, 83, 780-786.	3.8	38
104	Density Functional Theory Study of Single Metal Atoms Embedded into MBene for Electrocatalytic Conversion of N₂ to NH₃. ACS Applied Nano Materials, 2020, 3, 9870-9879.	5.0	35
105	Designing the Interface of Carbon Nanotube/Biomaterials for High-Performance Ultra-Broadband Photodetection. ACS Applied Materials & Interfaces, 2017, 9, 11016-11024.	8.0	34
106	Electronic Structure, Dielectric Response and Surface Charge Distribution of RGD (1FUV) Peptide. Scientific Reports, 2014, 4, 5605.	3.3	33
107	The Hydration Effect and Selectivity of Alkali Metal Ions on Poly(ethylene glycol) Models in Cyclic and Linear Topology. Journal of Physical Chemistry A, 2017, 121, 4721-4731.	2.5	32
108	Electronic structure and optical properties of amorphous GeO2 in comparison to amorphous SiO2. Journal of Non-Crystalline Solids, 2015, 428, 176-183.	3.1	31

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109	Impact of Hydrogen Bonding in the Binding Site between Capsid Protein and MS2 Bacteriophage ssRNA. Journal of Physical Chemistry B, 2017, 121, 6321-6330.	2.6	30
110	Electronic structures and physical properties of Na2O doped silicate glass. Journal of Applied Physics, 2017, 121, .	2.5	29
111	Electronic Structure of a Near Î£11 aâ€axis Tilt Grain Boundary in Î±â€A12O3. Journal of the American Ceramic Society, 1996, 79, 627-633.	3.8	28
112	Electronic Structure and Partial Charge Distribution of Doxorubicin in Different Molecular Environments. ChemPhysChem, 2015, 16, 1451-1460.	2.1	26
113	Ab initio Modeling of the Electronic Structures and Physical Properties of aâ€Si_{1â^'x}Ge_xO₂ Glass (x = 0 to 1). Journal of the American Ceramic Society, 2016, 99, 3677-3684.	3.8	24
114	Atomic-Scale Quantification of Interfacial Binding between Peptides and Inorganic Crystals: The Case of Calcium Carbonate Binding Peptide on Aragonite. Journal of Physical Chemistry C, 2017, 121, 28354-28363.	3.1	24
115	Thermodynamic Dissection of the Intercalation Binding Process of Doxorubicin to dsDNA with Implications of Ionic and Solvent Effects. Journal of Physical Chemistry B, 2020, 124, 7803-7818.	2.6	24
116	Mechanical properties of silica glass predicted by a pair-wise potential in molecular dynamics simulations. Journal of Non-Crystalline Solids, 2016, 445-446, 102-109.	3.1	23
117	Firstâ€principles study in an interâ€granular glassy film model of silicon nitride. Journal of the American Ceramic Society, 2018, 101, 2673-2688.	3.8	23
118	Electron states of YAG probed by energy-loss near-edge spectrometry and ab initio calculations. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1999, 79, 921-940.	0.6	22
119	X-ray absorption near edge structure/electron energy loss near edge structure calculation using the supercell orthogonalized linear combination of atomic orbitals method. Journal of Physics Condensed Matter, 2009, 21, 104202.	1.8	22
120	Geometry Optimization and Ground-State Properties of Complex Ceramic Oxides. Journal of the American Ceramic Society, 2001, 84, 801-805.	3.8	21
121	Deformation behavior of an amorphous zeolitic imidazolate framework â€“ from a supersoft material to a complex organometallic alloy. Physical Chemistry Chemical Physics, 2018, 20, 29001-29011.	2.8	21
122	Ultra-large-scale ab initio quantum chemical computation of bio-molecular systems: The case of spike protein of SARS-CoV-2 virus. Computational and Structural Biotechnology Journal, 2021, 19, 1288-1301.	4.1	21
123	Abâ€initio Calculation of Yttrium Substitutional Impurities in alphaâ€Al₂O₃. Journal of the American Ceramic Society, 1997, 80, 3199-3204.	3.8	20
124	Structure and properties of hydrogrossular mineral series. Journal of the American Ceramic Society, 2017, 100, 4317-4330.	3.8	20
125	Elastic and electronic properties of Ti2Al(C N1â^') solid solutions. Journal of the European Ceramic Society, 2015, 35, 3219-3227.	5.7	19
126	Charge distribution and hydrogen bonding of a collagen Î±₂â€chain in vacuum, hydrated, neutral, and charged structural models. International Journal of Quantum Chemistry, 2016, 116, 681-691.	2.0	18

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127	Polarityâ€Controlled Attachment of Cytochrome C for Highâ€Performance Cytochrome C/Graphene van der Waals Heterojunction Photodetectors. Advanced Functional Materials, 2018, 28, 1704797.	14.9	18
128	Amino acid interacting network in the receptor-binding domain of SARS-CoV-2 spike protein. RSC Advances, 2020, 10, 39831-39841.	3.6	18
129	Structural and physical properties of 99 complex bulk chalcogenides crystals using first-principles calculations. Scientific Reports, 2021, 11, 9921.	3.3	18
130	Mutations of Omicron Variant at the Interface of the Receptor Domain Motif and Human Angiotensin-Converting Enzyme-2. International Journal of Molecular Sciences, 2022, 23, 2870.	4.1	18
131	Optical properties and electronic transitions of DNA oligonucleotides as a function of composition and stacking sequence. Physical Chemistry Chemical Physics, 2015, 17, 4589-4599.	2.8	17
132	van der Waals Interactions on the Mesoscale: Open-Science Implementation, Anisotropy, Retardation, and Solvent Effects. Langmuir, 2015, 31, 10145-10153.	3.5	17
133	Temperature-Dependent Properties of Molten Li₂BeF₄ Salt Using Ab Initio Molecular Dynamics. ACS Omega, 2021, 6, 19822-19835.	3.5	17
134	Ab initio study on the adsorption mechanism of oxygen on Cr2AlC (0 0 0 1) surface. Applied Surface Science, 2014, 315, 45-54.	6.1	16
135	Ab initio calculations of thermomechanical properties and electronic structure of vitreloy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">Z</mml:mi><mml:msub><mml:mi mathvariant="normal">r</mml:mi><mml:mrow><mml:mn>41.2</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">T</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mrow><mml:mn>13.8</mml:mn></mml:mrow></mml:msub><mml:mi	3.2	16
136	Theoretical investigation of C-(A)-S-H(I) cement hydrates. Construction and Building Materials, 2018, 184, 536-548.	7.2	15
137	Anti-perovskite carbides and nitrides A3BX: A new family of damage tolerant ceramics. Journal of Materials Science and Technology, 2020, 40, 64-71.	10.7	15
138	First-principles calculation of lattice distortions in four single phase high entropy alloys with experimental validation. Materials and Design, 2021, 209, 110071.	7.0	15
139	First-Principles Simulation of Dielectric Function in Biomolecules. Materials, 2021, 14, 5774.	2.9	15
140	Computational Design of Miniproteins as SARS-CoV-2 Therapeutic Inhibitors. International Journal of Molecular Sciences, 2022, 23, 838.	4.1	15
141	Understanding the atomic and electronic origin of mechanical property in thaumasite and ettringite mineral crystals. Journal of the American Ceramic Society, 2018, 101, 5177-5187.	3.8	14
142	Ab initio molecular dynamics simulation of Na-doped aluminosilicate glasses and glass-water interaction. AIP Advances, 2019, 9, .	1.3	14
143	First-Principles Calculations of Thermoelectric Transport Properties of Quaternary and Ternary Bulk Chalcogenide Crystals. Materials, 2022, 15, 2843.	2.9	14
144	Oxidation of Cr2AlC (0001): Insights from Ab Initio Calculations. Jom, 2013, 65, 1487-1491.	1.9	13

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145	The bonding, charge distribution, spin ordering, optical, and elastic properties of four MAX phases Cr2AX (Aâ€‰=â€‰Al or Ge, Xâ€‰=â€‰C or N): From density functional theory study. Journal of Applied Physics, 2013, 114, .	2.2	13
146	Complex interplay of interatomic bonding in a multi-component pyrophosphate crystal: K 2 Mg (H 2 P 2) Tj ETQq0 0 0 rgBT /Overlock 10	2.4	13
147	Structural, electronic, and dielectric properties of a large random network model of amorphous zeolitic imidazolate frameworks and its analogues. Journal of the American Ceramic Society, 2019, 102, 4602-4611.	3.8	13
148	<I>Ab-initio</I> Calculation of Si-K and Si-L ELNES Edges in an Extended Inactive Defect Model of Crystalline Silicon. Materials Transactions, 2002, 43, 1430-1434.	1.2	11
149	Computational Study of a Heterostructural Model of Type I Collagen and Implementation of an Amino Acid Potential Method Applicable to Large Proteins. Polymers, 2014, 6, 491-514.	4.5	11
150	Conspicuous interatomic bonding in chalcogenide crystals and implications on electronic, optical, and elastic properties. AIP Advances, 2020, 10, .	1.3	11
151	DFT Study of Electronic Structure and Optical Properties of Kaolinite, Muscovite, and Montmorillonite. Crystals, 2021, 11, 618.	2.2	11
152	Delta Variant with P681R Critical Mutation Revealed by Ultra-Large Atomic-Scale Ab Initio Simulation: Implications for the Fundamentals of Biomolecular Interactions. Viruses, 2022, 14, 465.	3.3	11
153	Understanding the atomistic origin of hydration effects in single and mixed bulk alkaliâ€silicate glasses. Journal of the American Ceramic Society, 2019, 102, 207-221.	3.8	10
154	Synthesis of monodisperse rod-shaped silica particles through biotemplating of surface-functionalized bacteria. Nanoscale, 2020, 12, 8732-8741.	5.6	10
155	Unraveling the effects of linker substitution on structural, electronic and optical properties of amorphous zeolitic imidazolate frameworks-62 (a-ZIF-62) glasses: a DFT study. RSC Advances, 2020, 10, 14013-14024.	3.6	10
156	Solvent Effect on the Structure and Properties of RGD Peptide (1FUV) at Body Temperature (310 K) Using Ab Initio Molecular Dynamics. Polymers, 2021, 13, 3434.	4.5	10
157	Electronic Structure and Bonding in Crystalline Y₁₀[SiO₄]₆N₂. Journal of the American Ceramic Society, 2003, 86, 1424-1426.	3.8	9
158	Dielectric response variation and the strength of van der Waals interactions. Journal of Colloid and Interface Science, 2014, 417, 278-284.	9.4	9
159	Ab Initio Study of Hydrolysis Effects in Single and Ion-Exchanged Alkali Aluminosilicate Glasses. Journal of Physical Chemistry B, 2020, 124, 8418-8433.	2.6	9
160	Crystal Structure and Elastic Properties of Hypothesized <scp>MAX</scp> Phaseâ€Like Compound (<scp><scp>Cr</scp></scp>₂<scp><scp>Hf</scp></scp>)₂<scp><scp>Al</scp></scp>₃<scp><scp>C</scp></scp>₂. Journal of the American Ceramic Society, 2014, 97, 2646-2653.	3.8	8
161	Metallic Ternary Telluride with Sphalerite Superstructure. Inorganic Chemistry, 2016, 55, 2114-2122.	4.0	8
162	Interfacial Interaction between Suolunite Crystal and Silica Binding Peptide for Novel Bioinspired Cement. ACS Combinatorial Science, 2019, 21, 794-804.	3.8	8

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163	Subtle Variations of the Electronic Structure and Mechanical Properties of High Entropy Alloys With 50% Carbon Composites. Frontiers in Materials, 2020, 7, .	2.4	8
164	Prediction of a high-density phase of SiO2 with a high dielectric constant. Physica Status Solidi (B): Basic Research, 2005, 242, R64-R66.	1.5	7
165	Crystal Plasticity Modeling of Void Growth on Grain Boundaries in Ni-Based Superalloys. Jom, 2019, 71, 3859-3868.	1.9	7
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