Wai-Yim Ching

List of Publications by Year
in descending order

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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	Computational Design of Miniproteins as SARS-CoV-2 Therapeutic Inhibitors. International Journal of Molecular Sciences, 2022, 23, 838.	4.1	15
2	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
3	Role of chemical disorder on radiation-induced defect production and damage evolution in NiFeCoCr. Journal of Nuclear Materials, 2022, 565, 153689.	2.7	3
4	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
5	First-Principles Calculations of Thermoelectric Transport Properties of Quaternary and Ternary Bulk Chalcogenide Crystals. Materials, 2022, 15, 2843.	2.9	14
6	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
7	Ceramic Genomics: Total Bond Order Density. , 2021, , 441-474.		1
8	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
9	Structural and physical properties of 99 complex bulk chalcogenides crystals using first-principles calculations. Scientific Reports, 2021, 11, 9921.	3.3	18
10	DFT Study of Electronic Structure and Optical Properties of Kaolinite, Muscovite, and Montmorillonite. Crystals, 2021, 11, 618.	2.2	11
11	Temperature-Dependent Properties of Molten Li₂BeF₄ Salt Using Ab Initio Molecular Dynamics. ACS Omega, 2021, 6, 19822-19835.	3.5	17
12	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
13	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
14	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
15	First-Principles Simulation of Dielectric Function in Biomolecules. Materials, 2021, 14, 5774.	2.9	15
16	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
17	Origin of the existence of interâ€granular glassy films in Î²â€Si₃N₄. Journal of the American Ceramic Society, 2020, 103, 737-743.	3.8	4
18	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

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19	Amino acid interacting network in the receptor-binding domain of SARS-CoV-2 spike protein. RSC Advances, 2020, 10, 39831-39841.	3.6	18
20	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
21	Conspicuous interatomic bonding in chalcogenide crystals and implications on electronic, optical, and elastic properties. AIP Advances, 2020, 10, .	1.3	11
22	Effects of the halogenated imidazolate linker on the fundamental properties of amorphous zeolitic imidazolate frameworks. Journal of Non-Crystalline Solids, 2020, 536, 120005.	3.1	6
23	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
24	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
25	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
26	Atomic-level insights into the influence of zinc incorporation on clinker hydration reactivity. Open Ceramics, 2020, 1, 100004.	2.0	6
27	Fundamental electronic structure and multiatomic bonding in 13 biocompatible high-entropy alloys. Npj Computational Materials, 2020, 6, .	8.7	79
28	Synthesis of monodisperse rod-shaped silica particles through biotemplating of surface-functionalized bacteria. Nanoscale, 2020, 12, 8732-8741.	5.6	10
29	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
30	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
31	Ab initio molecular dynamics simulation of Na-doped aluminosilicate glasses and glass-water interaction. AIP Advances, 2019, 9, .	1.3	14
32	Crystal Plasticity Modeling of Void Growth on Grain Boundaries in Ni-Based Superalloys. Jom, 2019, 71, 3859-3868.	1.9	7
33	Electronic structure and mechanical properties of crystalline precipitate phases M₂₃C₆(M=Cr, W, Mo, Fe) in Ni-based superalloys. Materials Research Express, 2019, 6, 116323.	1.6	6
34	Molecular mechanism and binding free energy of doxorubicin intercalation in DNA. Physical Chemistry Chemical Physics, 2019, 21, 3877-3893.	2.8	70
35	Atomic-Scale Understanding of Structure and Properties of Complex Pyrophosphate Crystals by First-Principles Calculations. Applied Sciences (Switzerland), 2019, 9, 840.	2.5	6
36	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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37	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
38	First-Principles Calculation. Springer Handbooks, 2019, , 1097-1130.	0.6	3
39	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
40	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
41	Molecular Dynamic and Free Energy Analysis of Doxorubicin and DNA Complex. Biophysical Journal, 2018, 114, 528a.	0.5	2
42	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
43	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
44	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
45	Interaction between Capsid Coat Protein and MS2 Bacteriophage SSRNA with Different Loop Motif for Virus Assembly Process. Biophysical Journal, 2018, 114, 252a.	0.5	1
46	Theoretical investigation of C-(A)-S-H(I) cement hydrates. Construction and Building Materials, 2018, 184, 536-548.	7.2	15
47	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
48	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
49	Designing the Interface of Carbon Nanotube/Biomaterials for High-Performance Ultra-Broadband Photodetection. ACS Applied Materials & Interfaces, 2017, 9, 11016-11024.	8.0	34
50	Observation of reduced phase transition temperature in N-doped thermochromic film of monoclinic VO2. Applied Surface Science, 2017, 410, 363-372.	6.1	43
51	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
52	Structure and properties of hydrogrossular mineral series. Journal of the American Ceramic Society, 2017, 100, 4317-4330.	3.8	20
53	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
54	Electronic structures and physical properties of Na2O doped silicate glass. Journal of Applied Physics, 2017, 121, .	2.5	29

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55	Complex interplay of interatomic bonding in a multi-component pyrophosphate crystal: K 2 Mg (H 2 P 2) Tj ETQq1 1 0.784314 rgBT /O	2.4	13
56	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
57	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
58	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
59	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"><mml:mrow><mml:mn>13.8</mml:mn></mml:mrow></mml:msub><mml:mi	3.2	16
60	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
61	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
62	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
63	Materials Informatics Using Ab initio Data: Application to MAX Phases. Springer Series in Materials Science, 2016, , 187-212.	0.6	3
64	Metallic Ternary Telluride with Sphalerite Superstructure. Inorganic Chemistry, 2016, 55, 2114-2122.	4.0	8
65	Electronic Structure and Partial Charge Distribution of Doxorubicin in Different Molecular Environments. ChemPhysChem, 2015, 16, 1451-1460.	2.1	26
66	Approximate lattice thermal conductivity of MAX phases at high temperature. Journal of the European Ceramic Society, 2015, 35, 3203-3212.	5.7	78
67	Elastic and electronic properties of Ti2Al(C N1â^') solid solutions. Journal of the European Ceramic Society, 2015, 35, 3219-3227.	5.7	19
68	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
69	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
70	van der Waals Interactions on the Mesoscale: Open-Science Implementation, Anisotropy, Retardation, and Solvent Effects. Langmuir, 2015, 31, 10145-10153.	3.5	17
71	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
72	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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73	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
74	Dependence of the strength of van der Waals interactions on the details of the dielectric response variation. Materials Research Society Symposia Proceedings, 2014, 1648, 1.	0.1	0
75	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
76	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
77	Optical Properties and van der Waals-London Dispersion Interactions in Inorganic and Biomolecular Assemblies. Materials Research Society Symposia Proceedings, 2014, 1619, 1.	0.1	0
78	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
79	Densification of a continuous random network model of amorphous SiO₂glass. Physical Chemistry Chemical Physics, 2014, 16, 1500-1514.	2.8	56
80	Dielectric response variation and the strength of van der Waals interactions. Journal of Colloid and Interface Science, 2014, 417, 278-284.	9.4	9
81	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
82	High-Resolution Spectroscopy of Bonding in a Novel BeP2N4Compound. Microscopy and Microanalysis, 2014, 20, 664-670.	0.4	5
83	Quantum Mechanical Metric for Internal Cohesion in Cement Crystals. Scientific Reports, 2014, 4, 7332.	3.3	74
84	Electronic Structure, Dielectric Response and Surface Charge Distribution of RGD (1FUV) Peptide. Scientific Reports, 2014, 4, 5605.	3.3	33
85	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
86	Oxidation of Cr2AlC (0001): Insights from Ab Initio Calculations. Jom, 2013, 65, 1487-1491.	1.9	13
87	Intrinsic Mechanical Properties of 20 MAXâ€Phase Compounds. Journal of the American Ceramic Society, 2013, 96, 2292-2297.	3.8	95
88	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, .	2.3	13
89	Historical Account of the LCAO Method. , 2012, , 6-13.		0
90	Application to Semiconductors and Insulators. , 2012, , 53-89.		0

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91	Application to Biomolecular Systems. , 2012, , 197-212.		0
92	Application to Complex Crystals. , 2012, , 114-141.		0
93	Electronic Structure Methods in Materials Theory. , 2012, , 1-5.		3
94	Basic Theory and Techniques of the OLCAO Method. , 2012, , 14-34.		0
95	Calculation of Physical Properties Using the OLCAO Method. , 2012, , 35-52.		0
96	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
97	Application to Crystalline Metals and Alloys. , 2012, , 90-113.		0
98	Application to Non-Crystalline Solids and Liquids. , 2012, , 142-170.		0
99	Enhancement and Extension of the OLCAO Method. , 2012, , 241-259.		0
100	Application to Impurities, Defects, and Surfaces. , 2012, , 171-196.		0
101	Application to Core Level Spectroscopy. , 2012, , 213-240.		0
102	Higher-Order Continuum Theory Applied to Fracture Simulation of Nanoscale Intergranular Glassy Film. Journal of Nanomechanics & Micromechanics, 2011, 1, 60-71.	1.4	91
103	Mechanical properties, electronic structure and bonding of Î±- and Î²-tricalcium phosphates with surface characterization. Acta Biomaterialia, 2010, 6, 3763-3771.	8.3	83
104	Long range interactions in nanoscale science. Reviews of Modern Physics, 2010, 82, 1887-1944.	45.6	359
105	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
106	Ab initio elastic properties and tensile strength of crystalline hydroxyapatite. Acta Biomaterialia, 2009, 5, 3067-3075.	8.3	121
107	Ab Initio Calculation of Elastic Constants of Ceramic Crystals. Journal of the American Ceramic Society, 2007, 90, 3194-3204.	3.8	281
108	Grain Boundary Strengthening in Alumina by Rare Earth Impurities. Science, 2006, 311, 212-215.	12.6	391

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109	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
110	Recent Advances in New Hard High-Pressure Nitrides. Advanced Materials, 2006, 18, 2933-2948.	21.0	127
111	Ab initio theoretical tensile test on Y-doped Î£=3 grain boundary in Î±-Al2O3. Acta Materialia, 2005, 53, 403-410.	7.9	40
112	"Electronic Structure and Bonding of All Crystalline Phases in the Silica-Yttria-Silicon Nitride Phase Equilibrium Diagram". Journal of the American Ceramic Society, 2005, 88, 2011-2011.	3.8	2
113	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
114	Complex Nonlinear Deformation of Nanometer Intergranular Glassy Films inÎ²â^'Si3N4. Physical Review Letters, 2005, 95, 256103.	7.8	54
115	Electronic and optical properties of Â-Al2O3fromab initiotheory. Journal of Physics Condensed Matter, 2004, 16, 2891-2900.	1.8	47
116	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
117	Electronic Structure and Electrical Conductivity of Undoped LiFePO[sub 4]. Electrochemical and Solid-State Letters, 2004, 7, A131.	2.2	131
118	Accurate Redetermination of the X-ray Structure and Electronic Bonding in Adenosylcobalamin. Inorganic Chemistry, 2004, 43, 1235-1241.	4.0	83
119	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
120	Electronic Structure and Bonding in Crystalline Y₁₀[SiO₄]₆N₂. Journal of the American Ceramic Society, 2003, 86, 1424-1426.	3.8	9
121	Identification of ultradilute dopants in ceramics. Nature Materials, 2003, 2, 541-545.	27.5	78
122	<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
123	Structure and Properties of Advanced Nitrides. Journal of the American Ceramic Society, 2002, 85, 1-1.	3.8	3
124	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
125	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. Journal of the American Ceramic Society, 2002, 85, 75-80.	3.8	90
126	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

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127	Geometry Optimization and Ground-State Properties of Complex Ceramic Oxides. Journal of the American Ceramic Society, 2001, 84, 801-805.	3.8	21
128	Electron energy loss near-edge structures of cubic Si3N4. Applied Physics Letters, 2001, 78, 2134-2136.	3.3	49
129	Prediction of the new spinel phase ofTi3N4andSiTi2N4and the metal-insulator transition. Physical Review B, 2000, 61, 10609-10614.	3.2	50
130	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
131	Fullab initiogeometry optimization of all known crystalline phases ofSi3N4. Physical Review B, 2000, 61, 8696-8700.	3.2	82
132	Electronic structure and bonding in garnet crystalsGd3Sc2Ga3O12,Gd3Sc2Al3O12,andGd3Ga3O12compared toY3Al3O12. Physical Review B, 2000, 61, 1817-1824.	3.2	85
133	Electronic Structure and Bonding of Î²â€SiAlON. Journal of the American Ceramic Society, 2000, 83, 780-786.	3.8	38
134	Nonscalability and nontransferability in the electronic properties of the Y-Al-O system. Physical Review B, 1999, 59, 12815-12821.	3.2	112
135	Interesting Physical Properties of the New Spinel Phase ofSi3N4andC3N4. Physical Review Letters, 1999, 83, 5046-5049.	7.8	205
136	Electronic structure of a grain-boundary model inSrTiO3. Physical Review B, 1999, 60, 2416-2424.	3.2	86
137	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
138	Electronic structure of yttrium aluminum garnet(Y3Al5O12). Physical Review B, 1999, 59, 10530-10535.	3.2	158
139	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
140	Electronic and optical properties ofÎ¸â^'Al2O3and comparison toÎ±â^'Al2O3. Physical Review B, 1998, 57, 15219-15228.	3.2	105
141	Ab initiocalculations for the neutral and charged O vacancy in sapphire. Physical Review B, 1997, 56, 7277-7284.	3.2	50
142	Electronic, structural, and optical properties of crystalline yttria. Physical Review B, 1997, 56, 14993-15000.	3.2	139
143	Electronic and Structural Properties of Bulk Î³â€Al₂O₃. Journal of the American Ceramic Society, 1997, 80, 1193-1197.	3.8	73
144	Abâ€initio Calculation of Yttrium Substitutional Impurities in alphaâ€Al₂O₃. Journal of the American Ceramic Society, 1997, 80, 3199-3204.	3.8	20

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145	Electronic structures and optical properties of low- and high-pressure phases of crystallineB2O3. Physical Review B, 1996, 54, 13616-13622.	3.2	50
146	Critical point analysis of the interband transition strength of electrons. Journal Physics D: Applied Physics, 1996, 29, 1740-1750.	2.8	66
147	Electronic structure of normal, inverse, and partially inverse spinels in theMgAl2O4system. Physical Review B, 1996, 54, 16555-16561.	3.2	69
148	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
149	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
150	Electronic and optical properties of three phases of titanium dioxide: Rutile, anatase, and brookite. Physical Review B, 1995, 51, 13023-13032.	3.2	891
151	Band theory of linear and nonlinear susceptibilities of some binary ionic insulators. Physical Review B, 1995, 52, 1596-1611.	3.2	127
152	Optical properties of Î²-C3N4and its pressure dependence. Physical Review B, 1994, 50, 11231-11234.	3.2	52
153	First-principles calculation of the electronic and optical properties ofLiNbO3. Physical Review B, 1994, 50, 1992-1995.	3.2	84
154	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
155	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
156	Calculation of optical excitations in cubic semiconductors. I. Electronic structure and linear response. Physical Review B, 1993, 47, 9449-9463.	3.2	186
157	Calculation of optical excitations in cubic semiconductors. III. Third-harmonic generation. Physical Review B, 1993, 47, 9479-9491.	3.2	59
158	Electronic properties of negative-curvature periodic graphitic carbon surfaces. Physical Review B, 1993, 47, 1593-1606.	3.2	58
159	Electronic, optical, and structural properties of some wurtzite crystals. Physical Review B, 1993, 48, 4335-4351.	3.2	642
160	Calculation of optical excitations in cubic semiconductors. II. Second-harmonic generation. Physical Review B, 1993, 47, 9464-9478.	3.2	104
161	Electronic structure of aluminum nitride: Theory and experiment. Applied Physics Letters, 1993, 63, 1182-1184.	3.3	81
162	Electronic structures, total energies, and optical properties of Î±-rhombohedralB12and Î±-tetragonalB50crystals. Physical Review B, 1992, 45, 5895-5905.	3.2	50

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163	Optical properties of aCaF2crystal. Physical Review B, 1992, 45, 8248-8255.	3.2	63
164	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
165	Electronic and optical properties of all polymorphic forms of silicon dioxide. Physical Review B, 1991, 44, 11048-11059.	3.2	153
166	Optical properties of superconductingK3C60and insulatingK6C60. Physical Review B, 1991, 44, 13171-13174.	3.2	66
167	Analytic solution of a two-dimensional hydrogen atom. I. Nonrelativistic theory. Physical Review A, 1991, 43, 1186-1196.	2.5	236
168	First-principles calculation of optical properties of C_{60} in the fcc lattice. Physical Review Letters, 1991, 67, 2045-2048.	7.8	177
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