Eugene A Kotomin

List of Publications by Year in Descending Order

435 papers	9,631 citations	49 h-index	77 g-index
461 ext. papers	10,380 ext. citations	2.7 avg, IF	6.15 L-index

#	Paper	IF	Citations
435	Influence of Au, Ag, and Cu Adatoms on Optical Properties of TiO2 (110) Surface: Predictions from RT-TDDFT Calculations. *Crystals*, **2022**, 12, 452	2.3	
434	Evidence for the formation of two types of oxygen interstitials in neutron-irradiated □AlO single crystals. *Scientific Reports*, **2021**, 11, 20909	4.9	3
433	Water Splitting on Multifaceted SrTiO3 Nanocrystals: Computational Study. *Catalysts*, **2021**, 11, 1326	4	3
432	Extraction□Pyrolytic Method for TiO2 Polymorphs Production. *Crystals*, **2021**, 11, 431	2.3	19
431	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	7.1	3
430	BaCoO monoclinic structure and chemical bonding analysis: hybrid DFT calculations. *Physical Chemistry Chemical Physics*, **2021**, 23, 17493-17501	3.6	3
429	Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies. *Journal of Materials Chemistry C*, **2021**, 9, 1693-1700	7.1	11
428	The electronic properties of SrTiO with oxygen vacancies or substitutions. *Scientific Reports*, **2021**, 11, 23341	4.9	4
427	First principles calculations of the vibrational properties of single and dimer F-type centers in corundum crystals. *Journal of Chemical Physics*, **2020**, 153, 134107	3.9	0
426	Hybrid density functional theoretical study of NASICON-type NaTi(PO) (x = 1-4). *Physical Chemistry Chemical Physics*, **2020**, 22, 11861-11870	3.6	5
425	Distinctive features of diffusion-controlled radiation defect recombination in stoichiometric magnesium aluminate spinel single crystals and transparent polycrystalline ceramics. *Scientific Reports*, **2020**, 10, 7810	4.9	26
424	Interdependence of Oxygenation and Hydration in Mixed-Conducting (Ba,Sr)FeO3□Perovskites Studied by Density Functional Theory. *Journal of Physical Chemistry C*, **2020**, 124, 11780-11789	3.8	12
423	Ab initio calculations of pure and Co+2-doped MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2020**, 470, 10-14	1.2	1
422	First-principles comparative study of perfect and defective CsPbX (X = Br, I) crystals. *Physical Chemistry Chemical Physics*, **2020**, 22, 3914-3920	3.6	18
421	Oxygen Evolution Reaction on a N-Doped Co0.5-Terminated Co3o4 (001) Surface. *Proceedings of the Latvian Academy of Sciences*, **2020**, 74, 396-403	0.3	
420	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	0.7	8
419	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	1.2	7

418	First-Principles Modeling of Oxygen Adsorption on Ag-Doped LaMnO3 (001) Surface. *Journal of Electronic Materials*, **2020**, 49, 1421-1434	1.9	3
417	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	3.8	12
416	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	1.2	12
415	First principles calculations of oxygen reduction reaction at fuel cell cathodes. *Current Opinion in Electrochemistry*, **2020**, 19, 122-128	7.2	8
414	Atomic, electronic and magnetic structure of an oxygen interstitial in neutron-irradiated AlO single crystals. *Scientific Reports*, **2020**, 10, 15852	4.9	7
413	Low temperature structural transformations on the (001) surface of SrTiO3 single crystals. *Low Temperature Physics*, **2020**, 46, 740-750	0.7	6
412	Role of Intrinsic Dipoles in the Evaporation-Driven Assembly of Perovskite Nanocubes into Energy-Harvesting Composites. *Physica Status Solidi (A) Applications and Materials Science*, **2020**, 217, 1900533	1.6	2
411	On the Way to Optoionics. *Helvetica Chimica Acta*, **2020**, 103, e2000073	2	11
410	Thermodynamic stability of non-stoichiometric SrFeO: a hybrid DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 3918-3931	3.6	18
409	Ab initio simulation of (Ba,Sr)TiO3 and (Ba,Ca)TiO3 perovskite solid solutions. *Solid State Ionics*, **2019**, 337, 76-81	3.3	9
408	Defect-Induced Effects in Nanomaterials. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1900181	1.3	
407	Manifestation of dipole-induced disorder in self-assembly of ferroelectric and ferromagnetic nanocubes. *Nanoscale*, **2019**, 11, 7293-7303	7.7	7
406	First principles calculations on CeO2 doped with Tb3+ ions. *Optical Materials*, **2019**, 90, 76-83	3.3	2
405	First-principles calculations of iodine-related point defects in CsPbI. *Physical Chemistry Chemical Physics*, **2019**, 21, 7841-7846	3.6	17
404	Nitrogen interstitial defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. *Materials Today Communications*, **2019**, 21, 100616	2.5	8
403	Interface-induced enhancement of piezoelectricity in the (SrTiO)/(BaTiO) superlattice for energy harvesting applications. *Physical Chemistry Chemical Physics*, **2019**, 21, 23541-23551	3.6	6
402	The first principles calculations of CO2 adsorption on (101□0) ZnO surface **2019**,		5
401	Theoretical and Experimental Study of (Ba,Sr)TiO3 Perovskite Solid Solutions and BaTiO3/SrTiO3 Heterostructures. *Journal of Physical Chemistry C*, **2019**, 123, 2031-2036	3.8	15

400	First Principles Simulations on Migration Paths of Oxygen Interstitials in MgAl2O4. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800282	1.3	6
399	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	1.3	2
398	Kinetics of the electronic center annealing in Al2O3 crystals. *Journal of Nuclear Materials*, **2018**, 502, 295-300	3.3	15
397	Ab initio modelling of the initial stages of the ODS particle formation process. *Nuclear Instruments & Methods in Physics Research B*, **2018**, 435, 70-73	1.2	4
396	Ab initio simulations on charged interstitial oxygen migration in corundum. *Nuclear Instruments & Methods in Physics Research B*, **2018**, 435, 74-78	1.2	10
395	Anomalous Kinetics of Diffusion-Controlled Defect Annealing in Irradiated Ionic Solids. *Journal of Physical Chemistry A*, **2018**, 122, 28-32	2.8	23
394	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	1.2	0
393	Kinetic Monte Carlo modeling of Y2O3 nano-cluster formation in radiation resistant matrices. *Nuclear Instruments & Methods in Physics Research B*, **2018**, 434, 13-22	1.2	
392	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	1.2	24
391	First-Principles Modelling of N-Doped Co3O4. *Latvian Journal of Physics and Technical Sciences*, **2018**, 55, 36-42	0.5	1
390	Kinetics of dimer F2 type center annealing in MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2018**, 435, 79-82	1.2	12
389	Theoretical investigations of nitrogen doping on Co3O4 for water dissociation catalytically activity. *Journal of Physics: Conference Series*, **2018**, 1115, 032032	0.3	1
388	Transition levels of acceptor impurities in ZnO crystals by DFT-LCAO calculations. *Journal of Physics: Conference Series*, **2018**, 1115, 042064	0.3	0
387	Dopant solubility in ceria: alloy thermodynamics combined with the DFT+U calculations. *Solid State Ionics*, **2018**, 325, 258-264	3.3	1
386	Impact of point defects on the elastic properties of BaZrO3: Comprehensive insight from experiments and ab initio calculations. *Acta Materialia*, **2018**, 160, 247-256	8.4	14
385	Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes. *Journal of Materials Chemistry A*, **2018**, 6, 11929-11940	13	28
384	Use of site symmetry in supercell models of defective crystals: polarons in CeO. *Physical Chemistry Chemical Physics*, **2017**, 19, 8340-8348	3.6	14
383	(Invited) The Effect of (La,Sr)MnO 3 Cathode Surface Termination on Its Electronic Structure. *ECS Transactions*, **2017**, 77, 67-73	1	2

382	Thermodynamic stability of stoichiometric LaFeO and BiFeO: a hybrid DFT study. *Physical Chemistry Chemical Physics*, **2017**, 19, 3738-3755	3.6	16
381	Analysis of self-trapped hole mobility in alkali halides and metal halides. *Solid State Ionics*, **2017**, 302, 3-6	3.3	21
380	First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 25245-25251	3.6	14
379	Electromechanical Properties of BaSrTiO Perovskite Solid Solutions from First-Principles Calculations. *Journal of Physical Chemistry A*, **2017**, 121, 9409-9414	2.8	10
378	First-principles Study of Perovskite Ultrathin Films: Stability and Confinement Effects. *Israel Journal of Chemistry*, **2017**, 57, 509-521	3.4	7
377	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	2.3	8
376	Stabilization of primary mobile radiation defects in MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 374, 24-28	1.2	28
375	Kinetics of F center annealing and colloid formation in Al2O3. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 374, 107-110	1.2	33
374	Ab initio simulations on migration paths of interstitial oxygen in corundum. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 374, 29-34	1.2	13
373	Charged oxygen interstitials in corundum: first principles simulations. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2016**, 13, 932-936		2
372	Ab initio modelling of YO cluster formation in Fe lattice. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 2136-2143	1.3	4
371	Theoretical analysis of the kinetics of low-temperature defect recombination in alkali halide crystals. *Low Temperature Physics*, **2016**, 42, 588-593	0.7	22
370	Surface Segregation Entropy of Protons and Oxygen Vacancies in BaZrO3. *Chemistry of Materials*, **2016**, 28, 1363-1368	9.6	32
369	First principles study of confinement effects for oxygen vacancies in BaZrO(001) ultra-thin films. *Physical Chemistry Chemical Physics*, **2016**, 18, 9902-8	3.6	13
368	Large-Scale Modeling of Defects in Advanced Oxides: Oxygen Vacancies in BaZrO3 Crystals **2016**, 187-198		
367	Void lattice formation in electron irradiated CaF2: Statistical analysis of experimental data and cellular automata simulations. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 368, 138-143	1.2	5
366	First Principles Modeling of Pd-doped (La,Sr)(Co,Fe)O3 Complex Perovskites. *Fuel Cells*, **2016**, 16, 267-271	1.9	5
365	Low-temperature radiation effects in wide gap materials. *Low Temperature Physics*, **2016**, 42, 537-538	0.7	

364	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	0.3	1
363	Ab initio modelling of oxygen vacancies and protonic defects in La1−xSrxFeO3−δ perovskite solid solutions. *Journal of Materials Chemistry A*, **2016**, 4, 13093-13104	13	28
362	The effective diffusion coefficient in a one-dimensional discrete lattice with the inclusions. *Physica B: Condensed Matter*, **2015**, 470-471, 50-52	2.8	3
361	Ab Initio Study of BiFeO3: Thermodynamic Stability Conditions. *Journal of Physical Chemistry Letters* , **2015**, 6, 2847-51	6.4	38
360	First principles modeling of Ag adsorption on the LaMnO3 (001) surfaces. *Solid State Ionics*, **2015**, 273, 46-50	3.3	1
359	Hydration entropy of BaZrO3 from first principles phonon calculations. *Journal of Materials Chemistry A*, **2015**, 3, 7639-7648	13	53
358	Thermodynamic properties of neutral and charged oxygen vacancies in BaZrO3 based on first principles phonon calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 20765-74	3.6	39
357	Ab initio simulations on Frenkel pairs of radiation defects in corundum. *IOP Conference Series: Materials Science and Engineering*, **2015**, 77, 012001	0.4	4
356	Water interaction with perfect and fluorine-doped Co3O4 (100) surface. *Solid State Ionics*, **2015**, 277, 77-82	3.3	19
355	Confinement effects for the F center in non-stoichiometric BaZrO3 ultrathin films. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 139-143	1.3	6
354	Ab initio modeling of radiation damage in MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2014**, 326, 314-317	1.2	14
353	Hydrogen induced metallization of ZnO (11 00) surface: Ab initio study. *Thin Solid Films*, **2014**, 553, 38-42	2.2	13
352	Theory of non-equilibrium critical phenomena in three-dimensional condensed systems of charged mobile nanoparticles. *Physical Chemistry Chemical Physics*, **2014**, 16, 13974-83	3.6	5
351	Static and dynamic screening effects in the electrostatic self-assembly of nano-particles. *Physical Chemistry Chemical Physics*, **2014**, 16, 25449-60	3.6	10
350	Hydrogen adsorption on the ZnO $(1bar{1}00)$ surface: ab initio hybrid density functional linear combination of atomic orbitals calculations. *Physica Scripta*, **2014**, 89, 045801	2.6	12
349	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	3.8	22
348	Ab Initio Thermodynamics of Oxygen Vacancies and Zinc Interstitials in ZnO. *Journal of Physical Chemistry Letters*, **2014**, 5, 4238-42	6.4	13
347	Statistical characterization of self-assembled charged nanoparticle structures. *Physica Status Solidi (A) Applications and Materials Science*, **2014**, 211, 288-293	1.6	3

346	Radiation defects in complex perovskite solid solutions. *Nuclear Instruments & Methods in Physics Research B*, **2014**, 326, 243-246	1.2	1
345	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	13	22
344	Theoretical modeling of antiferrodistortive phase transition for SrTiO3 ultrathin films. *Physical Review B*, **2013**, 88,	3.3	10
343	First-principles modeling of the H color centers in MgF2 crystals. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2013**, 10, 160-164		4
342	Theoretical modeling of the complexes of iron impurities and oxygen vacancies in SrTiO3. *Applied Physics Letters*, **2013**, 102, 112913	3.4	28
341	Ab initio study of phase competition in (La1 □t,Src)CoO3 solid solutions. *Solid State Ionics*, **2013**, 230, 32-36	3.3	14
340	Combined theoretical and experimental analysis of processes determining cathode performance in solid oxide fuel cells. *Physical Chemistry Chemical Physics*, **2013**, 15, 5443-71	3.6	208
339	Formation and migration of oxygen vacancies in La(1-x)Sr(x)Co(1-y)Fe(y)O(3-□perovskites: insight from ab initio calculations and comparison with Ba(1-x)Sr(x)Co(1-y)Fe(y)O(3-□ *Physical Chemistry Chemical Physics*, **2013**, 15, 911-8	3.6	95
338	First principles calculations of (Ba,Sr)(Co,Fe)O3□structural stability. *Solid State Ionics*, **2013**, 230, 21-26	3.3	14
337	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. *Journal of Nuclear Materials*, **2013**, 435, 102-106	3.3	16
336	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	3.8	68
335	Atomic and electronic structure of hydrogen on ZnO (11 00) surface: ab initio hybrid calculations. *IOP Conference Series: Materials Science and Engineering*, **2013**, 49, 012054	0.4	
334	Phase competition in (La1 □t,Src)CoO3 solid solutions: ab initio thermodynamic study. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 864-869	1.3	10
333	The first-principles treatment of the electron-correlation and spin-orbital effects in uranium mononitride nuclear fuels. *Physical Chemistry Chemical Physics*, **2012**, 14, 4482-90	3.6	63
332	The Intrinsic Defects, Disordering, and Structural Stability of BaxSr1□CoyFe1□O3□Perovskite Solid Solutions. *Journal of Physical Chemistry C*, **2012**, 116, 18605-18611	3.8	53
331	Note: Effective diffusion coefficient in heterogeneous media. *Journal of Chemical Physics*, **2012**, 137, 166101	3.9	7
330	Jahn-Teller effect in the phonon properties of defective SrTiO3 from first principles. *Physical Review B*, **2012**, 85,	3.3	46
329	Ab initiomodelling of UN grain boundary interfaces. *IOP Conference Series: Materials Science and Engineering*, **2012**, 38, 012058	0.4	

328	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	0.2	1
327	First-principles phonon calculations of Fe impurity in SrTiO *Journal of Physics Condensed Matter*, **2012**, 24, 104024	1.8	3
326	Oxygen exchange kinetics on solid oxide fuel cell cathode materials general trends and their mechanistic interpretation. *Journal of Materials Research*, **2012**, 27, 2000-2008	2.5	76
325	Ab initiocalculations of theFcenters in MgF2bulk and on the (001) surface. *Physica Scripta*, **2012**, 86, 035304	2.6	8
324	Ab initiocalculations of theHcenters in MgF2crystals. *IOP Conference Series: Materials Science and Engineering*, **2012**, 38, 012041	0.4	
323	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	0.4	4
322	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	0.2	2
321	Pattern formation kinetics for charged molecules on surfaces: microscopic correlation function analysis. *Journal of Physical Chemistry B*, **2011**, 115, 14626-33	3.4	5
320	Phonon calculations in cubic and tetragonal phases of SrTiO3: A comparative LCAO and plane-wave study. *Physical Review B*, **2011**, 83,	3.3	71
319	The non-equilibrium charge screening effects in diffusion-driven systems with pattern formation. *Journal of Chemical Physics*, **2011**, 135, 034702	3.9	10
318	Modeling of yttrium, oxygen atoms and vacancies in ron lattice. *Journal of Nuclear Materials*, **2011**, 416, 40-44	3.3	7
317	Ab initio modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies. *Journal of Nuclear Materials*, **2011**, 416, 200-204	3.3	29
316	Simulations on the mechanism of CNT bundle growth upon smooth and nanostructured Ni as well as Al2O3 catalysts. *Open Physics*, **2011**, 9,	1.3	3
315	Ab initio calculations of the atomic and electronic structure of MgF2 (011) and (111) surfaces. *Open Physics*, **2011**, 9,	1.3	4
314	First principles calculations of oxygen vacancy formation and migration in mixed conducting Ba0.5Sr0.5Co1 FeyO3 perovskites. *Solid State Ionics*, **2011**, 188, 1-5	3.3	80
313	Confinement effects for ionic carriers in SrTiO3 ultrathin films: first-principles calculations of oxygen vacancies. *Physical Chemistry Chemical Physics*, **2011**, 13, 923-6	3.6	13
312	First Principles Calculations of Oxygen Vacancy Formation and Migration in Ba1 SrxCo1 FeyO3 Perovskites. *Journal of the Electrochemical Society*, **2011**, 159, B219-B226	3.9	74
311	A Comparative Hybrid DFT Study of Phonons in Several SrTiO3 Phases. *Integrated Ferroelectrics*, **2011**, 123, 18-25	0.8	3

310	First-Principles Modeling of Oxygen Interaction with SrTiO3(001) Surface: Comparative Density-Functional LCAO and Plane-Wave Study. *Integrated Ferroelectrics*, **2011**, 123, 10-17	0.8	11
309	DFT calculations of point defects on UN(001) surface. *Surface Science*, **2011**, 605, 396-400	1.8	22
308	Atomistic theory of mesoscopic pattern formation induced by bimolecular surface reactions between oppositely charged molecules. *Journal of Chemical Physics*, **2011**, 135, 224503	3.9	5
307	First Principles Modeling of Oxygen Mobility in Perovskite SOFC Cathode and Oxygen Permeation Membrane Materials. *ECS Transactions*, **2011**, 35, 823-830	1	10
306	The Structural Disorder and Lattice Stability of (Ba,Sr)(Co,Fe)O3 Complex Perovskites. *ECS Transactions*, **2011**, 35, 2077-2084	1	8
305	Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for (La, Sr)MnO3 *Journal of Physical Chemistry C*, **2010**, 114, 3017-3027	3.8	142
304	Microscopic approach to the kinetics of pattern formation of charged molecules on surfaces. *Physical Review E*, **2010**, 82, 021602	2.4	8
303	First-principles modelling of complex perovskite (Ba1-xSrx)(Co1-yFey)O3- for solid oxide fuel cell and gas separation membrane applications. *Energy and Environmental Science*, **2010**, 3, 1544	35.4	70
302	Ab initio calculations of MgF2 (001) and (011) surface structure. *Physica B: Condensed Matter*, **2010**, 405, 2125-2127	2.8	25
301	Ab initio simulation of yttrium oxide nanocluster formation on fcc Fe lattice. *Journal of Nuclear Materials*, **2010**, 406, 345-350	3.3	18
300	Ab initio calculations of Nb doped SrTiO3. *Physica B: Condensed Matter*, **2010**, 405, 3164-3166	2.8	12
299	Void superlattice formation in electron irradiated CaF2: Theoretical analysis. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3055-3058	1.2	4
298	Basic properties of the F-type centers in halides, oxides and perovskites. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3084-3089	1.2	126
297	Helium behavior in oxide nuclear fuels: First principles modeling. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3090-3094	1.2	29
296	Implementing first principles calculations of defect migration in a fuel performance code for UN simulations. *Journal of Nuclear Materials*, **2009**, 393, 292-299	3.3	23
295	A comparative ab initio study of bulk and surface oxygen vacancies in PbTiO3, PbZrO3 and SrTiO3 perovskites. *Solid State Communications*, **2009**, 149, 1359-1362	1.6	44
294	First principles calculations of oxygen adsorption on the UN(001) surface. *Surface Science*, **2009**, 603, 50-53	1.8	20
293	Atomic, electronic and thermodynamic properties of cubic and orthorhombic LaMnO3 surfaces. *Surface Science*, **2009**, 603, 326-335	1.8	94

292	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations. *Journal of Nuclear Materials*, **2009**, 393, 504-507	3.3	23
291	First-principles study of bulk and surface oxygen vacancies in SrTiO3 crystal. *European Physical Journal B*, **2009**, 72, 53-57	1.2	81
290	Ab initio DFT+U study of He atom incorporation into UO(2) crystals. *Physical Chemistry Chemical Physics*, **2009**, 11, 7241-7	3.6	65
289	The Effect of Oxygen Vacancies on the Atomic and Electronic Structure of Cubic ABO3 Perovskite Bulk and the (001) Surface: Ab initio Calculations. *Ferroelectrics*, **2009**, 379, 191-198	0.6	11
288	Oxygen Incorporation Reaction into Mixed Conducting Perovskites: a Mechanistic Analysis for (La,Sr)MnO3 Based on DFT Calculations. *ECS Transactions*, **2009**, 25, 2753-2760	1	9
287	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	3.4	73
286	Hybrid DFT calculations of theFcenters in cubic ABO3perovskites. *Journal of Physics: Conference Series*, **2008**, 117, 012019	0.3	6
285	Adsorption of atomic and molecular oxygen on the LaMnO3(001) surface: ab initio supercell calculations and thermodynamics. *Physical Chemistry Chemical Physics*, **2008**, 10, 4644-9	3.6	104
284	The electronic properties of an oxygen vacancy at ZrO(2)-terminated (001) surfaces of a cubic PbZrO(3): computer simulations from the first principles. *Physical Chemistry Chemical Physics*, **2008**, 10, 4258-63	3.6	22
283	First-Principles Modeling of LaMnO3 SOFC Cathode Material. *ECS Transactions*, **2008**, 13, 301-306	1	4
282	Ab initio modeling of spin and charge ordering and lattice dynamics in CaFeO(3) crystals. *Journal of Chemical Physics*, **2008**, 129, 214704	3.9	5
281	Electronic structure and thermodynamic stability of LaMnO3 and La1⊠SrxMnO3 (001) surfaces: Ab initio calculations. *Physical Review B*, **2008**, 78,	3.3	79
280	Ab initiostudy of bulk and surface iron defects in SrTiO3. *Journal of Physics: Conference Series*, **2008**, 117, 012001	0.3	2
279	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	1.3	3
278	Atomistic Modeling of a New Storage. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2008**, 634, 2055-2055	1.3	
277	A first-principles DFT study of UN bulk and (001) surface: comparative LCAO and PW calculations. *Journal of Computational Chemistry*, **2008**, 29, 2079-87	3.5	36
276	First principles modelling of oxygen impurities in UN nuclear fuels. *Journal of Nuclear Materials*, **2008**, 377, 492-495	3.3	23
275	First-principles modelling of radiation defects in advanced nuclear fuels. *Nuclear Instruments & Methods in Physics Research B*, **2008**, 266, 2671-2675	1.2	13

274	Jahn-Teller distortion around Fe4+ in Sr(FexTi1−x)O3−δ from x-ray absorption spectroscopy, x-ray diffraction, and vibrational spectroscopy. *Physical Review B*, **2007**, 76,	3.3	102
273	Differences in the metallic film growth mode between perfect and defective MgO surfaces. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 255, 219-222	1.2	8
272	First-principles modelling of defects in advanced nuclear fuels. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2007**, 4, 1193-1196		24
271	Periodic models in quantum chemical simulations of F centers in crystalline metal oxides. *International Journal of Quantum Chemistry*, **2007**, 107, 2956-2985	2.1	69
270	Enhanced lithium storage and chemical diffusion in metal-LiF nanocomposites: Experimental and theoretical results. *Physical Review B*, **2007**, 76,	3.3	31
269	Electronic structure and thermodynamic stability of double-layered SrTiO3(001) surfaces: Ab initio simulations. *Physical Review B*, **2007**, 75,	3.3	83
268	Electronic and magnetic structure of La0.875Sr0.125MnO3 calculated by means of hybrid density-functional theory. *Physical Review B*, **2007**, 76,	3.3	24
267	Atomic scale DFT simulations of point defects in uranium nitride. *Journal of Physics Condensed Matter*, **2007**, 19, 106208	1.8	40
266	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	3.2	31
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