Eugene A Kotomin

List of Publications by Year
in descending order

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456 papers	11,099 citations	36303 51 h-index	58581 82 g-index
461 all docs	461 docs citations	461 times ranked	7062 citing authors

#	Article	IF	Citations
1	Theoretical and Experimental Studies of Charge Ordering in CaFeO₃ and SrFeO₃ Crystals. Physica Status Solidi (B): Basic Research, 2022, 259, 2100238.	1.5	6
2	Photo de-mixing in mixed halide perovskites: the roles of ions and electrons. JPhys Energy, 2022, 4, 011001.	5.3	6
3	Comparative ab initio calculations of SrTiO3, BaTiO3, PbTiO3, and SrZrO3 (001) and (111) surfaces as well as oxygen vacancies. Low Temperature Physics, 2022, 48, 80-88.	0.6	4
4	Influence of Au, Ag, and Cu Adatoms on Optical Properties of TiO2 (110) Surface: Predictions from RT-TDDFT Calculations. Crystals, 2022, 12, 452.	2.2	4
5	Oxygen Vacancy Formation and Migration within the Antiphase Boundaries in Lanthanum Scandate-Based Oxides: Computational Study. Materials, 2022, 15, 2695.	2.9	0
6	Water Splitting on Multifaceted SrTiO3 Nanocrystals: Calculations of Raman Vibrational Spectrum. Materials, 2022, 15, 4233.	2.9	5
7	The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments. Journal of Materials Chemistry C, 2021, 9, 4948-4960.	5.5	7
8	BaCoO3 monoclinic structure and chemical bonding analysis: hybrid DFT calculations. Physical Chemistry Chemical Physics, 2021, 23, 17493-17501.	2.8	4
9	Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies. Journal of Materials Chemistry C, 2021, 9, 1693-1700.	5.5	22
10	Extractionâ€“Pyrolytic Method for TiO2 Polymorphs Production. Crystals, 2021, 11, 431.	2.2	41
11	Small radius electron and hole polarons in PbX₂ (X = F, Cl, Br) crystals: a computational study. Journal of Materials Chemistry C, 2021, 9, 16536-16544.	5.5	8
12	Evidence for the formation of two types of oxygen interstitials in neutron-irradiated Î±-Al2O3 single crystals. Scientific Reports, 2021, 11, 20909.	3.3	14
13	Water Splitting on Multifaceted SrTiO3 Nanocrystals: Computational Study. Catalysts, 2021, 11, 1326.	3.5	7
14	The electronic properties of SrTiO3-Î´ with oxygen vacancies or substitutions. Scientific Reports, 2021, 11, 23341.	3.3	14
15	Role of Intrinsic Dipoles in the Evaporationâ€Driven Assembly of Perovskite Nanocubes into Energyâ€Harvesting Composites. Physica Status Solidi (A) Applications and Materials Science, 2020, 217, 1900533.	1.8	2
16	Hybrid density functional calculations of hyperfine coupling tensor for hole-type defects in MgAl2O4. Nuclear Instruments & Methods in Physics Research B, 2020, 464, 60-64.	1.4	15
17	First-Principles Modeling of Oxygen Adsorption on Ag-Doped LaMnO3 (001) Surface. Journal of Electronic Materials, 2020, 49, 1421-1434.	2.2	4
18	Proton, Hydroxide Ion, and Oxide Ion Affinities of Closed-Shell Oxides: Importance for the Hydration Reaction and Correlation to Electronic Structure. Journal of Physical Chemistry C, 2020, 124, 1277-1284.	3.1	23

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19	Thermal annealing of radiation damage produced by swift 132Xe ions in MgO single crystals. Nuclear Instruments & Methods in Physics Research B, 2020, 462, 163-168.	1.4	17
20	First principles calculations of oxygen reduction reaction at fuel cell cathodes. Current Opinion in Electrochemistry, 2020, 19, 122-128.	4.8	23
21	Atomic, electronic and magnetic structure of an oxygen interstitial in neutron-irradiated Al2O3 single crystals. Scientific Reports, 2020, 10, 15852.	3.3	18
22	Low temperature structural transformations on the (001) surface of SrTiO3 single crystals. Low Temperature Physics, 2020, 46, 740-750.	0.6	11
23	First principles calculations of the vibrational properties of single and dimer F-type centers in corundum crystals. Journal of Chemical Physics, 2020, 153, 134107.	3.0	5
24	Hybrid density functional theoretical study of NASICON-type Na_xTi₂(PO₄)₃ (x = 1â€“4). Physical Chemistry Chemical Physics, 2020, 22, 11861-11870.	2.8	6
25	Distinctive features of diffusion-controlled radiation defect recombination in stoichiometric magnesium aluminate spinel single crystals and transparent polycrystalline ceramics. Scientific Reports, 2020, 10, 7810.	3.3	50
26	Interdependence of Oxygenation and Hydration in Mixed-Conducting (Ba,Sr)FeO_{3â˜Î´} Perovskites Studied by Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 11780-11789.	3.1	24
27	Ab initio calculations of pure and Co+2-doped MgF2 crystals. Nuclear Instruments & Methods in Physics Research B, 2020, 470, 10-14.	1.4	5
28	First-principles comparative study of perfect and defective CsPbX₃ (X = Br, I) crystals. Physical Chemistry Chemical Physics, 2020, 22, 3914-3920.	2.8	37
29	On the Way to Optoionics. Helvetica Chimica Acta, 2020, 103, e2000073.	1.6	16
30	Ab initio calculations of structural, electronic and vibrational properties of BaTiO3 and SrTiO3 perovskite crystals with oxygen vacancies. Low Temperature Physics, 2020, 46, 1185-1195.	0.6	26
31	Oxygen Evolution Reaction on a N-Doped Co_{0.5}-Terminated Co₃o₄ (001) Surface. Proceedings of the Latvian Academy of Sciences, 2020, 74, 396-403.	0.1	0
32	Nitrogen interstitial defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Materials Today Communications, 2019, 21, 100616.	1.9	9
33	Thermodynamic stability of non-stoichiometric SrFeO_{3â˜Î´}: a hybrid DFT study. Physical Chemistry Chemical Physics, 2019, 21, 3918-3931.	2.8	30
34	Ab initio simulation of (Ba,Sr)TiO3 and (Ba,Ca)TiO3 perovskite solid solutions. Solid State Ionics, 2019, 337, 76-81.	2.7	13
35	Defectâ€Induced Effects in Nanomaterials. Physica Status Solidi (B): Basic Research, 2019, 256, 1900181.	1.5	0
36	Manifestation of dipole-induced disorder in self-assembly of ferroelectric and ferromagnetic nanocubes. Nanoscale, 2019, 11, 7293-7303.	5.6	10

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37	First principles calculations on CeO2 doped with Tb3+ ions. Optical Materials, 2019, 90, 76-83.	3.6	3
38	First-principles calculations of iodine-related point defects in CsPbI₃. Physical Chemistry Chemical Physics, 2019, 21, 7841-7846.	2.8	29
39	Interface-induced enhancement of piezoelectricity in the (SrTiO₃)_m/(BaTiO₃)_{Mâ^'m} superlattice for energy harvesting applications. Physical Chemistry Chemical Physics, 2019, 21, 23541-23551.	2.8	9
40	The first principles calculations of CO2 adsorption on (101Â¯0) ZnO surface. AIP Conference Proceedings, 2019, , .	0.4	9
41	Theoretical and Experimental Study of (Ba,Sr)TiO₃ Perovskite Solid Solutions and BaTiO₃/SrTiO₃ Heterostructures. Journal of Physical Chemistry C, 2019, 123, 2031-2036.	3.1	18
42	First Principles Simulations on Migration Paths of Oxygen Interstitials in MgAl₂O₄. Physica Status Solidi (B): Basic Research, 2019, 256, 1800282.	1.5	7
43	Ab Initio Modeling of Y and O Solute Atom Interaction in Small Clusters within the bcc Iron Lattice. Physica Status Solidi (B): Basic Research, 2019, 256, 1800346.	1.5	2
44	Kinetics of the electronic center annealing in Al2O3 crystals. Journal of Nuclear Materials, 2018, 502, 295-300.	2.7	21
45	Ab initio modelling of the initial stages of the ODS particle formation process. Nuclear Instruments & Methods in Physics Research B, 2018, 435, 70-73.	1.4	5
46	Ab initio simulations on charged interstitial oxygen migration in corundum. Nuclear Instruments & Methods in Physics Research B, 2018, 435, 74-78.	1.4	14
47	Anomalous Kinetics of Diffusion-Controlled Defect Annealing in Irradiated Ionic Solids. Journal of Physical Chemistry A, 2018, 122, 28-32.	2.5	46
48	Kinetics of dimer F type center annealing in MgF2 crystals. Nuclear Instruments & Methods in Physics Research B, 2018, 435, 79-82.	1.4	16
49	Theoretical investigations of nitrogen doping on Co3O4 for water dissociation catalytically activity. Journal of Physics: Conference Series, 2018, 1115, 032032.	0.4	1
50	Transition levels of acceptor impurities in ZnO crystals by DFT-LCAO calculations. Journal of Physics: Conference Series, 2018, 1115, 042064.	0.4	1
51	Dopant solubility in ceria: alloy thermodynamics combined with the DFT+U calculations. Solid State Ionics, 2018, 325, 258-264.	2.7	1
52	Impact of point defects on the elastic properties of BaZrO3: Comprehensive insight from experiments and ab initio calculations. Acta Materialia, 2018, 160, 247-256.	7.9	21
53	Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes. Journal of Materials Chemistry A, 2018, 6, 11929-11940.	10.3	38
54	Ab initio modelling of the Y, O, and Ti solute interaction in fcc-Fe matrix. Nuclear Instruments & Methods in Physics Research B, 2018, 433, 106-110.	1.4	3

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55	Kinetic Monte Carlo modeling of Y2O3 nano-cluster formation in radiation resistant matrices. Nuclear Instruments & Methods in Physics Research B, 2018, 434, 13-22.	1.4	0
56	Comparison of the F-type center thermal annealing in heavy-ion and neutron irradiated Al2O3 single crystals. Nuclear Instruments & Methods in Physics Research B, 2018, 433, 93-97.	1.4	47
57	First-Principles Modelling of N-Doped Co₃O₄. Latvian Journal of Physics and Technical Sciences, 2018, 55, 36-42.	0.6	1
58	Use of site symmetry in supercell models of defective crystals: polarons in CeO₂. Physical Chemistry Chemical Physics, 2017, 19, 8340-8348.	2.8	20
59	(Invited) The Effect of (La,Sr)MnO 3 Cathode Surface Termination on Its Electronic Structure. ECS Transactions, 2017, 77, 67-73.	0.5	2
60	Thermodynamic stability of stoichiometric LaFeO₃ and BiFeO₃: a hybrid DFT study. Physical Chemistry Chemical Physics, 2017, 19, 3738-3755.	2.8	27
61	Analysis of self-trapped hole mobility in alkali halides and metal halides. Solid State Ionics, 2017, 302, 3-6.	2.7	29
62	First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. Physical Chemistry Chemical Physics, 2017, 19, 25245-25251.	2.8	19
63	Electromechanical Properties of Ba_(1â€“x)Sr_xTiO₃ Perovskite Solid Solutions from First-Principles Calculations. Journal of Physical Chemistry A, 2017, 121, 9409-9414.	2.5	11
64	Firstâ€principles Study of Perovskite Ultrathin Films: Stability and Confinement Effects. Israel Journal of Chemistry, 2017, 57, 509-521.	2.3	7
65	Analysis of the U L 3 -edge X-ray absorption spectra in UO 2 using molecular dynamics simulations. Progress in Nuclear Energy, 2017, 94, 187-193.	2.9	8
66	(Invited) The Effect of (La,Sr)MnO3 Cathode Surface Termination on Its Electronic Structure. ECS Meeting Abstracts, 2017, , .	0.0	0
67	First Principles Modeling of Pdâ€doped (La,Sr)(Co,Fe)O₃ Complex Perovskites. Fuel Cells, 2016, 16, 267-271.	2.4	5
68	Low-temperature radiation effects in wide gap materials. Low Temperature Physics, 2016, 42, 537-538.	0.6	0
69	Interpretation of the U L₃-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations. Journal of Physics: Conference Series, 2016, 712, 012091.	0.4	1
70	Defect-induced Effects in Nanomaterials. Physica Status Solidi C: Current Topics in Solid State Physics, 2016, 13, 868-869.	0.8	0
71	Ab initio modelling of oxygen vacancies and protonic defects in La_{1â^'x}Sr_xFeO_{3â^'Î´} perovskite solid solutions. Journal of Materials Chemistry A, 2016, 4, 13093-13104.	10.3	33
72	Charged oxygen interstitials in corundum: first principles simulations. Physica Status Solidi C: Current Topics in Solid State Physics, 2016, 13, 932-936.	0.8	5

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73	Ab initio modelling of Yâ€“O cluster formation in Î³â€Fe lattice. Physica Status Solidi (B): Basic Research, 2016, 253, 2136-2143.	1.5	4
74	Defectâ€induced Effects in Nanomaterials. Physica Status Solidi (B): Basic Research, 2016, 253, 2097-2098.	1.5	0
75	Theoretical analysis of the kinetics of low-temperature defect recombination in alkali halide crystals. Low Temperature Physics, 2016, 42, 588-593.	0.6	27
76	Surface Segregation Entropy of Protons and Oxygen Vacancies in BaZrO₃. Chemistry of Materials, 2016, 28, 1363-1368.	6.7	42
77	First principles study of confinement effects for oxygen vacancies in BaZrO₃ (001) ultra-thin films. Physical Chemistry Chemical Physics, 2016, 18, 9902-9908.	2.8	20
78	Void lattice formation in electron irradiated CaF 2 : Statistical analysis of experimental data and cellular automata simulations. Nuclear Instruments & Methods in Physics Research B, 2016, 368, 138-143.	1.4	6
79	Stabilization of primary mobile radiation defects in MgF2 crystals. Nuclear Instruments & Methods in Physics Research B, 2016, 374, 24-28.	1.4	42
80	Kinetics of F center annealing and colloid formation in Al2O3. Nuclear Instruments & Methods in Physics Research B, 2016, 374, 107-110.	1.4	46
81	Ab initio simulations on migration paths of interstitial oxygen in corundum. Nuclear Instruments & Methods in Physics Research B, 2016, 374, 29-34.	1.4	21
82	Ab initio simulations on Frenkel pairs of radiation defects in corundum. IOP Conference Series: Materials Science and Engineering, 2015, 77, 012001.	0.6	4
83	Water interaction with perfect and fluorine-doped Co3O4 (100) surface. Solid State Ionics, 2015, 277, 77-82.	2.7	24
84	Defect-induced effects in nanomaterials. Physica Status Solidi C: Current Topics in Solid State Physics, 2015, 12, 9-9.	0.8	1
85	Confinement effects for the F center in non-stoichiometric BaZrO₃ ultrathin films. Physica Status Solidi (B): Basic Research, 2015, 252, 139-143.	1.5	6
86	The effective diffusion coefficient in a one-dimensional discrete lattice with the inclusions. Physica B: Condensed Matter, 2015, 470-471, 50-52.	2.7	3
87	Ab Initio Study of BiFeO₃: Thermodynamic Stability Conditions. Journal of Physical Chemistry Letters, 2015, 6, 2847-2851.	4.6	48
88	First principles modeling of Ag adsorption on the LaMnO3 (001) surfaces. Solid State Ionics, 2015, 273, 46-50.	2.7	1
89	Hydration entropy of BaZrO₃ from first principles phonon calculations. Journal of Materials Chemistry A, 2015, 3, 7639-7648.	10.3	68
90	Thermodynamic properties of neutral and charged oxygen vacancies in BaZrO₃ based on first principles phonon calculations. Physical Chemistry Chemical Physics, 2015, 17, 20765-20774.	2.8	47

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91	Comparison of Permeation Measurements and Hybrid Density-Functional Calculations on Oxygen Vacancy Transport in Complex Perovskite Oxides. Journal of Physical Chemistry C, 2014, 118, 29542-29553.	3.1	25
92	Ab Initio Thermodynamics of Oxygen Vacancies and Zinc Interstitials in ZnO. Journal of Physical Chemistry Letters, 2014, 5, 4238-4242.	4.6	14
93	Statistical characterization of selfâ€assembled charged nanoparticle structures. Physica Status Solidi (A) Applications and Materials Science, 2014, 211, 288-293.	1.8	3
94	Radiation defects in complex perovskite solid solutions. Nuclear Instruments & Methods in Physics Research B, 2014, 326, 243-246.	1.4	1
95	Ab initio modeling of radiation damage in MgF2 crystals. Nuclear Instruments & Methods in Physics Research B, 2014, 326, 314-317.	1.4	15
96	Hydrogen induced metallization of ZnO (11Ì…00) surface: Ab initio study. Thin Solid Films, 2014, 553, 38-42.	1.8	15
97	Theory of non-equilibrium critical phenomena in three-dimensional condensed systems of charged mobile nanoparticles. Physical Chemistry Chemical Physics, 2014, 16, 13974-13983.	2.8	5
98	Static and dynamic screening effects in the electrostatic self-assembly of nano-particles. Physical Chemistry Chemical Physics, 2014, 16, 25449-25460.	2.8	11
99	Hydrogen adsorption on the ZnO $(1ar{1}00)$ surface: ab initio hybrid density functional linear combination of atomic orbitals calculations. Physica Scripta, 2014, 89, 045801.	2.5	12
100	Ab initio thermodynamic study of (Ba,Sr)(Co,Fe)O3 perovskite solid solutions for fuel cell applications. Journal of Materials Chemistry A, 2013, 1, 14320.	10.3	28
101	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
102	First-principles modeling of theHcolor centers in MgF2crystals. Physica Status Solidi C: Current Topics in Solid State Physics, 2013, 10, 160-164.	0.8	4
103	Theoretical modeling of the complexes of iron impurities and oxygen vacancies in SrTiO3. Applied Physics Letters, 2013, 102, .	3.3	29
104	Ab initio study of phase competition in (La1â^'c,Src)CoO3 solid solutions. Solid State Ionics, 2013, 230, 32-36.	2.7	15
105	Combined theoretical and experimental analysis of processes determining cathode performance in solid oxide fuel cells. Physical Chemistry Chemical Physics, 2013, 15, 5443.	2.8	240
106	Formation and migration of oxygen vacancies in La_{1â^'x}Sr_xCo_{1â^'y}Fe_yO_{3â^'Î´}perovskites: insight from ab initio calculations and comparison with Ba_{1â^'x}Sr_xCo_{1â^'y}Fe_yO_{3â^'Î´}. Physical Chemistry Chemical Physics, 2013, 15, 911-918.	2.8	111
107	First principles calculations of (Ba,Sr)(Co,Fe)O3â^'Î´ structural stability. Solid State Ionics, 2013, 230, 21-26.	2.7	18
108	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. Journal of Nuclear Materials, 2013, 435, 102-106.	2.7	18

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109	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
110	Atomic and electronic structure of hydrogen on ZnO (11Ì„00) surface: ab initio hybrid calculations. IOP Conference Series: Materials Science and Engineering, 2013, 49, 012054.	0.6	0
111	Defect-induced Effects in Nanomaterials. Physica Status Solidi C: Current Topics in Solid State Physics, 2013, 10, 601-602.	0.8	1
112	Phase competition in (La_{1â€‰â€‰â€‰c},Sr_c)CoO₃ solid solutions: ab initio thermodynamic study. Physica Status Solidi (B): Basic Research, 2013, 250, 864-869.	1.5	10
113	Oxygen exchange kinetics on solid oxide fuel cell cathode materialsâ€”general trends and their mechanistic interpretation. Journal of Materials Research, 2012, 27, 2000-2008.	2.6	85
114	Ab initiocalculations of theFcenters in MgF2bulk and on the (001) surface. Physica Scripta, 2012, 86, 035304.	2.5	9
115	Ab initiocalculations of theHcenters in MgF2crystals. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012041.	0.6	0
116	The effect of Zn vacancies and Ga dopants on the electronic structure of ZnO:Ab initiosimulations. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012015.	0.6	4
117	The first-principles treatment of the electron-correlation and spinâ€“orbital effects in uranium mononitride nuclear fuels. Physical Chemistry Chemical Physics, 2012, 14, 4482.	2.8	70
118	The Intrinsic Defects, Disordering, and Structural Stability of Ba_xSr_{1â€“x}Co_yFe_{1â€“y}O_{3â^'Î´} Perovskite Solid Solutions. Journal of Physical Chemistry C, 2012, 116, 18605-18611.	3.3	56
119	Note: Effective diffusion coefficient in heterogeneous media. Journal of Chemical Physics, 2012, 137, 166101.	3.0	7
120	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
121	Ab initiomodelling of UN grain boundary interfaces. IOP Conference Series: Materials Science and Engineering, 2012, 38, 012058.	0.6	0
122	CNT Arrays Grown upon Catalytic Nickel Particles as Applied in the Nanoelectronic Devices: Ab Initio Simulation of Growth Mechanism. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 101-114.	0.3	1
123	First-principles phonon calculations of Fe⁴⁺impurity in SrTiO₃. Journal of Physics Condensed Matter, 2012, 24, 104024.	1.8	3
124	Interaction Between Oxygen and Yttrium Impurity Atoms as well as Vacancies in fcc Iron Lattice: Ab Initio Modeling. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 149-159.	0.3	2
125	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
126	First Principles Calculations of Oxygen Vacancy Formation and Migration in Ba_{1â^'x}Sr_xCo_{1â^'y}Fe_yO_{3â^'Î´}Perovskites. Journal of the Electrochemical Society, 2011, 159, B219-B226.	2.9	84

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127	A Comparative Hybrid DFT Study of Phonons in Several SrTiO₃ Phases. Integrated Ferroelectrics, 2011, 123, 18-25.	0.7	4
128	First-Principles Modeling of Oxygen Interaction with SrTiO₃(001) Surface: Comparative Density-Functional LCAO and Plane-Wave Study. Integrated Ferroelectrics, 2011, 123, 10-17.	0.7	11
129	Pattern Formation Kinetics for Charged Molecules on Surfaces: Microscopic Correlation Function Analysis. Journal of Physical Chemistry B, 2011, 115, 14626-14633.	2.6	5
130	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
131	The non-equilibrium charge screening effects in diffusion-driven systems with pattern formation. Journal of Chemical Physics, 2011, 135, 034702.	3.0	10
132	Modeling of yttrium, oxygen atoms and vacancies in Î³-iron lattice. Journal of Nuclear Materials, 2011, 416, 40-44.	2.7	7
133	Ab initio modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies. Journal of Nuclear Materials, 2011, 416, 200-204.	2.7	33
134	Simulations on the mechanism of CNT bundle growth upon smooth and nanostructured Ni as well as Î¸-Al2O3 catalysts. Open Physics, 2011, 9, 530-541.	1.7	3
135	Ab initio calculations of the atomic and electronic structure of MgF2 (011) and (111) surfaces. Open Physics, 2011, 9, .	1.7	5
136	First principles calculations of oxygen vacancy formation and migration in mixed conducting Ba0.5Sr0.5Co1â^'yFeyO3â^'Î´ perovskites. Solid State Ionics, 2011, 188, 1-5.	2.7	98
137	DFT calculations of point defects on UN(001) surface. Surface Science, 2011, 605, 396-400.	1.9	26
138	Atomistic theory of mesoscopic pattern formation induced by bimolecular surface reactions between oppositely charged molecules. Journal of Chemical Physics, 2011, 135, 224503.	3.0	5
139	First Principles Modeling of Oxygen Mobility in Perovskite SOFC Cathode and Oxygen Permeation Membrane Materials. ECS Transactions, 2011, 35, 823-830.	0.5	10
140	The Structural Disorder and Lattice Stability of (Ba,Sr)(Co,Fe)O₃ Complex Perovskites. ECS Transactions, 2011, 35, 2077-2084.	0.5	8
141	FIRST PRINCIPLES SIMULATIONS ON DISSOCIATIVE ADSORPTION OF METHANE MOLECULES UPON NICKEL SUBSTRATE RESULTING IN A GROWTH OF NANOTUBES. , 2011, , .		0
142	Ab initio calculations of MgF2 (001) and (011) surface structure. Physica B: Condensed Matter, 2010, 405, 2125-2127.	2.7	27
143	Ab initio simulation of yttrium oxide nanocluster formation on fcc Fe lattice. Journal of Nuclear Materials, 2010, 406, 345-350.	2.7	22
144	Ab initio calculations of Nb doped SrTiO3. Physica B: Condensed Matter, 2010, 405, 3164-3166.	2.7	13

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145	Void superlattice formation in electron irradiated CaF2: Theoretical analysis. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3055-3058.	1.4	4
146	Basic properties of the F-type centers in halides, oxides and perovskites. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3084-3089.	1.4	159
147	Helium behavior in oxide nuclear fuels: First principles modeling. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3090-3094.	1.4	30
148	Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for (La, Sr)MnO_{3â˜Î´}. Journal of Physical Chemistry C, 2010, 114, 3017-3027.	3.1	160
149	Microscopic approach to the kinetics of pattern formation of charged molecules on surfaces. Physical Review E, 2010, 82, 021602.	2.1	8
150	First-principles modelling of complex perovskite (Ba1-xSrx)(Co1-yFey)O3-Î´ for solid oxide fuel cell and gas separation membrane applications. Energy and Environmental Science, 2010, 3, 1544.	30.8	75
151	Implementing first principles calculations of defect migration in a fuel performance code for UN simulations. Journal of Nuclear Materials, 2009, 393, 292-299.	2.7	25
152	A comparative ab initio study of bulk and surface oxygen vacancies in PbTiO3, PbZrO3 and SrTiO3 perovskites. Solid State Communications, 2009, 149, 1359-1362.	1.9	55
153	First principles calculations of oxygen adsorption on the UN(001) surface. Surface Science, 2009, 603, 50-53.	1.9	22
154	Atomic, electronic and thermodynamic properties of cubic and orthorhombic LaMnO3 surfaces. Surface Science, 2009, 603, 326-335.	1.9	106
155	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations. Journal of Nuclear Materials, 2009, 393, 504-507.	2.7	25
156	First-principles study of bulk and surface oxygen vacancies in SrTiO3 crystal. European Physical Journal B, 2009, 72, 53-57.	1.5	94
157	Ab initio DFT+U study of He atom incorporation into UO2 crystals. Physical Chemistry Chemical Physics, 2009, 11, 7241.	2.8	72
158	The Effect of Oxygen Vacancies on the Atomic and Electronic Structure of Cubic ABO₃Perovskite Bulk and the (001) Surface:Abinitio Calculations. Ferroelectrics, 2009, 379, 191-198.	0.6	12
159	Oxygen Incorporation Reaction into Mixed Conducting Perovskites: a Mechanistic Analysis for (La,Sr)MnO₃ Based on DFT Calculations. ECS Transactions, 2009, 25, 2753-2760.	0.5	9
160	A comparative ab initio study of Cu overlayers on BaTiO₃(001) and MgO(001) substrates. Physica Status Solidi (B): Basic Research, 2008, 245, 980-985.	1.5	3
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