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	Kinetics of bimolecular reactions in condensed media: critical phenomena and microscopic self-organisation. Reports on Progress in Physics, 1988, 51, 1479-1523.	20.1	261
2	Ab initiomodeling of surface structure forSrTiO3perovskite crystals. Physical Review B, 2001, 64, .	3.2	256
3	Radiation-induced point defects in simple oxides. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 1-15.	1.4	248
4	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
5	Evidence for Interfacial-Storage Anomaly in Nanocomposites for Lithium Batteries from First-Principles Simulations. Physical Review Letters, 2006, 96, 058302.	7.8	200
6	Nano-ionics in the context of lithium batteries. Journal of Power Sources, 2006, 159, 171-178.	7.8	185
7	Hybrid DFT calculations of the atomic and electronic structure for ABO3 perovskite (001) surfaces. Surface Science, 2005, 575, 75-88.	1.9	177
8	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
9	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
10	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
11	First-principles calculations for SrTiO3() surface structure. Surface Science, 2002, 513, 211-220.	1.9	120
12	Jahn-Teller distortion around<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi mathvariant="normal">Fe</mml:mi><mml:mrow><mml:mn>4</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mat xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi		

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19	Atomic and electronic structure of the corundum (0001) surface: comparison with surface spectroscopies. Surface Science, 1997, 370, 190-200.	1.9	99
20	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
21	First-principles and semiempirical calculations for bound-hole polarons inKNbO3. Physical Review B, 1999, 60, 1-5.	3.2	97
22	First-principles study of bulk and surface oxygen vacancies in SrTiO3 crystal. European Physical Journal B, 2009, 72, 53-57.	1.5	94
23	Electronic structure and thermodynamic stability of double-layeredSrTiO3(001)surfaces:Ab initiosimulations. Physical Review B, 2007, 75, .	3.2	92
24	Phenomenological kinetics of Frenkel defect recombination and accumulation in ionic solids. Reports on Progress in Physics, 1992, 55, 2079-2188.	20.1	89
25	Ab initiocalculations of theSrTiO3(110) polar surface. Physical Review B, 2004, 69, .	3.2	86
26	Electronic structure and thermodynamic stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaMnO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>La</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> Physical Review B, 2008, 78, .	3.2	85
27	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
28	Ab InitioModeling of Metal Adhesion on Oxide Surfaces with Defects. Physical Review Letters, 2000, 84, 1256-1259.	7.8	84
29	Comparative density-functional LCAO and plane-wave calculations ofLaMnO3surfaces. Physical Review B, 2005, 72, .	3.2	84
30	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
31	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
32	Enhanced interfacial lithium storage in nanocomposites of transition metals with LiF and Li2O: Comparison of DFT calculations and experimental studies. Solid State Sciences, 2008, 10, 491-495.	3.2	78
33	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
34	Ab initio DFT+U study of He atom incorporation into UO2 crystals. Physical Chemistry Chemical Physics, 2009, 11, 7241.	2.8	72
35	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
36	Calculations of the geometry and optical properties ofFMgcenters and dimer (F2-type) centers in corundum crystals. Physical Review B, 1995, 51, 8770-8778.	3.2	70

#	Article	IF	Citations
37	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
38	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
39	Interstitial-oxygen-atom diffusion in MgO. Physical Review B, 1996, 53, 7731-7735.	3.2	68
40	Hydration entropy of BaZrO₃ from first principles phonon calculations. Journal of Materials Chemistry A, 2015, 3, 7639-7648.	10.3	68
41	Single impurities in insulators:â€ƒAb initiostudy of Fe-dopedSrTiO3. Physical Review B, 2003, 67, .	3.2	67
42	First-principles and semiempirical calculations forFcenters inKNbO3. Physical Review B, 1997, 56, 8599-8604.	3.2	66
43	Polaronic-type excitons in ferroelectric oxides: Microscopic calculations and experimental manifestation. Physical Review B, 2002, 65, .	3.2	66
44	Quantum-chemical simulation of impurity-induced trapping of a hole: (Li)0centre in MgO. Journal of Physics C: Solid State Physics, 1986, 19, 4183-4199.	1.5	62
45	A periodic ab initio Hartree-Fock calculation on corundum. Chemical Physics Letters, 1987, 140, 120-123.	2.6	58
46	Ab initiothermodynamics ofBacSr(1â^'c)TiO3solid solutions. Physical Review B, 2005, 71, .	3.2	56
47	The Intrinsic Defects, Disordering, and Structural Stability of Ba_xSr_{1â€“x}Co_yFe_{1â€“y}O_{3â3'Î} Perovskite Solid Solutions. Journal of Physical Chemistry C, 2012, 116, 18605-18611.		56
48	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
49	DFT plane wave calculations of the atomic and electronic structure of LaMnO3(001) surface. Physical Chemistry Chemical Physics, 2005, 7, 2346.	2.8	54
50	Formation of anion-vacancy clusters and nanocavities in thermochemically reduced MgO single crystals. Physical Review B, 2000, 62, 9299-9304.	3.2	52
51	The adhesion properties of the Ag/Î±-Al2O3() interface: an ab initio study. Surface Science, 2002, 513, 343-358.	1.9	52
52	Ab initio study of the SrTiO3, BaTiO3 and PbTiO3 (001) surfaces. Ceramics International, 2004, 30, 1989-1992.	4.8	51
53	Calculations for antiferrodistortive phase of SrTiO3perovskite: hybrid density functional study. Journal of Physics Condensed Matter, 2006, 18, 4845-4851.	1.8	51
54	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

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55	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
56	Defect energies for pure corundum and for corundum doped with transition metal ions. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 68, 695-709.	0.6	49
57	The adhesion nature of the Ag/MgO(100) interface: an ab initio study. Chemical Physics Letters, 1998, 283, 395-401.	2.6	49
58	Quantum chemical modelling of "green" luminescence in ABO $ mathsf {_3}$ perovskites. European Physical Journal B, 2002, 27, 483-486.	1.5	48
59	Ab Initio Study of BiFeO₃: Thermodynamic Stability Conditions. Journal of Physical Chemistry Letters, 2015, 6, 2847-2851.	4.6	48
60	Theory of the growth mode for a thin metallic film on an insulating substrate. Surface Science, 2002, 499, 24-40.	1.9	47
61	Ab initio calculations of the BaTiO3 (100) and (110) surfaces. Journal of Electroceramics, 2006, 16, 289-292.	2.0	47
62	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
63	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
64	Kinetics of F center annealing and colloid formation in Al2O3. Nuclear Instruments & Methods in Physics Research B, 2016, 374, 107-110.	1.4	46
65	Anomalous Kinetics of Diffusion-Controlled Defect Annealing in Irradiated Ionic Solids. Journal of Physical Chemistry A, 2018, 122, 28-32.	2.5	46
66	Quantum chemical simulations of hole self-trapping in corundum. Journal of Physics Condensed Matter, 1992, 4, 7531-7544.	1.8	44
67	Atomic scale DFT simulations of point defects in uranium nitride. Journal of Physics Condensed Matter, 2007, 19, 106208.	1.8	44
68	The kinetics of defect aggregation and metal colloid formation in ionic solids under irradiation. Radiation Effects and Defects in Solids, 2001, 155, 113-125.	1.2	43
69	Quantum chemical simulation of the self-trapped hole in Î±-Al2O3crystals. Physical Review Letters, 1992, 69, 1411-1414.	7.8	42
70	Photoconversion ofF-type centers in thermochemically reduced MgO single crystals. Physical Review B, 1999, 59, 4786-4790.	3.2	42
71	Surface Segregation Entropy of Protons and Oxygen Vacancies in BaZrO₃. Chemistry of Materials, 2016, 28, 1363-1368.	6.7	42
72	Stabilization of primary mobile radiation defects in MgF2 crystals. Nuclear Instruments & Methods in Physics Research B, 2016, 374, 24-28.	1.4	42

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73	Extractionâ€“Pyrolytic Method for TiO2 Polymorphs Production. Crystals, 2021, 11, 431.	2.2	41
74	Semi-empirical simulations of the electron centers in MgO crystal. Computational Materials Science, 1996, 5, 298-306.	3.0	40
75	Quantum chemical calculations of the electron center diffusion in MgO crystals. Physica Status Solidi (B): Basic Research, 1996, 195, 61-66.	1.5	40
76	Photoconversion and dynamic hole recycling process in anion vacancies in neutron-irradiated MgO crystals. Physical Review B, 1999, 60, 3787-3791.	3.2	40
77	A new phase in ferroelectric oxides: The phase of charge transfer vibronic excitons. Europhysics Letters, 2001, 56, 702-708.	2.0	40
78	Ab initio calculations of atomic an electronic structure of LaMnO and SrMnO. Solid State Ionics, 2004, 173, 107-111.	2.7	40
79	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
80	Dynamics of F-center annihilation in thermochemically reduced MgO single crystals. Solid State Communications, 2001, 118, 163-167.	1.9	39
81	Adsorption of single Ag and Cu atoms on regular and defective MgO(001) substrates: an ab initio study. Vacuum, 2004, 74, 235-240.	3.5	39
82	Theory of tunneling recombination of defects stimulated by their motion I. General formalism. Physica Status Solidi (B): Basic Research, 1982, 114, 9-34.	1.5	38
83	Calculations of the atomic and electronic structure for SrTiO3 perovskite thin films. Thin Solid Films, 2001, 400, 76-80.	1.8	38
84	Semi-empirical calculations of the electronic and atomic structure of polarons and excitons in ABO 3 perovskite crystals. Computational Materials Science, 2003, 27, 81-86.	3.0	38
85	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
86	Theory of tunneling recombination of defects stimulated by their motion II. Three recombination mechanisms. Physica Status Solidi (B): Basic Research, 1982, 114, 287-318.	1.5	37
87	Kinetics of nanocavity formation based onF-center aggregation in thermochemically reduced MgO single crystals. Physical Review B, 2001, 64, .	3.2	37
88	Atomic and electronic structure of perfect and defective PbZrO3 perovskite: Hybrid DFT calculations of cubic and orthorhombic phases. Computational Materials Science, 2007, 41, 195-201.	3.0	37
89	First-principles comparative study of perfect and defective CsPbX₃ (X = Br, I) crystals. Physical Chemistry Chemical Physics, 2020, 22, 3914-3920.	2.8	37
90	Photoconversion of F+ centers in neutron-irradiated MgO. Nuclear Instruments & Methods in Physics Research B, 2000, 166-167, 220-224.	1.4	36

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91	Quantum chemical modelling of electron polarons and excitons in ABO3perovskites. Journal of Physics Condensed Matter, 2000, 12, L557-L562.	1.8	36
92	Theoretical Analysis of the Growth Mode for Thin Metallic Films on Oxide Substrates. Physical Review Letters, 2000, 85, 4333-4336.	7.8	36
93	Quantum chemical modelling of electron polarons and charge-transfer vibronic excitons in BaTiO3perovskite crystals. Journal of Physics Condensed Matter, 2002, 14, 3735-3741.	1.8	36
94	Modelling of defects and surfaces in perovskite ferroelectrics. Physica Status Solidi (B): Basic Research, 2003, 236, 253-264.	1.5	33
95	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
96	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
97	Charge distribution and optical properties of and F centres in crystals. Journal of Physics Condensed Matter, 1997, 9, L315-L321.	1.8	32
98	Comparative theoretical study of the Agâ€“MgO (100) and (110) interfaces. Surface Science, 1999, 441, 373-383.	1.9	32
99	Enhanced lithium storage and chemical diffusion in metal-LiF nanocomposites: Experimental and theoretical results. Physical Review B, 2007, 76, .	3.2	32
100	Some problems of recombination kinetics. I. Chemical Physics, 1983, 76, 479-487.	1.9	31
101	Thermodynamic stability and disordering in La Sr1â^'MnO3 solid solutions. Solid State Ionics, 2006, 177, 217-222.	2.7	31
102	Atomistic simulation of the [001]surface structure in BaTiO3. Thin Solid Films, 1997, 296, 76-78.	1.8	30
103	DFT study of a singleF center in cubic SrTiO3 perovskite. International Journal of Quantum Chemistry, 2006, 106, 2173-2183.	2.0	30
104	Helium behavior in oxide nuclear fuels: First principles modeling. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3090-3094.	1.4	30
105	Thermodynamic stability of non-stoichiometric SrFeO_{3â^'Î´}: a hybrid DFT study. Physical Chemistry Chemical Physics, 2019, 21, 3918-3931.	2.8	30
106	Quantum chemical simulations of the optical properties and diffusion of electron centres in mgo crystals. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 212-214.	3.5	29
107	Ab initio study of the F centers in CaF2: Calculations of the optical absorption, diffusion and binding energies. Solid State Communications, 1998, 106, 285-288.	1.9	29
108	Quantum chemical modelling of perovskite solid solutions. Journal of Physics Condensed Matter, 2000, 12, L431-L434.	1.8	29

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109	Theory of bound polarons in oxide compounds. Physical Review B, 2001, 63, .	3.2	29
110	Ab initio Hartree-Fock calculations of LaMnO3 (110) surfaces. Solid State Communications, 2003, 127, 367-371.	1.9	29
111	Comparative study of polar perovskite surfaces. Surface Science, 2004, 566-568, 231-235.	1.9	29
112	DFT LCAO and plane wave calculations of SrZrO3. Physica Status Solidi (B): Basic Research, 2005, 242, R11-R13.	1.5	29
113	Theoretical modeling of the complexes of iron impurities and oxygen vacancies in SrTiO3. Applied Physics Letters, 2013, 102, .	3.3	29
114	Analysis of self-trapped hole mobility in alkali halides and metal halides. Solid State Ionics, 2017, 302, 3-6.	2.7	29
115	First-principles calculations of iodine-related point defects in CsPbI₃. Physical Chemistry Chemical Physics, 2019, 21, 7841-7846.	2.8	29
116	Some problems of recombination kinetics. II. Chemical Physics, 1983, 81, 335-347.	1.9	28
117	Modified Maxwell-Garnett equation for the effective transport coefficients in inhomogeneous media. Journal of Physics A, 1998, 31, 7227-7234.	1.6	28
118	Experimental and theoretical studies of polaron optical properties in KNbO3 perovskite. Solid State Communications, 2004, 129, 691-696.	1.9	28
119	The electronic properties of an oxygen vacancy at ZrO2-terminated (001) surfaces of a cubic PbZrO3: computer simulations from the first principles. Physical Chemistry Chemical Physics, 2008, 10, 4258.	2.8	28
120	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
121	The MgO(110) surface and CO adsorption thereon. I. Clean (110) surface. Journal of Physics C: Solid State Physics, 1987, 20, 4983-4990.	1.5	27
122	Correlated annealing of radiation defects in alkali halide crystals. Journal of Physics Condensed Matter, 1992, 4, 5901-5910.	1.8	27
123	Hartree - Fock simulation of the Ag/MgO interface structure. Journal of Physics Condensed Matter, 1996, 8, 6577-6584.	1.8	27
124	F center aggregation kinetics in low-energy electron irradiated LiF. Solid State Communications, 1998, 108, 629-633.	1.9	27
125	Ab initio calculations of the LaMnO3 surface properties. Applied Surface Science, 2004, 238, 457-463.	6.1	27
126	First principles modelling of oxygen impurities in UN nuclear fuels. Journal of Nuclear Materials, 2008, 377, 492-495.	2.7	27

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127	Ab initio calculations of MgF2 (001) and (011) surface structure. Physica B: Condensed Matter, 2010, 405, 2125-2127.	2.7	27
128	Theoretical analysis of the kinetics of low-temperature defect recombination in alkali halide crystals. Low Temperature Physics, 2016, 42, 588-593.	0.6	27
129	Thermodynamic stability of stoichiometric LaFeO₃ and BiFeO₃: a hybrid DFT study. Physical Chemistry Chemical Physics, 2017, 19, 3738-3755.	2.8	27
130	The theory of diffusion-limited recombination of donorâ€"acceptor pairs. Journal of Luminescence, 1975, 9, 502-513.	3.1	26
131	Quantum chemical simulations of hole self-trapping in semi-ionic crystals. International Journal of Quantum Chemistry, 1994, 52, 1177-1198.	2.0	26
132	A novel model for F+to F photoconversion in corundum crystals. Journal of Physics Condensed Matter, 1994, 6, L569-L573.	1.8	26
133	Transient optical absorption in KNbO3 crystals irradiated with pulsed electron beam. Solid State Communications, 1997, 104, 327-330.	1.9	26
134	The kinetics of CaF2 metallization induced by low-energy electron irradiation. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 79-84.	1.4	26
135	Generalised Maxwell-Garnett equation: application to electrical and chemical transport. Physical Chemistry Chemical Physics, 2006, 8, 1310.	2.8	26
136	Electronic and magnetic structure ofLa0.875Sr0.125MnO3calculated by means of hybrid density-functional theory. Physical Review B, 2007, 76, .	3.2	26
137	First-principles modelling of defects in advanced nuclear fuels. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 1193-1196.	0.8	26
138	DFT calculations of point defects on UN(001) surface. Surface Science, 2011, 605, 396-400.	1.9	26
139	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
140	Calculation of energies of radiative tunneling transitions between defects in alkali halides. Solid State Communications, 1982, 42, 749-752.	1.9	25
141	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
142	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations. Journal of Nuclear Materials, 2009, 393, 504-507.	2.7	25
143	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
144	Role of tunnelling recombination in radiation-induced F-centre creation in alkali halide crystals at liquid helium temperatures. Journal of Physics C: Solid State Physics, 1975, 8, 2366-2375.	1.5	24

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145	Water interaction with perfect and fluorine-doped Co3O4 (100) surface. Solid State Ionics, 2015, 277, 77-82.	2.7	24
146	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
147	Kinetics of non-steady state diffusion-controlled tunnelling recombination of defects in insulating crystals. Journal of Physics Condensed Matter, 1989, 1, 6777-6785.	1.8	23
148	A mesoscopic approach to radiation-induced defect aggregation in alkali halides stimulated by the elastic interaction of mobile Frenkel defects. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1994, 70, 313-327.	0.6	23
149	Discrete-lattice theory for Frenkel-defect aggregation in irradiated ionic solids. Physical Review B, 1998, 58, 8454-8463.	3.2	23
150	Atomistic simulation of SrTiO3 and BaTiO3 (110) surface relaxations. Thin Solid Films, 2000, 358, 1-5.	1.8	23
151	Quantum chemical modelling of electron polarons and ÂgreenÂ luminescence in PbTiO3perovskite crystals. Journal of Physics Condensed Matter, 2002, 14, L647-L653.	1.8	23
152	Study of the electronic and atomic structure of thermally treated SrTiO3(110) surfaces. Surface and Interface Analysis, 2003, 35, 998-1003.	1.8	23
153	First principles simulations ofF centers in cubic SrTiO3. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 153-158.	0.8	23
154	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
155	First principles calculations of oxygen reduction reaction at fuel cell cathodes. Current Opinion in Electrochemistry, 2020, 19, 122-128.	4.8	23
156	Generalised theory of diffusion-controlled defect annealing. Journal of Physics C: Solid State Physics, 1980, 13, L499-L502.	1.5	22
157	Semiempirical Calculations of Defect Properties in LiF Crystal. Physica Status Solidi (B): Basic Research, 1981, 108, 673-681.	1.5	22
158	The semiempirical approach to electronic structure of ionic crystal surface. Journal of Physics C: Solid State Physics, 1982, 15, 847-861.	1.5	22
159	Semiempirical Calculations of Defect Properties in LiF Crystal. II. Electron and Hole Centres and Their Recombination. Physica Status Solidi (B): Basic Research, 1982, 109, 75-81.	1.5	22
160	Atomistic simulation of surface relaxation. Journal of Physics Condensed Matter, 1998, 10, L347-L353.	1.8	22
161	First principles calculations of oxygen adsorption on the UN(001) surface. Surface Science, 2009, 603, 50-53.	1.9	22
162	Ab initio simulation of yttrium oxide nanocluster formation on fcc Fe lattice. Journal of Nuclear Materials, 2010, 406, 345-350.	2.7	22

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163	Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies. Journal of Materials Chemistry C, 2021, 9, 1693-1700.	5.5	22
164	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
165	Kinetics of the electronic center annealing in Al2O3 crystals. Journal of Nuclear Materials, 2018, 502, 295-300.	2.7	21
166	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
167	The MgO(110) surface and CO adsorption thereon. II. CO adsorption. Journal of Physics C: Solid State Physics, 1987, 20, 4991-4997.	1.5	20
168	Luminescence properties of KNbO3 crystals. Journal of Luminescence, 1997, 72-74, 672-674.	3.1	20
169	Semi-empirical defect calculations for the perovskite KNbO3. Journal of Physics Condensed Matter, 2000, 12, 569-574.	1.8	20
170	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
171	Use of site symmetry in supercell models of defective crystals: polarons in CeO₂. Physical Chemistry Chemical Physics, 2017, 19, 8340-8348.	2.8	20
172	Kinetics of Defect Accumulation and Recombination: II. Diffusionâ€Controlled Defect Annihilation. Physica Status Solidi (B): Basic Research, 1981, 108, 37-44.	1.5	19
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