Robert A Evarestov

List of Publications by Year
in descending order

305 papers	5,797 citations	109321 35 h-index	114465 63 g-index
311 all docs	311 docs citations	311 times ranked	5271 citing authors

#	Article	IF	Citations
1	Phonon dispersion and Raman scattering in hexagonal GaN and AlN. Physical Review B, 1998, 58, 12899-12907.	3.2	741
2	Special points of the brillouin zone and their use in the solid state theory. Physica Status Solidi (B): Basic Research, 1983, 119, 9-40.	1.5	176
3	First-principles calculations of the atomic and electronic structure ofFcenters in the bulk and on the (001) surface ofSrTiO3. Physical Review B, 2006, 73, .	3.2	152
4	Electronic structure and properties ofCu2O. Physical Review B, 1997, 56, 7189-7196.	3.2	146
5	Adsorption of Water on the TiO2(Rutile) (110) Surface:Â A Comparison of Periodic and Embedded Cluster Calculations. Journal of Physical Chemistry B, 2004, 108, 7844-7853.	2.6	126
6	Modification of the Monkhorst-Pack special points meshes in the Brillouin zone for density functional theory and Hartree-Fock calculations. Physical Review B, 2004, 70, .	3.2	103
7	Electronic and magnetic structure of ScMnO3. Physica Status Solidi (B): Basic Research, 2006, 243, R10-R12.	1.5	98
8	First-principles study of bulk and surface oxygen vacancies in SrTiO3 crystal. European Physical Journal B, 2009, 72, 53-57.	1.5	94
9	Firstâ€principles calculations on the four phases of BaTiO₃. Journal of Computational Chemistry, 2012, 33, 1123-1130.	3.3	89
10	Site Symmetry in Crystals. Springer Series in Solid-state Sciences, 1997, , .	0.3	87
11	Comparative density-functional LCAO and plane-wave calculations ofLaMnO3surfaces. Physical Review B, 2005, 72, .	3.2	84
12	Phonon calculations in cubic and tetragonal phases of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: A comparative LCAO and plane-wave study. Physical Review B, 2011, 83, .	3.2	81
13	Large unit cell calculations of solids in the CNDO approximation. Physica Status Solidi (B): Basic Research, 1977, 79, 743-751.	1.5	77
14	Adsorption of water on (001) surface of SrTiO3 and SrZrO3 cubic perovskites: Hybrid HF-DFT LCAO calculations. Surface Science, 2007, 601, 1844-1856.	1.9	77
15	A Comparative Ab Initio Thermodynamic Study of Oxygen Vacancies in ZnO and SrTiO₃: Emphasis on Phonon Contribution. Journal of Physical Chemistry C, 2013, 117, 13776-13784.	3.1	72
16	Periodic models in quantum chemical simulations of F centers in crystalline metal oxides. International Journal of Quantum Chemistry, 2007, 107, 2956-2985.	2.0	69
17	From anatase (101) surface to TiO2 nanotubes: Rolling procedure and first principles LCAO calculations. Surface Science, 2009, 603, L117-L120.	1.9	68
18	Single impurities in insulators:â€ƒAb initiostudy of Fe-dopedSrTiO3. Physical Review B, 2003, 67, .	3.2	67

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19	The Energy Band Structure of Corundum. Physica Status Solidi (B): Basic Research, 1980, 99, 387-396.	1.5	56
20	DFT plane wave calculations of the atomic and electronic structure of LaMnO3(001) surface. Physical Chemistry Chemical Physics, 2005, 7, 2346.	2.8	54
21	Ab initio study of the electronic and atomic structure of the wolframite-type ZnWO4. Solid State Communications, 2009, 149, 425-428.	1.9	54
22	Jahn-Teller effect in the phonon properties of defective SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2012, 85, .	3.2	51
23	Quantum Chemistry of Solids. Springer Series in Solid-state Sciences, 2012, , .	0.3	51
24	Titania nanotubes modeled from 3- and 6-layered (101) anatase sheets: Line group symmetry and comparative ab initio LCAO calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 43, 266-278.	2.7	49
25	Hybrid density functional theory LCAO calculations on phonons in Ba(Ti,Zr,Hf)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	3.2	49
26	Ab initio LCAO study of the atomic, electronic and magnetic structures and the lattice dynamics of triclinic CuWO4. Acta Materialia, 2013, 61, 371-378.	7.9	49
27	Quantum-chemical definition of the atomic valence in molecules and crystals. Theoretica Chimica Acta, 1991, 81, 95-103.	0.8	47
28	Symmetry and Models of Single-Wall BN and TiO₂ Nanotubes with Hexagonal Morphology. Journal of Physical Chemistry C, 2010, 114, 21061-21069.	3.1	46
29	The translational symmetry in the molecular models of solids. Physica Status Solidi (B): Basic Research, 1975, 68, 453-461.	1.5	42
30	Use of representative points of the Brillouin zone for the selfâ€consistent calculations of solids in the large unit cell approach. Physica Status Solidi (B): Basic Research, 1975, 72, 569-578.	1.5	40
31	A firstâ€principles DFT study of UN bulk and (001) surface: Comparative LCAO and PW calculations. Journal of Computational Chemistry, 2008, 29, 2079-2087.	3.3	40
32	Hybrid HFâ€“DFT modeling of monolayer water adsorption on (001) surface of cubic BaHfO3 and BaZrO3 crystals. Surface Science, 2010, 604, 1591-1597.	1.9	40
33	Use of the Symmetryâ€Adapted Atomic Orbitals in the Large Unit Cell Approach to Solids. Physica Status Solidi (B): Basic Research, 1979, 93, 469-482.	1.5	39
34	Ab initiostudy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sr</mml:mi><mml:msub><mml:mi mathvariant="normal">Fe</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>: Jahn-Teller distortion and electronic structure. Physical Review B, 2008, 77, .	3.2	38
35	First-principles comparative study of perfect and defective CsPbX₃ (X = Br, I) crystals. Physical Chemistry Chemical Physics, 2020, 22, 3914-3920.	2.8	37
36	Local characteristics of crystal electronic structure in the Hartree-Fock method. Physics of the Solid State, 1999, 41, 1286-1290.	0.6	33

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37	Quantum mechanicsâ€“molecular dynamics approach to the interpretation of x-ray absorption spectra. Journal of Physics Condensed Matter, 2009, 21, 055401.	1.8	33
38	Symmetry and Models of Double-Wall BN and TiO₂Nanotubes with Hexagonal Morphology. Journal of Physical Chemistry C, 2011, 115, 14067-14076.	3.1	33
39	Thermodynamic stability and disordering in La Sr1âˆ'MnO3 solid solutions. Solid State Ionics, 2006, 177, 217-222.	2.7	31
40	Ab initio structure modeling of ZrO2 nanosheets and single-wall nanotubes. Computational Materials Science, 2012, 65, 395-405.	3.0	31
41	HF and DFT calculations of MgO surface energy and electrostatic potential using two- and three-periodic models. International Journal of Quantum Chemistry, 2004, 100, 452-459.	2.0	30
42	DFT study of a singleF center in cubic SrTiO3 perovskite. International Journal of Quantum Chemistry, 2006, 106, 2173-2183.	2.0	30
43	Plain DFT and hybrid HF-DFT LCAO calculations of SnO2 (110) and (100) bare and hydroxylated surfaces. Physica Status Solidi (B): Basic Research, 2006, 243, 1823-1834.	1.5	30
44	Ab initio Hartree-Fock calculations of LaMnO3 (110) surfaces. Solid State Communications, 2003, 127, 367-371.	1.9	29
45	DFT LCAO and plane wave calculations of SrZrO3. Physica Status Solidi (B): Basic Research, 2005, 242, R11-R13.	1.5	29
46	Theoretical modeling of the complexes of iron impurities and oxygen vacancies in SrTiO3. Applied Physics Letters, 2013, 102, .	3.3	29
47	First-principles calculations of iodine-related point defects in CsPbI₃. Physical Chemistry Chemical Physics, 2019, 21, 7841-7846.	2.8	29
48	Wannier-type atomic functions and chemical bonding in crystals. International Journal of Quantum Chemistry, 2002, 88, 642-651.	2.0	28
49	Ab initio calculations of the LaMnO3 surface properties. Applied Surface Science, 2004, 238, 457-463.	6.1	27
50	Hybrid HF-DFT comparative study of SrZrO3 and SrTiO3(001) surface properties. Physica Status Solidi (B): Basic Research, 2006, 243, 2756-2763.	1.5	27
51	First-Principles Evaluation of the Morphology of WS₂ Nanotubes for Application as Visible-Light-Driven Water-Splitting Photocatalysts. ACS Omega, 2019, 4, 1434-1442.	3.5	27
52	Calculations of the Electronic Structure of Colour Centres in Ionic Crystals (II). Physica Status Solidi (B): Basic Research, 1970, 40, 433-460.	1.5	26
53	Oxygen vacancy formation energies in Sr-doped complex perovskites: ab initio thermodynamic study. Solid State Ionics, 2014, 254, 11-16.	2.7	26
54	First-principles periodic and semiempirical cyclic cluster calculations for single oxygen vacancies in crystalline Al2O3. Physica Status Solidi (B): Basic Research, 2004, 241, 1032-1040.	1.5	25

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55	Electronic Structure of La₂O₃ and LaF₃ Crystals. Physica Status Solidi (B): Basic Research, 1992, 170, 145-153.	1.5	24
56	Quasi-two-dimensional behavior of phonon subsystems and the superconductivity mechanism in perovskitelike compounds. Physical Review B, 1994, 49, 9933-9943.	3.2	24
57	TiS₂and ZrS₂single- and double-wall nanotubes: First-principles study. Journal of Computational Chemistry, 2014, 35, 395-405.	3.3	24
58	Phonon spectra, electronic, and thermodynamic properties of WS₂ nanotubes. Journal of Computational Chemistry, 2017, 38, 2581-2593.	3.3	24
59	Hartreeâ€fock exchange and LCAO approximation in the band structure calculations of solids. Physica Status Solidi (B): Basic Research, 1983, 117, 417-427.	1.5	23
60	Investigation of the chemical bonding in nickel mixed oxides from electronic structure calculations. Journal of Physics and Chemistry of Solids, 1996, 57, 1839-1850.	4.0	23
61	Electronic structure of crystalline uranium nitrides UN, U₂N₃and UN₂: LCAO calculations with the basis set optimization. Journal of Physics: Conference Series, 2008, 117, 012015.	0.4	23
62	Allâ€electron LCAO calculations of the LiF crystal phonon spectrum: Influence of the basis set, the exchangeâ€correlation functional, and the supercell size. Journal of Computational Chemistry, 2009, 30, 2645-2655.	3.3	23
63	Surface modelling on heavy atom crystalline compounds: HfO2 and UO2 fluorite structures. Acta Materialia, 2009, 57, 600-606.	7.9	23
64	First-principles LCAO study of phonons in NiWO4. Open Physics, 2011, 9, .	1.7	23
65	Origin of pressureâ€induced insulatorâ€toâ€metal transition in the van der Waals compound FePS₃ from firstâ€principles calculations. Journal of Computational Chemistry, 2020, 41, 1337-1344.	3.3	23
66	Site Symmetry in Crystals. Springer Series in Solid-state Sciences, 1993, , .	0.3	23
67	The origin of energy functional in Roothaan open shellSCF theory. International Journal of Quantum Chemistry, 1990, 37, 35-50.	2.0	22
68	Local properties of the electronic structure of cubic SrTiO3, BaTiO3 and PbTiO3 crystals, analysed using Wannier-type atomic functions. Solid State Communications, 2003, 127, 423-426.	1.9	22
69	The water adsorption on the surfaces of SrMO₃(M= Ti, Zr, and Hf) crystalline oxides: quantum and classical modelling. Journal of Physics: Conference Series, 2007, 93, 012001.	0.4	22
70	Electronic structure of crystalline uranium nitride: LCAO DFT calculations. Physica Status Solidi (B): Basic Research, 2008, 245, 114-122.	1.5	22
71	First principles calculations of oxygen adsorption on the UN(001) surface. Surface Science, 2009, 603, 50-53.	1.9	22
72	Hybrid density-functional calculations of phonons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaCoO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: Physical Review B, 2010, 82, .	3.2	22

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73	Structure and stability of SnS2-based single- and multi-wall nanotubes. Surface Science, 2015, 641, 6-15.	1.9	22
74	Functionalized Pt(II) and Ir(III) NIR Emitters and Their Covalent Conjugates with Polymer-Based Nanocarriers. Bioconjugate Chemistry, 2020, 31, 1327-1343.	3.6	22
75	Monovalent Mercuryâ€Like Ion Dimer Centres in Alkali Halide Crystals. Physica Status Solidi (B): Basic Research, 1975, 70, 749-758.	1.5	21
76	Comparison of the Large Unit Cell and Small Periodic Cluster Approaches to the Quasimolecular Calculations of the Band Spectra of Crystals. Physica Status Solidi (B): Basic Research, 1976, 76, 377-383.	1.5	21
77	FIRST-PRINCIPLES LCAO CALCULATIONS ON 5D TRANSITION METAL OXIDES: ELECTRONIC AND PHONON PROPERTIES. Integrated Ferroelectrics, 2009, 108, 1-10.	0.7	21
78	Symmetry and models of single-walled TiO2 nanotubes with rectangular morphology. Open Physics, 2011, 9, 492-501.	1.7	21
79	Symmetry and Stability of the Rutile-Based TiO₂ Nanowires: Models and Comparative LCAO-Plane Wave DFT Calculations. Journal of Physical Chemistry C, 2012, 116, 13395-13402.	3.1	21
80	Molecular Cluster Approach to Smallâ€Radius Impurity Centres in Solids. Physica Status Solidi (B): Basic Research, 1974, 64, 635-642.	1.5	20
81	Four-faceted nanowires generated from densely-packed TiO2 rutile surfaces: Ab initio calculations. Surface Science, 2013, 608, 226-240.	1.9	20
82	Hybrid Hartreeâ€“Fock-density functional theory study of V2O5 three phases: Comparison of bulk and layer stability, electron and phonon properties. Acta Materialia, 2014, 75, 246-258.	7.9	20
83	Use of site symmetry in supercell models of defective crystals: polarons in CeO₂. Physical Chemistry Chemical Physics, 2017, 19, 8340-8348.	2.8	20
84	Near-Infrared [Ir(N^{â^§}C)₂(N^{â^§}N)]⁺ Emitters and Their Noncovalent Adducts with Human Serum Albumin: Synthesis and Photophysical and Computational Study. Organometallics, 2019, 38, 3740-3751.	2.3	20
85	Symmetrical transformation of basic translation vectors in the supercell model of imperfect crystals and in the theory of special points of the Brillouin zone. Journal of Physics Condensed Matter, 1997, 9, 3023-3031.	1.8	19
86	Connection between slab and cluster models for crystalline surfaces. Physics of the Solid State, 2001, 43, 1774-1782.	0.6	19
87	Structure reconstruction of TiO2-based multi-wall nanotubes: first-principles calculations. Physical Chemistry Chemical Physics, 2014, 16, 14781.	2.8	19
88	First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. Physical Chemistry Chemical Physics, 2017, 19, 25245-25251.	2.8	19
89	Luminescent organic dyes containing a phenanthro[9,10-D]imidazole core and [Ir(N^C)(N^N)]⁺ complexes based on the cyclometalating and diimine ligands of this type. Dalton Transactions, 2020, 49, 6751-6763.	3.3	19
90	Supercell Model of V-Doped TiO2: Unrestricted Hartree-Fock Calculations. Physica Status Solidi (B): Basic Research, 1999, 215, 949-956.	1.5	18

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91	Interpretation of EXAFS in ReO₃using molecular dynamics simulations. Journal of Physics: Conference Series, 2009, 190, 012080.	0.4	18
92	The Electronic Structure of Copper Oxide Crystalline Compounds. I. LUCâ€CNDO Approach to the Electronic Structure of Cu₂O and CuO Crystals. Physica Status Solidi (B): Basic Research, 1990, 157, 281-291.	1.5	17
93	The hartree-fock method and density-functional theory as applied to an infinite crystal and to a cyclic cluster. Physics of the Solid State, 2002, 44, 1656-1670.	0.6	17
94	Confinement effects for ionic carriers in SrTiO₃ultrathin films: first-principles calculations of oxygen vacancies. Physical Chemistry Chemical Physics, 2011, 13, 923-926.	2.8	17
95	Interpretation of unexpected behavior of infrared absorption spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScF</mml:mi><mml:mn>3</mml:mn></mml:msub></m the quasiharmonic approximation. Physical Review B, 2016, 93, .	3.2	17
96	Colossal Spin Splitting in the Monolayer of the Collinear Antiferromagnet MnF₂. Journal of Physical Chemistry Letters, 2021, 12, 2363-2369.	4.6	17
97	Application of the Band Representations of Space Groups in the Theory of Electronic States of Crystalline Solids. I. General Consideration of the Band Representations. Physica Status Solidi (B): Basic Research, 1984, 122, 231-238.	1.5	16
98	The Electronic Structure of Crystalline Lead Oxides. I. Crystal Structure and LUCâ€CNDO Calculations. Physica Status Solidi (B): Basic Research, 1991, 165, 401-410.	1.5	16
99	Full inclusion of symmetry in constructing Wannier functions: Chemical bonding in MgO and TiO2 crystals. Physics of the Solid State, 2003, 45, 2072-2082.	0.6	16
100	HYBRID HF-DFT MODELLING OF WATER ADSORPTION ON (001) SURFACE OF ORTHORHOMBIC AND CUBIC SrHfO₃. Integrated Ferroelectrics, 2009, 108, 37-45.	0.7	16
101	Quantum chemical simulations of doped ZnO nanowires for photocatalytic hydrogen generation. Physica Status Solidi (B): Basic Research, 2016, 253, 2120-2128.	1.5	16
102	Ab Initio Calculations on the Electronic Structure and Photocatalytic Properties of Twoâ€Dimensional WS₂ (0001) Nanolayers of Varying Thickness. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800253.	2.4	16
103	Symmetry Groups of Cyclic Systems in Crystals. Physica Status Solidi (B): Basic Research, 1985, 128, 275-285.	1.5	15
104	The Electronic Structure of Copper Oxide Crystalline Compounds. II. Chemical Bonding in Copperâ€“Oxygen Crystals. Physica Status Solidi (B): Basic Research, 1990, 158, 201-212.	1.5	15
105	Oxygen interstitials in magnesium oxide: A band-model study. Physical Review B, 1996, 54, 8969-8972.	3.2	15
106	Electron state symmetries and optical transitions in semiconductor superlattices: I. grown along the [001] direction. Journal of Physics Condensed Matter, 1997, 9, 257-276.	1.8	15
107	Hartree-Fock calculations of electronic structure of (110)-surface of rutile TiO2: Comparison of single (2D) and periodic (3D) slab models. International Journal of Quantum Chemistry, 2004, 96, 282-291.	2.0	15
108	Surface relaxation and tilting in SrHfO3 orthorhombic perovskite: Hybrid HF-DFT LCAO calculations. Surface Science, 2008, 602, 3674-3682.	1.9	15

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109	BaTiO₃â€based nanolayers and nanotubes: Firstâ€principles calculations. Journal of Computational Chemistry, 2013, 34, 175-186.	3.3	15
110	Doped 1D Nanostructures of Transitionâ€metal Oxides: Firstâ€principles Evaluation of Photocatalytic Suitability. Israel Journal of Chemistry, 2017, 57, 461-476.	2.3	15
111	Calculations of the Electronic Structure of Colour Centres in Ionic Crystals (I). Physica Status Solidi (B): Basic Research, 1970, 40, 9-29.	1.5	14
112	Use of the Large Unit Cell Approach for Generating Special Points of the Brillouin Zone. Physica Status Solidi (B): Basic Research, 1980, 99, 463-470.	1.5	14
113	Semiempirical Calculations of the Impurity Level Positions with Respect to the Perfect Crystal Bands. Physica Status Solidi (B): Basic Research, 1981, 103, 581-587.	1.5	14
114	Calculations of the Electronic Structure of Crystalline SrZrO[sub 3] in the Framework of the Density-Functional Theory in the LCAO Approximation. Physics of the Solid State, 2005, 47, 2248.	0.6	14
115	Energetic stability and photocatalytic activity of SrTiO3 nanowires: ab initio simulations. RSC Advances, 2015, 5, 24115-24125.	3.6	14
116	Site group analysis of normal modes in semiconductor superlattices. The Journal of Physical Chemistry, 1991, 95, 10772-10776.	2.9	13
117	Hartree-Fock Study of the Chemical Bonding in Crystalline Titanium Oxides: TiO2, Ti2O3, TiO. Physica Status Solidi (B): Basic Research, 1997, 203, R3-R4.	1.5	13
118	Symmetry and stability of nanotubes based on titanium dioxide. Russian Journal of General Chemistry, 2010, 80, 1152-1167.	0.8	13
119	Theoretical modeling of antiferrodistortive phase transition for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>SrTi</mml:mtext><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>ultrathin films. Physical Review B, 2013, 88, .	3.2	13
120	Application of zoneâ€folding approach to the firstâ€principles estimation of thermodynamic properties of carbon and <scp>ZrS</scp>₂â€based nanotubes. Journal of Computational Chemistry, 2016, 37, 641-652.	3.3	13
121	Molecular cluster approach to magnesium and calcium oxide crystals. I. Perfect crystals. Physica Status Solidi (B): Basic Research, 1975, 72, 787-794.	1.5	12
122	Large unit cell calculations of the band structure of ionic crystals using the Mullikenâ€Ruedenberg approximation. Physica Status Solidi (B): Basic Research, 1978, 86, 47-55.	1.5	12
123	Electronic structure and chemical bonding in Bi₂O₃. Physica Status Solidi (B): Basic Research, 1994, 183, K15.	1.5	12
124	Wannier functions and chemical bonding in crystals with the perovskite-like structure: SrTiO3, BaTiO3, PbTi3, and LaMnO3. International Journal of Quantum Chemistry, 2004, 100, 352-359.	2.0	12
125	Ab initio calculations of charged point defects in GaN. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 507-510.	0.8	12
126	Firstâ€principles calculations on thermodynamic properties of BaTiO₃ rhombohedral phase. Journal of Computational Chemistry, 2012, 33, 1554-1563.	3.3	12

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127	A Rare Type of Rhenium(I) Diimine Complexes with Unsupported Coordinated Phosphine Oxide Ligands: Synthesis, Structural Characterization, Photophysical and Theoretical Study. European Journal of Inorganic Chemistry, 2019, 2019, 4350-4357.	2.0	12
128	Quantum mechanics-classical molecular dynamics approach to EXAFS. Journal of Physics: Conference Series, 2009, 190, 012024.	0.4	11
129	Site symmetry approach applied to the supercell model of MgAl2O4 spinel with oxygen interstitials: Ab initio calculations. Computational Materials Science, 2018, 150, 517-523.	3.0	11
130	Antiferromagnetism-Induced Spin Splitting in Systems Described by Magnetic Layer Groups. Journal of Physical Chemistry C, 2021, 125, 16147-16154.	3.1	11
131	Point Defects in Lithium Hydride Crystals. Physica Status Solidi (B): Basic Research, 1974, 66, 687-694.	1.5	10
132	The Quasimolecular Approach to the Electronic Structure Calculations for Silver and Copper Halides. Physica Status Solidi (B): Basic Research, 1983, 118, 191-203.	1.5	10
133	Electronic structure of fluorite-type crystals. Journal of Physics Condensed Matter, 1989, 1, 6603-6609.	1.8	10
134	The electronic structure of crystalline nickel oxides. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 555-563.	1.7	10
135	Computer modeling of C2 cluster addition to fullerene C60. International Journal of Quantum Chemistry, 2002, 88, 652-662.	2.0	10
136	Atomistic modeling of polar LaMnO3 surfaces. Sensors and Actuators B: Chemical, 2004, 100, 81-87.	7.8	10
137	Ab initio calculations and analysis of chemical bonding in SrTiO3 and SrZrO3 cubic crystals. International Journal of Quantum Chemistry, 2006, 106, 2191-2200.	2.0	10
138	Temperature dependence of Youngâ€™s modulus of titanium dioxide (TIO2) nanotubes: Molecular mechanics modeling. Physics of the Solid State, 2015, 57, 2464-2472.	0.6	10
139	New insight on cubicâ€“tetragonalâ€“monoclinic phase transitions in ZrO₂: ab initio study and symmetry analysis. Journal of Applied Crystallography, 2016, 49, 1572-1578.	4.5	10
140	Simulation of Youngâ€™s moduli for hexagonal ZnO [0â€‰0â€‰0â€‰1]-oriented nanowires: first principles and molecular mechanical calculations. Materials Research Express, 2017, 4, 085014.	1.6	10
141	Comparison of vibrational and thermodynamic properties of MoS₂ and WS₂ nanotubes: first principles study. Materials Research Express, 2018, 5, 115028.	1.6	10
142	The site-symmetry induced representations of layer groups on the Bilbao Crystallographic Server. Journal of Applied Crystallography, 2019, 52, 1214-1221.	4.5	10
143	Selfâ€consistent energy band structure of tetragonal lead oxide. Physica Status Solidi (B): Basic Research, 1983, 115, K15.	1.5	9
144	Normal modes of Biî—¸Srî—¸Caî—¸Cuî—¸O high-temperature superconductors: layer-by-layer approach. Physica C: Superconductivity and Its Applications, 1992, 190, 477-482.	1.2	9

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145	The Electronic Structure and the Chemical Bonding in NiO and La₂NiO₄ Crystals. A Comparison with CuO and La₂CuO₄. Physica Status Solidi (B): Basic Research, 1993, 179, 441-451.	1.5	9
146	Trends in calculation of point and extended defects in wide-gap solids: periodic models of aperiodic systems. Physica Status Solidi A, 2005, 202, 235-242.	1.7	9
147	Calculations of electronic structure of the UF6 molecule and the UO2 crystal with a relativistic pseudopotential. Russian Journal of General Chemistry, 2008, 78, 1823-1835.	0.8	9
148	Nanolayered solid electrolyte (GeSe2)30(Sb2Se3)30(AgI)40/AgI: A new hypothesis for the conductivity mechanism in layered AgI. Solid State Ionics, 2016, 294, 82-89.	2.7	9
149	Multi-walled MoS2 nanotubes. First principles and molecular mechanics computer simulation. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114183.	2.7	9
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