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	Antiferromagnetism-induced spin splitting in monolayers of layered and non-layered crystals: Symmetry-based analysis and Density Functional Theory calculation. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 139, 115118.	2.7	4
2	Spin Splitting in Systems Described by Magnetic Rod Groups. Journal of Physical Chemistry C, 2022, 126, 5362-5367.	3.1	3
3	Spin splitting in monoperiodic systems described by magnetic line groups. Journal of Physics Condensed Matter, 2022, 34, 315803.	1.8	2
4	Lattice Dynamics and Thermodynamic Properties of Bulk Phases and Monolayers of GaTe and InTe: A Comparison from Firstâ€Principles Calculations. European Journal of Inorganic Chemistry, 2021, 2021, 126-138.	2.0	9
5	Argentophillic interactions in argentum chalcogenides: First principles calculations and topological analysis of electron density. Journal of Computational Chemistry, 2021, 42, 242-247.	3.3	7
6	Colossal Spin Splitting in the Monolayer of the Collinear Antiferromagnet MnF₂. Journal of Physical Chemistry Letters, 2021, 12, 2363-2369.	4.6	17
7	The Nature of Chemical Bonds in the Tetragonal Polymorph of InTe: Firstâ€Principlesâ€Based Topological Analysis. Physica Status Solidi (B): Basic Research, 2021, 258, 2100072.	1.5	2
8	Antiferromagnetism-Induced Spin Splitting in Systems Described by Magnetic Layer Groups. Journal of Physical Chemistry C, 2021, 125, 16147-16154.	3.1	11
9	Structure and stability of GaS, GaTe, and Janus-Ga2STe multi-walled nanotubes. Molecular mechanics simulation. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 133, 114779.	2.7	4
10	Firstâ€Principles Calculations of Phonons and Thermodynamic Properties of Zr(Hf)S₂â€Based Nanotubes. Journal of Computational Chemistry, 2020, 41, 759-768.	3.3	5
11	Topological analysis of chemical bonding in the layered <scp>FePSe₃</scp> upon pressureâ€induced phase transitions. Journal of Computational Chemistry, 2020, 41, 2610-2623.	3.3	4
12	Multi-walled MoS2 nanotubes. First principles and molecular mechanics computer simulation. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114183.	2.7	9
13	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
14	Nonempirical Calculations of the Structure and Stability of Nanotubes Based on Gallium Monochalcogenides. Physics of the Solid State, 2020, 62, 1017-1023.	0.6	5
15	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
16	First-principles comparative study of perfect and defective CsPbX₃ (X = Br, I) crystals. Physical Chemistry Chemical Physics, 2020, 22, 3914-3920.	2.8	37
17	Parameterization of dilute Ising model for iron-containing lanthanum gallate and aluminate solid solutions based on first-principles calculations. Solid State Ionics, 2020, 348, 115283.	2.7	0
18	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

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19	Binary Oxides of Transition Metals: ZnO, TiO$$_2$$, ZrO$$_2$$, HfO$$_2$$. Nanoscience and Technology, 2020, , 255-451.	1.5	0
20	First-Principles Simulations of Bulk Crystal and Nanolayer Properties. Nanoscience and Technology, 2020, , 123-219.	1.5	0
21	Ternary Oxides. Nanoscience and Technology, 2020, , 519-629.	1.5	0
22	Binary Oxides of Transition Metals: V$$_2$$O$$_5$$. Nanoscience and Technology, 2020, , 453-518.	1.5	0
23	Simulations of Nanotube Properties. Nanoscience and Technology, 2020, , 221-252.	1.5	0
24	Chalcogenides. Nanoscience and Technology, 2020, , 631-833.	1.5	0
25	The Symmetry Groups in Three-Dimensional Space. Nanoscience and Technology, 2020, , 9-121.	1.5	0
26	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
27	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
28	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
29	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
30	Development of the Local (Site) Symmetry Method in the Supercell Model for a Crystal with an Impurity. Physics of the Solid State, 2019, 61, 994-1006.	0.6	0
31	First-principles calculations of iodine-related point defects in CsPbI₃. Physical Chemistry Chemical Physics, 2019, 21, 7841-7846.	2.8	29
32	First principles evaluation on photocatalytic suitability of 2H structured and [0001] oriented WS2 nanosheets and nanotubes. IOP Conference Series: Materials Science and Engineering, 2019, 503, 012002.	0.6	4
33	The site-symmetry induced representations of layer groups on the Bilbao Crystallographic Server. Journal of Applied Crystallography, 2019, 52, 1214-1221.	4.5	10
34	Supercell-zone folding transformation for bulk crystals and nanotubes. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	6
35	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
36	Calculation of Youngâ€™s Modulus of MoS2-Based Single-Wall Nanotubes Using Force-Field and Hybrid Density Functional Theory. Physics of the Solid State, 2018, 60, 2551-2558.	0.6	4

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37	Ab initio (DFT) calculations of corundum (Î±-Al2O3) oxygen isotope fractionation. European Journal of Mineralogy, 2018, 30, 1063-1070.	1.3	3
38	Binuclear platinum(II) complexes based on a new bis-bidentate 3,6-di(thien-2-yl)pyridazine skeleton, a novel type of deep-red phosphorescent emitters: Synthesis and nonempirical calculations. Inorganic Chemistry Communication, 2018, 98, 105-110.	3.9	3
39	Infrared and Raman active vibrational modes in MoS 2 â€based nanotubes: Symmetry analysis and firstâ€principles calculations. Journal of Computational Chemistry, 2018, 39, 2163-2172.	3.3	8
40	Temperature dependence of thermodynamic properties of MoS2 monolayer and single-wall nanotubes: Application of the developed three-body force field. Journal of Molecular Graphics and Modelling, 2018, 85, 212-222.	2.4	4
41	Comparison of vibrational and thermodynamic properties of MoS₂ and WS₂ nanotubes: first principles study. Materials Research Express, 2018, 5, 115028.	1.6	10
42	First-principles calculations of CdS-based nanolayers and nanotubes. Materials Research Express, 2018, 5, 055036.	1.6	5
43	Use of site symmetry in supercell models of defective crystals: polarons in CeO₂. Physical Chemistry Chemical Physics, 2017, 19, 8340-8348.	2.8	20
44	Use of Wyckoff position splittings in the supercell model of crystals with point defects. Journal of Applied Crystallography, 2017, 50, 893-900.	4.5	8
45	Firstâ€principles modeling of hafniaâ€based nanotubes. Journal of Computational Chemistry, 2017, 38, 2088-2099.	3.3	7
46	Atomâ€“atom force field for simulation of zirconia bulk, nanosheets and nanotubes. Molecular Simulation, 2017, 43, 886-899.	2.0	7
47	Doped 1D Nanostructures of Transitionâ€metal Oxides: Firstâ€principles Evaluation of Photocatalytic Suitability. Israel Journal of Chemistry, 2017, 57, 461-476.	2.3	15
48	Phonon spectra, electronic, and thermodynamic properties of WS₂ nanotubes. Journal of Computational Chemistry, 2017, 38, 2581-2593.	3.3	24
49	Water adsorption on Î±-V2O5 surface and absorption in V2O5â™nH2O xerogel: DFT study of electronic structure. Surface Science, 2017, 666, 76-83.	1.9	4
50	First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. Physical Chemistry Chemical Physics, 2017, 19, 25245-25251.	2.8	19
51	First-principles calculations on Fe-Pt nanoclusters of various morphologies. Scientific Reports, 2017, 7, 10579.	3.3	2
52	Site symmetry approach in the supercell model of carbon-doped ZnO bulk. Chemical Physics Letters, 2017, 682, 91-95.	2.6	6
53	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
54	Firstâ€principles Calculations of InSâ€based Nanotubes. Israel Journal of Chemistry, 2017, 57, 490-500.	2.3	5

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55	Temperature dependence of strain energy and thermodynamic properties of V₂O₅â€based singleâ€walled nanotubes: Zoneâ€folding approach. Journal of Computational Chemistry, 2016, 37, 1442-1450.	3.3	8
56	Synchrotron-based far-infrared spectroscopy of nickel tungstate. Low Temperature Physics, 2016, 42, 552-555.	0.6	5
57	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
58	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
59	Simulation of structure and stability of carbon nanoribbons. Russian Journal of General Chemistry, 2016, 86, 1777-1786.	0.8	2
60	Quantum chemical simulations of doped ZnO nanowires for photocatalytic hydrogen generation. Physica Status Solidi (B): Basic Research, 2016, 253, 2120-2128.	1.5	16
61	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
62	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
63	Young's modulus and Poisson's ratio for TiO2-based nanotubes and nanowires: modelling of temperature dependence. RSC Advances, 2016, 6, 16037-16045.	3.6	6
64	Thermodynamic properties of nanotubes: zone-folding approach. Lithuanian Journal of Physics, 2016, 56, 164-172.	0.4	7
65	Theoretical study of Î±- and Î³-V₂O₅ double-walled nanotubes. Lithuanian Journal of Physics, 2016, 56, .	0.4	0
66	Theoretical Study of Î±â€V₂O₅â€Based Doubleâ€Wall Nanotubes. ChemPhysChem, 2015, 16, 3007-3014.	2.1	8
67	Quantum Chemical Study of Water Adsorption on the Surfaces of SrTiO₃ Nanotubes. ChemPhysChem, 2015, 16, 2192-2198.	2.1	2
68	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
69	Energetic stability and photocatalytic activity of SrTiO3 nanowires: ab initio simulations. RSC Advances, 2015, 5, 24115-24125.	3.6	14
70	Symmetry classification of electron and phonon states in TiO₂â€based nanowires and nanotubes. Journal of Computational Chemistry, 2015, 36, 957-969.	3.3	5
71	Structure and stability of SnS2-based single- and multi-wall nanotubes. Surface Science, 2015, 641, 6-15.	1.9	22
72	Ab initio modeling of single wall nanotubes folded from Î±- and Î³-V2O5 monolayers: structural, electronic and vibrational properties. CrystEngComm, 2015, 17, 3277-3285.	2.6	5

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73	Ab initio modeling of wall structure and shape in perovskite-based nanotubes. Computational Materials Science, 2015, 96, 124-133.	3.0	6
74	Ternary Oxides. Nanoscience and Technology, 2015, , 545-610.	1.5	1
75	Sulfides. Nanoscience and Technology, 2015, , 611-651.	1.5	0
76	Nitrides of Boron and Group III Metals. Nanoscience and Technology, 2015, , 347-427.	1.5	0
77	Group IV Semiconductors. Nanoscience and Technology, 2015, , 253-346.	1.5	0
78	First-Principles Simulations of Bulk Crystal and Nanolayer Properties. Nanoscience and Technology, 2015, , 113-214.	1.5	0
79	Binary Oxides of Transition Metals. Nanoscience and Technology, 2015, , 429-543.	1.5	0
80	The Symmetry Groups in Three-Dimensional Space. Nanoscience and Technology, 2015, , 9-112.	1.5	0
81	First-principles calculations of single-walled nanotubes in sulfides MS2(M = Ti, Zr). Physica Scripta, 2014, 89, 044001.	2.5	8
82	Oxygen vacancy formation energies in Sr-doped complex perovskites: ab initio thermodynamic study. Solid State Ionics, 2014, 254, 11-16.	2.7	26
83	TiS₂and ZrS₂single- and double-wall nanotubes: First-principles study. Journal of Computational Chemistry, 2014, 35, 395-405.	3.3	24
84	Structure reconstruction of TiO2-based multi-wall nanotubes: first-principles calculations. Physical Chemistry Chemical Physics, 2014, 16, 14781.	2.8	19
85	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
86	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
87	Theoretical modeling of the complexes of iron impurities and oxygen vacancies in SrTiO3. Applied Physics Letters, 2013, 102, .	3.3	29
88	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
89	Quantum mechanics based classical molecular dynamics study of water adsorption on (001) SrMO3 surfaces (M=Ti, Zr). Surface Science, 2013, 611, 10-24.	1.9	5
90	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

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91	Four-faceted nanowires generated from densely-packed TiO2 rutile surfaces: Ab initio calculations. Surface Science, 2013, 608, 226-240.	1.9	20
92	BaTiO₃â€based nanolayers and nanotubes: Firstâ€principles calculations. Journal of Computational Chemistry, 2013, 34, 175-186.	3.3	15
93	Nanotubes folded from cubic and orthorhombic SrZrO3: First-principles study. IOP Conference Series: Materials Science and Engineering, 2013, 49, 012009.	0.6	3
94	SYMMETRY AND CALCULATIONS OF NANOTUBES AND NANOWIRES BASED ON RUTILE AND PEROVSKITE STRUCTURES. , 2013, , .		0
95	LCAO Calculations on Uranium Nitrides. Springer Series in Solid-state Sciences, 2012, , 603-630.	0.3	0
96	Ab initiosimulations on rutile-based titania nanowires. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012005.	0.6	2
97	Rod groups and their settings as special geometric realisations of line groups. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 582-588.	0.3	5
98	Ab initio structure modeling of ZrO2 nanosheets and single-wall nanotubes. Computational Materials Science, 2012, 65, 395-405.	3.0	31
99	Hartreeâ€“Fock LCAO Method for Periodic Systems. Springer Series in Solid-state Sciences, 2012, , 109-155.	0.3	1
100	Semiempirical LCAO Methods for Molecules and Periodic Systems. Springer Series in Solid-state Sciences, 2012, , 207-249.	0.3	0
101	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
102	Quantum Chemistry of Solids. Springer Series in Solid-state Sciences, 2012, , .	0.3	51
103	Firstâ€principles calculations on thermodynamic properties of BaTiO₃ rhombohedral phase. Journal of Computational Chemistry, 2012, 33, 1554-1563.	3.3	12
104	Firstâ€principles calculations on the four phases of BaTiO₃. Journal of Computational Chemistry, 2012, 33, 1123-1130.	3.3	89
105	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
106	Symmetry and Non-empirical Calculations of Structure and Properties of Single- and Double-Wall SrTiO3 Nanotubes. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 75-85.	0.3	6
107	Electron Correlations in Molecules and Crystals. Springer Series in Solid-state Sciences, 2012, , 157-206.	0.3	0
108	Basis Sets and Pseudopotentials in Periodic LCAO Calculations. Springer Series in Solid-state Sciences, 2012, , 305-356.	0.3	0

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109	Modeling and LCAO Calculations of Point Defects in Crystals. Springer Series in Solid-state Sciences, 2012, , 489-540.	0.3	0
110	Symmetry and Modeling of BN, TiO2, and SrTiO3 Nanotubes. Springer Series in Solid-state Sciences, 2012, , 631-690.	0.3	0
111	Surface Modeling in LCAO Calculations of Metal Oxides. Springer Series in Solid-state Sciences, 2012, , 541-601.	0.3	0
112	LCAO Calculations of Perfect-Crystal Properties. Springer Series in Solid-state Sciences, 2012, , 357-488.	0.3	0
113	Symmetry and Localization of Crystalline Orbitals. Springer Series in Solid-state Sciences, 2012, , 47-107.	0.3	0
114	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
115	LCAO Calculations of (001) Surface Oxygen Vacancy Structure in Y-Doped BaZrO3. Integrated Ferroelectrics, 2011, 123, 1-9.	0.7	4
116	Symmetry and Models of Double-Wall BN and TiO₂Nanotubes with Hexagonal Morphology. Journal of Physical Chemistry C, 2011, 115, 14067-14076.	3.1	33
117	A Comparative Hybrid DFT Study of Phonons in Several SrTiO₃ Phases. Integrated Ferroelectrics, 2011, 123, 18-25.	0.7	4
118	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
119	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
120	LCAO calculations of SrTiO3nanotubes. IOP Conference Series: Materials Science and Engineering, 2011, 23, 012013.	0.6	8
121	First-principles LCAO study of phonons in NiWO4. Open Physics, 2011, 9, .	1.7	23
122	Symmetry and models of single-walled TiO2 nanotubes with rectangular morphology. Open Physics, 2011, 9, 492-501.	1.7	21
123	LCAO calculation of water adsorption on (001) surface of Y-doped BaZrO3. Solid State Ionics, 2011, 188, 25-30.	2.7	8
124	First-principles calculations on double-walled inorganic nanotubes with hexagonal chiralities. IOP Conference Series: Materials Science and Engineering, 2011, 23, 012014.	0.6	2
125	Symmetry and structure of SrTiO₃nanotubes. IOP Conference Series: Materials Science and Engineering, 2011, 23, 012012.	0.6	6
126	Symmetry and stability of nanotubes based on titanium dioxide. Russian Journal of General Chemistry, 2010, 80, 1152-1167.	0.8	13

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127	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
128	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
129	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:msub></mml:mrow></mml:math> Physical Review B, 2010, 82, .	3.2	22
130	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
131	FIRST-PRINCIPLES LCAO CALCULATIONS ON 5D TRANSITION METAL OXIDES: ELECTRONIC AND PHONON PROPERTIES. Integrated Ferroelectrics, 2009, 108, 1-10.	0.7	21
132	HYBRID HF-DFT MODELLING OF WATER ADSORPTION ON (001) SURFACE OF ORTHORHOMBIC AND CUBIC SrHfO₃. Integrated Ferroelectrics, 2009, 108, 37-45.	0.7	16
133	Quantum mechanicsâ€“molecular dynamics approach to the interpretation of x-ray absorption spectra. Journal of Physics Condensed Matter, 2009, 21, 055401.	1.8	33
134	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
135	Ab initio study of the electronic and atomic structure of the wolframite-type ZnWO4. Solid State Communications, 2009, 149, 425-428.	1.9	54
136	First principles calculations of oxygen adsorption on the UN(001) surface. Surface Science, 2009, 603, 50-53.	1.9	22
137	From anatase (101) surface to TiO2 nanotubes: Rolling procedure and first principles LCAO calculations. Surface Science, 2009, 603, L117-L120.	1.9	68
138	Surface modelling on heavy atom crystalline compounds: HfO2 and UO2 fluorite structures. Acta Materialia, 2009, 57, 600-606.	7.9	23
139	First-principles study of bulk and surface oxygen vacancies in SrTiO3 crystal. European Physical Journal B, 2009, 72, 53-57.	1.5	94
140	Quantum-chemical calculations of the variance of phonons in crystals: Convergence of results depending on cyclic cluster growth. Russian Journal of General Chemistry, 2009, 79, 509-510.	0.8	0
141	Interpretation of EXAFS in ReO₃using molecular dynamics simulations. Journal of Physics: Conference Series, 2009, 190, 012080.	0.4	18
142	Quantum mechanics-classical molecular dynamics approach to EXAFS. Journal of Physics: Conference Series, 2009, 190, 012024.	0.4	11
143	Electronic structure of crystalline uranium nitride: LCAO DFT calculations. Physica Status Solidi (B): Basic Research, 2008, 245, 114-122.	1.5	22
144	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

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145	Surface relaxation and tilting in SrHfO3 orthorhombic perovskite: Hybrid HF-DFT LCAO calculations. Surface Science, 2008, 602, 3674-3682.	1.9	15
146	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
147	Ab initio modeling of spin and charge ordering and lattice dynamics in CaFeO3 crystals. Journal of Chemical Physics, 2008, 129, 214704.	3.0	7
148	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
149	<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
150	Ab initiostudy of bulk and surface iron defects in SrTiO₃. Journal of Physics: Conference Series, 2008, 117, 012001.	0.4	3
151	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
152	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
153	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
154	Electronic structure of crystalline uranium nitride: LCAO DFT calculations. Journal of Structural Chemistry, 2007, 48, S125-S133.	1.0	2
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