Eugene A Kotomin

List of Publications by Citations

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	Kinetics of bimolecular reactions in condensed media: critical phenomena and microscopic self-organisation. *Reports on Progress in Physics*, **1988**, 51, 1479-1523	14.4	248
434	Ab initio modeling of surface structure for SrTiO3 perovskite crystals. *Physical Review B*, **2001**, 64,	3.3	232
433	Radiation-induced point defects in simple oxides. *Nuclear Instruments & Methods in Physics Research B*, **1998**, 141, 1-15	1.2	218
432	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
431	Evidence for interfacial-storage anomaly in nanocomposites for lithium batteries from first-principles simulations. *Physical Review Letters*, **2006**, 96, 058302	7.4	172
430	Nano-ionics in the context of lithium batteries. *Journal of Power Sources*, **2006**, 159, 171-178	8.9	164
429	Hybrid DFT calculations of the atomic and electronic structure for ABO3 perovskite (0 0 1) surfaces. *Surface Science*, **2005**, 575, 75-88	1.8	160
428	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
427	First-principles calculations of the atomic and electronic structure of F centers in the bulk and on the (001) surface of SrTiO3. *Physical Review B*, **2006**, 73,	3.3	138
426	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
425	First-principles calculations for SrTiO3() surface structure. *Surface Science*, **2002**, 513, 211-220	1.8	111
424	Semi-empirical simulations of surface relaxation for perovskite titanates. *Surface Science*, **2000**, 462, 19-35	1.8	107
423	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
422	Calculations of the ground and excited states of F-type centers in corundum crystals. *Physical Review B*, **1994**, 49, 14854-14858	3.3	103
421	Jahn-Teller distortion around Fe4+ in Sr(FexTi1)O3 from x-ray absorption spectroscopy, x-ray diffraction, and vibrational spectroscopy. *Physical Review B*, **2007**, 76,	3.3	102
420	Calculations of the effective diffusion coefficient for inhomogeneous media. *Journal of Physics and Chemistry of Solids*, **2002**, 63, 449-456	3.9	100
419	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

418	Atomic, electronic and thermodynamic properties of cubic and orthorhombic LaMnO3 surfaces. *Surface Science*, **2009**, 603, 326-335	1.8	94
417	Atomic and electronic structure of the corundum (0001) surface: comparison with surface spectroscopies. *Surface Science*, **1997**, 370, 190-200	1.8	90
416	Electronic structure and thermodynamic stability of double-layered SrTiO3(001) surfaces: Ab initio simulations. *Physical Review B*, **2007**, 75,	3.3	83
415	Ab initio modeling of metal adhesion on oxide surfaces with defects. *Physical Review Letters*, **2000**, 84, 1256-9	7.4	82
414	First-principles study of bulk and surface oxygen vacancies in SrTiO3 crystal. *European Physical Journal B*, **2009**, 72, 53-57	1.2	81
413	First principles calculations of oxygen vacancy formation and migration in mixed conducting Ba0.5Sr0.5Co1−yFeyO3−δ perovskites. *Solid State Ionics*, **2011**, 188, 1-5	3.3	80
412	Electronic structure and thermodynamic stability of LaMnO3 and La1−xSrxMnO3 (001) surfaces: Ab initio calculations. *Physical Review B*, **2008**, 78,	3.3	79
411	Ab initio calculations of the SrTiO3 (110) polar surface. *Physical Review B*, **2004**, 69,	3.3	79
410	First-principles and semiempirical calculations for bound-hole polarons in KNbO3. *Physical Review B* , **1999**, 60, 1-5	3.3	79
409	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
408	Comparative density-functional LCAO and plane-wave calculations of LaMnO3 surfaces. *Physical Review B*, **2005**, 72,	3.3	75
407	Phenomenological kinetics of Frenkel defect recombination and accumulation in ionic solids. *Reports on Progress in Physics*, **1992**, 55, 2079-2188	14.4	75
406	First Principles Calculations of Oxygen Vacancy Formation and Migration in Ba1−xSrxCo1−yFeyO3−δ Perovskites. *Journal of the Electrochemical Society*, **2011**, 159, B219-B226	3.9	74
405	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
404	Phonon calculations in cubic and tetragonal phases of SrTiO3: A comparative LCAO and plane-wave study. *Physical Review B*, **2011**, 83,	3.3	71
403	First-principles modelling of complex perovskite (Ba1-xSrx)(Co1-yFey)O3-δ for solid oxide fuel cell and gas separation membrane applications. *Energy and Environmental Science*, **2010**, 3, 1544	35.4	70
402	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
401	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

400	Ab initio DFT+U study of He atom incorporation into UO(2) crystals. *Physical Chemistry Chemical Physics*, **2009**, 11, 7241-7	3.6	65
399	Polaronic-type excitons in ferroelectric oxides: Microscopic calculations and experimental manifestation. *Physical Review B*, **2002**, 65,	3.3	64
398	Interstitial-oxygen-atom diffusion in MgO. *Physical Review B*, **1996**, 53, 7731-7735	3.3	64
397	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
396	Calculations of the geometry and optical properties of FMg centers and dimer (F2-type) centers in corundum crystals. *Physical Review B*, **1995**, 51, 8770-8778	3.3	63
395	First-principles and semiempirical calculations for F centers in KNbO3. *Physical Review B*, **1997**, 56, 8599-8604	3.3	62
394	Single impurities in insulators: Ab initio study of Fe-doped SrTiO3. *Physical Review B*, **2003**, 67,	3.3	62
393	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		58
392	A periodic ab initio Hartree-Fock calculation on corundum. *Chemical Physics Letters*, **1987**, 140, 120-123	2.5	55
391	Hydration entropy of BaZrO3 from first principles phonon calculations. *Journal of Materials Chemistry A*, **2015**, 3, 7639-7648	13	53
390	The Intrinsic Defects, Disordering, and Structural Stability of BaxSr1−xCoyFe1−yO3−δ Perovskite Solid Solutions. *Journal of Physical Chemistry C*, **2012**, 116, 18605-18611	3.8	53
389	Ab initio thermodynamics of BacSr(1−c)TiO3 solid solutions. *Physical Review B*, **2005**, 71,	3.3	53
388	DFT plane wave calculations of the atomic and electronic structure of LaMnO3 (001) surface. *Physical Chemistry Chemical Physics*, **2005**, 7, 2346-50	3.6	49
387	Ab initio study of the SrTiO3, BaTiO3 and PbTiO3 (001) surfaces. *Ceramics International*, **2004**, 30, 1989-1992	5.1	49
386	The adhesion properties of the Ag/α-Al2O3() interface: an ab initio study. *Surface Science*, **2002**, 513, 343-358	1.8	49
385	Formation of anion-vacancy clusters and nanocavities in thermochemically reduced MgO single crystals. *Physical Review B*, **2000**, 62, 9299-9304	3.3	49
384	Jahn-Teller effect in the phonon properties of defective SrTiO3 from first principles. *Physical Review B*, **2012**, 85,	3.3	46
383	Calculations for antiferrodistortive phase of SrTiO3perovskite: hybrid density functional study. *Journal of Physics Condensed Matter*, **2006**, 18, 4845-4851	1.8	46

382	Quantum chemical modelling of □green□luminescence in ABO perovskites. *European Physical Journal B*, **2002**, 27, 483-486	1.2	46
381	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		45
380	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
379	The adhesion nature of the Ag/MgO(100) interface: an ab initio study. *Chemical Physics Letters*, **1998**, 283, 395-401	2.5	44
378	Ab initio calculations of the BaTiO3 (100) and (110) surfaces. *Journal of Electroceramics*, **2006**, 16, 289-292	2.5	44
377	Theory of the growth mode for a thin metallic film on an insulating substrate. *Surface Science*, **2002**, 499, 24-40	1.8	43
376	Quantum chemical simulations of hole self-trapping in corundum. *Journal of Physics Condensed Matter*, **1992**, 4, 7531-7544	1.8	41
375	Quantum chemical simulation of the self-trapped hole in alpha -Al2O3 crystals. *Physical Review Letters*, **1992**, 69, 1411-1414	7.4	41
374	Atomic scale DFT simulations of point defects in uranium nitride. *Journal of Physics Condensed Matter*, **2007**, 19, 106208	1.8	40
373	A new phase in ferroelectric oxides: The phase of charge transfer vibronic excitons. *Europhysics Letters*, **2001**, 56, 702-708	1.6	40
372	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
371	Adsorption of single Ag and Cu atoms on regular and defective MgO(0 0 1) substrates: an ab initio study. *Vacuum*, **2004**, 74, 235-240	3.7	39
370	Ab initio calculations of atomic an electronic structure of LaMnO and SrMnO. *Solid State Ionics*, **2004**, 173, 107-111	3.3	39
369	Ab Initio Study of BiFeO3: Thermodynamic Stability Conditions. *Journal of Physical Chemistry Letters* , **2015**, 6, 2847-51	6.4	38
368	Semi-empirical simulations of the electron centers in MgO crystal. *Computational Materials Science*, **1996**, 5, 298-306	3.2	37
367	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
366	Dynamics of F-center annihilation in thermochemically reduced MgO single crystals. *Solid State Communications*, **2001**, 118, 163-167	1.6	35
365	The kinetics of defect aggregation and metal colloid formation in ionic solids under irradiation. *Radiation Effects and Defects in Solids*, **2001**, 155, 113-125	0.9	35

364	Kinetics of nanocavity formation based on F-center aggregation in thermochemically reduced MgO single crystals. *Physical Review B*, **2001**, 64,	3.3	35
363	Quantum chemical calculations of the electron center diffusion in MgO crystals. *Physica Status Solidi (B): Basic Research*, **1996**, 195, 61-66	1.3	35
362	Calculations of the atomic and electronic structure for SrTiO3 perovskite thin films. *Thin Solid Films*, **2001**, 400, 76-80	2.2	34
361	Theoretical analysis of the growth mode for thin metallic films on oxide substrates. *Physical Review Letters*, **2000**, 85, 4333-6	7.4	34
360	Kinetics of F center annealing and colloid formation in Al2O3. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 374, 107-110	1.2	33
359	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	3.2	33
358	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	33
357	Photoconversion of F+ centers in neutron-irradiated MgO. *Nuclear Instruments & Methods in Physics Research B*, **2000**, 166-167, 220-224	1.2	33
356	Theory of tunneling recombination of defects stimulated by their motion I. General formalism. *Physica Status Solidi (B): Basic Research*, **1982**, 114, 9-34	1.3	33
355	Surface Segregation Entropy of Protons and Oxygen Vacancies in BaZrO3. *Chemistry of Materials*, **2016**, 28, 1363-1368	9.6	32
354	Photoconversion and dynamic hole recycling process in anion vacancies in neutron-irradiated MgO crystals. *Physical Review B*, **1999**, 60, 3787-3791	3.3	32
353	Photoconversion of F-type centers in thermochemically reduced MgO single crystals. *Physical Review B*, **1999**, 59, 4786-4790	3.3	32
352	Charge distribution and optical properties of and F centres in crystals. *Journal of Physics Condensed Matter*, **1997**, 9, L315-L321	1.8	31
351	Thermodynamic stability and disordering in La Sr1−MnO3 solid solutions. *Solid State Ionics*, **2006**, 177, 217-222	3.3	31
350	Enhanced lithium storage and chemical diffusion in metal-LiF nanocomposites: Experimental and theoretical results. *Physical Review B*, **2007**, 76,	3.3	31
349	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
348	Quantum chemical modelling of electron polarons and excitons in ABO3perovskites. *Journal of Physics Condensed Matter*, **2000**, 12, L557-L562	1.8	31
347	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

346	Helium behavior in oxide nuclear fuels: First principles modeling. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3090-3094	1.2	29
345	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	3.1	29
344	Stabilization of primary mobile radiation defects in MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 374, 24-28	1.2	28
343	Theoretical modeling of the complexes of iron impurities and oxygen vacancies in SrTiO3. *Applied Physics Letters*, **2013**, 102, 112913	3.4	28
342	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	1.6	28
341	DFT study of a single F center in cubic SrTiO3 perovskite. *International Journal of Quantum Chemistry*, **2006**, 106, 2173-2183	2.1	28
340	Theory of tunneling recombination of defects stimulated by their motion II. Three recombination mechanisms. *Physica Status Solidi (B): Basic Research*, **1982**, 114, 287-318	1.3	28
339	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
338	Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes. *Journal of Materials Chemistry A*, **2018**, 6, 11929-11940	13	28
337	Comparative study of polar perovskite surfaces. *Surface Science*, **2004**, 566-568, 231-235	1.8	27
336	Ab initio calculations of the LaMnO3 surface properties. *Applied Surface Science*, **2004**, 238, 457-463	6.7	27
335	Modelling of defects and surfaces in perovskite ferroelectrics. *Physica Status Solidi (B): Basic Research*, **2003**, 236, 253-264	1.3	27
334	Comparative theoretical study of the Ag/MgO (100) and (110) interfaces. *Surface Science*, **1999**, 441, 373-383	1.8	27
333	The MgO(110) surface and CO adsorption thereon. I. Clean (110) surface. *Journal of Physics C: Solid State Physics*, **1987**, 20, 4983-4990		27
332	Some problems of recombination kinetics. I. *Chemical Physics*, **1983**, 76, 479-487	2.3	27
331	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
330	Atomistic simulation of the [001]surface structure in BaTiO3. *Thin Solid Films*, **1997**, 296, 76-78	2.2	26
329	Transient optical absorption in KNbO3 crystals irradiated with pulsed electron beam. *Solid State Communications*, **1997**, 104, 327-330	1.6	26

328	Ab initio Hartree-Fock calculations of LaMnO3 (110) surfaces. *Solid State Communications*, **2003**, 127, 367-371	1.6	26
327	DFT LCAO and plane wave calculations of SrZrO3. *Physica Status Solidi (B): Basic Research*, **2005**, 242, R11-R13	1.3	26
326	Theory of bound polarons in oxide compounds. *Physical Review B*, **2001**, 63,	3.3	26
325	Ab initio calculations of MgF2 (001) and (011) surface structure. *Physica B: Condensed Matter*, **2010**, 405, 2125-2127	2.8	25
324	Hartree - Fock simulation of the Ag/MgO interface structure. *Journal of Physics Condensed Matter*, **1996**, 8, 6577-6584	1.8	25
323	F center aggregation kinetics in low-energy electron irradiated LiF. *Solid State Communications*, **1998**, 108, 629-633	1.6	25
322	Quantum chemical modelling of perovskite solid solutions. *Journal of Physics Condensed Matter*, **2000**, 12, L431-L434	1.8	25
321	Quantum chemical simulations of hole self-trapping in semi-ionic crystals. *International Journal of Quantum Chemistry*, **1994**, 52, 1177-1198	2.1	25
320	Calculation of energies of radiative tunneling transitions between defects in alkali halides. *Solid State Communications*, **1982**, 42, 749-752	1.6	25
319	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
318	First-principles modelling of defects in advanced nuclear fuels. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2007**, 4, 1193-1196		24
317	Electronic and magnetic structure of La0.875Sr0.125MnO3 calculated by means of hybrid density-functional theory. *Physical Review B*, **2007**, 76,	3.3	24
316	Generalised Maxwell-Garnett equation: application to electrical and chemical transport. *Physical Chemistry Chemical Physics*, **2006**, 8, 1310-4	3.6	24
315	Some problems of recombination kinetics. II. *Chemical Physics*, **1983**, 81, 335-347	2.3	24
314	Anomalous Kinetics of Diffusion-Controlled Defect Annealing in Irradiated Ionic Solids. *Journal of Physical Chemistry A*, **2018**, 122, 28-32	2.8	23
313	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
312	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations. *Journal of Nuclear Materials*, **2009**, 393, 504-507	3.3	23
311	First principles modelling of oxygen impurities in UN nuclear fuels. *Journal of Nuclear Materials*, **2008**, 377, 492-495	3.3	23

310	Experimental and theoretical studies of polaron optical properties in KNbO3 perovskite. *Solid State Communications*, **2004**, 129, 691-696	1.6	23
309	Theoretical analysis of the kinetics of low-temperature defect recombination in alkali halide crystals. *Low Temperature Physics*, **2016**, 42, 588-593	0.7	22
308	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
307	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
306	DFT calculations of point defects on UN(001) surface. *Surface Science*, **2011**, 605, 396-400	1.8	22
305	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
304	Study of the electronic and atomic structure of thermally treated SrTiO3(110) surfaces. *Surface and Interface Analysis*, **2003**, 35, 998-1003	1.5	22
303	Modified Maxwell-Garnett equation for the effective transport coefficients in inhomogeneous media. *Journal of Physics A*, **1998**, 31, 7227-7234		22
302	Discrete-lattice theory for Frenkel-defect aggregation in irradiated ionic solids. *Physical Review B*, **1998**, 58, 8454-8463	3.3	22
301	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	22
300	Semiempirical Calculations of Defect Properties in LiF Crystal. *Physica Status Solidi (B): Basic Research*, **1981**, 108, 673-681	1.3	22
299	Analysis of self-trapped hole mobility in alkali halides and metal halides. *Solid State Ionics*, **2017**, 302, 3-6	3.3	21
298	The kinetics of CaF2 metallization induced by low-energy electron irradiation. *Nuclear Instruments & Methods in Physics Research B*, **1998**, 141, 79-84	1.2	21
297	First principles simulations of F centers in cubic SrTiO3. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2005**, 2, 153-158		21
296	Atomistic simulation of SrTiO3 and BaTiO3 (110) surface relaxations. *Thin Solid Films*, **2000**, 358, 1-5	2.2	21
295	Atomistic simulation of surface relaxation. *Journal of Physics Condensed Matter*, **1998**, 10, L347-L353	1.8	21
294	The semiempirical approach to electronic structure of ionic crystal surface. *Journal of Physics C: Solid State Physics*, **1982**, 15, 847-861		21
293	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	1.3	21

292	The theory of diffusion-limited recombination of donor–acceptor pairs. *Journal of Luminescence*, **1975**, 9, 502-513	3.8	21
291	First principles calculations of oxygen adsorption on the UN(001) surface. *Surface Science*, **2009**, 603, 50-53	1.8	20
290	Water interaction with perfect and fluorine-doped Co3O4 (100) surface. *Solid State Ionics*, **2015**, 277, 77-82	3.3	19
289	Ab initio simulations of silver film adhesion on α-Al2O3 (0 0 0 1) and MgO (1 0 0) surfaces. *Nuclear Instruments & Methods in Physics Research B*, **1998**, 141, 73-78	1.2	19
288	Semi-empirical defect calculations for the perovskite KNbO3. *Journal of Physics Condensed Matter*, **2000**, 12, 569-574	1.8	19
287	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		19
286	A novel model for F+to F photoconversion in corundum crystals. *Journal of Physics Condensed Matter*, **1994**, 6, L569-L573	1.8	19
285	The MgO(110) surface and CO adsorption thereon. II. CO adsorption. *Journal of Physics C: Solid State Physics*, **1987**, 20, 4991-4997		19
284	Generalised theory of diffusion-controlled defect annealing. *Journal of Physics C: Solid State Physics*, **1980**, 13, L499-L502		19
283	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		19
282	Extraction Pyrolytic Method for TiO2 Polymorphs Production. *Crystals*, **2021**, 11, 431	2.3	19
281	Thermodynamic stability of non-stoichiometric SrFeO: a hybrid DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 3918-3931	3.6	18
280	First-principles comparative study of perfect and defective CsPbX (X = Br, I) crystals. *Physical Chemistry Chemical Physics*, **2020**, 22, 3914-3920	3.6	18
279	Ab initio simulation of yttrium oxide nanocluster formation on fcc Fe lattice. *Journal of Nuclear Materials*, **2010**, 406, 345-350	3.3	18
278	Luminescence properties of KNbO3 crystals. *Journal of Luminescence*, **1997**, 72-74, 672-674	3.8	18
277	Metal film growth on regular and defective MgO(0 0 1) surface: A comparative ab initio simulation and thermodynamic study. *Surface Science*, **2006**, 600, L99-L104	1.8	18
276	Semi-empirical calculations of the Nb-ion positions in doped crystals. *Journal of Physics Condensed Matter*, **1998**, 10, 6271-6276	1.8	18
275	Correlated annealing of radiation defects in alkali halide crystals. *Journal of Physics Condensed Matter*, **1992**, 4, 5901-5910	1.8	18

274	Kinetics of Defect Accumulation and Recombination: II. Diffusion-Controlled Defect Annihilation. *Physica Status Solidi (B): Basic Research*, **1981**, 108, 37-44	1.3	18
273	First-principles calculations of iodine-related point defects in CsPbI. *Physical Chemistry Chemical Physics*, **2019**, 21, 7841-7846	3.6	17
272	Adhesion trends and growth mode of ultra-thin copper films on MgO. *Journal of Physics Condensed Matter*, **2004**, 16, 4881-4896	1.8	17
271	Quantum chemical modelling of electron polarons and □green□luminescence in PbTiO3perovskite crystals. *Journal of Physics Condensed Matter*, **2002**, 14, L647-L653	1.8	17
270	Modelling of silver adhesion on MgO(100) surface with defects. *Journal of Physics Condensed Matter*, **2000**, 12, 55-66	1.8	17
269	A Contradiction between Pulsed and Steady-State Studies in the Recombination Kinetics of Close Frenkel Defects in KBr and KCl Crystals. *Journal of the Physical Society of Japan*, **1994**, 63, 2602-2611	1.5	17
268	Quantum-chemical calculations of electronic and hole centres and surface of NaCl crystals (I). *Physica Status Solidi (B): Basic Research*, **1979**, 96, 91-99	1.3	17
267	Thermodynamic stability of stoichiometric LaFeO and BiFeO: a hybrid DFT study. *Physical Chemistry Chemical Physics*, **2017**, 19, 3738-3755	3.6	16
266	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. *Journal of Nuclear Materials*, **2013**, 435, 102-106	3.3	16
265	A comparative analysis of electron spectroscopy and first-principles studies on Cu(Pd) adsorption on MgO. *Surface Science*, **2006**, 600, 3815-3820	1.8	16
264	Atomistic simulations of the LaMnO3(110) polar surface. *Physical Chemistry Chemical Physics*, **2003**, 5, 4180	3.6	16
263	Hartree□Fock study of adhesion and charge redistribution on the Ag/MgO(0 0 1) interface. *Surface Science*, **2001**, 482-485, 66-72	1.8	16
262	Ab initio and semiempirical calculations of H□centers in MgO crystals. *Physical Review B*, **1999**, 59, 1885-1890	3.3	16
261	Many-particle effects in accumulation kinetics of Frenkel defects in crystals. *Journal of Physics C: Solid State Physics*, **1984**, 17, 2283-2292		16
260	Kinetics of Defect Accumulation and Recombination. I. General Formalism. *Physica Status Solidi (B): Basic Research*, **1981**, 105, 789-801	1.3	16
259	Kinetics of the electronic center annealing in Al2O3 crystals. *Journal of Nuclear Materials*, **2018**, 502, 295-300	3.3	15
258	The electronic and atomic structure of SrTiO3, BaTiO3, and PbTiO3(001) surfaces: Ab initio DFT/HF hybrid calculations. *Microelectronic Engineering*, **2005**, 81, 472-477	2.5	15
257	Dynamic particle aggregation in the bimolecular A+B->0 reaction. *Journal of Chemical Physics*, **1993**, 98, 9107-9114	3.9	15

256	Modeling of Point Defects in Corundum Crystals. *Journal of the American Ceramic Society*, **1994**, 77, 2505-2508	3.6	15
255	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
254	Use of site symmetry in supercell models of defective crystals: polarons in CeO. *Physical Chemistry Chemical Physics*, **2017**, 19, 8340-8348	3.6	14
253	Ab initio modeling of radiation damage in MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2014**, 326, 314-317	1.2	14
252	Ab initio study of phase competition in (La1 □,Src)CoO3 solid solutions. *Solid State Ionics*, **2013**, 230, 32-36	3.3	14
251	First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 25245-25251	3.6	14
250	First principles calculations of (Ba,Sr)(Co,Fe)O3□ structural stability. *Solid State Ionics*, **2013**, 230, 21-26	3.3	14
249	Calculations of Diffusion Energies for Defects in MgO Crystals. *Defect and Diffusion Forum*, **1997**, 143-147, 1231-1236	0.7	14
248	Semi-Empirical Calculations of Hole Polarons in MgO and KNbO3 Crystals. *Physica Status Solidi (B): Basic Research*, **1998**, 208, 15-20	1.3	14
247	Modeling of primary defect aggregation in tracks of swift heavy ions in LiF. *Physical Review B*, **2001**, 64,	3.3	14
246	Quantum chemical modelling of point defects in KNbO3 perovskite crystals. *Computational Materials Science*, **2000**, 17, 290-298	3.2	14
245	The kinetics of defect accumulation under irradiation: many-particle effects. *Physica Scripta*, **1993**, 47, 585-595	2.6	14
244	Semiempirical Calculations of the Impurity Level Positions with Respect to the Perfect Crystal Bands. *Physica Status Solidi (B): Basic Research*, **1981**, 103, 581-587	1.3	14
243	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
242	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
241	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
240	Hydrogen induced metallization of ZnO (11 00) surface: Ab initio study. *Thin Solid Films*, **2014**, 553, 38-42	2.2	13
239	Ab Initio Thermodynamics of Oxygen Vacancies and Zinc Interstitials in ZnO. *Journal of Physical Chemistry Letters*, **2014**, 5, 4238-42	6.4	13

238	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
237	First-principles modelling of radiation defects in advanced nuclear fuels. *Nuclear Instruments & Methods in Physics Research B*, **2008**, 266, 2671-2675	1.2	13
236	Characterization of the Metal□Ceramic Bonding in the Ag/MgO(001) Interface from ab Initio Calculations. *Journal of Physical Chemistry B*, **2003**, 107, 11893-11899	3.4	13
235	Theoretical and experimental study of primary radiation defects in KNbO3 perovskite crystals. *Nuclear Instruments & Methods in Physics Research B*, **2000**, 166-167, 299-304	1.2	13
234	Mechanism of self-trapped hole motion in corundum crystals. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1993**, 67, 557-567		13
233	A theoretical study of H-centre migration in alkali halide crystals KCl and NaCl. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1993**, 68, 1359-1367		13
232	Effect of nonequilibrium charge screening in A + B -> 0 bimolecular reactions in condensed matter. *Journal of Statistical Physics*, **1993**, 72, 127-144	1.5	13
231	Radiation-stimulated aggregation of Frenkel defects in solids. *Uspekhi Fizicheskikh Nauk*, **1990**, 33, 793-811		13
230	The adsorption of SiO molecules on MgO Surfaces as a model for the silicon lever atomic force microscope (AFM). *Surface Science*, **1990**, 232, 399-406	1.8	13
229	Some problems of recombination kinetics. III. *Chemical Physics*, **1985**, 98, 351-360	2.3	13
228	Effect of reagent density fluctuations on bimolecular reaction kinetics. *Chemical Physics Letters*, **1982**, 87, 575-578	2.5	13
227	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
226	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
225	Ab initio calculations of Nb doped SrTiO3. *Physica B: Condensed Matter*, **2010**, 405, 3164-3166	2.8	12
224	Computer Modelling of Radiation Damage in Cation Sublattice of Corundum. *Physica Status Solidi (B): Basic Research*, **1998**, 207, 69-73	1.3	12
223	A comparative study of Ag and Cu adhesion on an MgO(001) surface. *Superlattices and Microstructures*, **2004**, 36, 63-72	2.8	12
222	Theory of Point Defects and Vacancy Motion in Corundum Crystals. *Journal of Solid State Chemistry*, **1993**, 106, 27-34	3.3	12
221	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

220	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
219	Kinetics of dimer F2 type center annealing in MgF2 crystals. *Nuclear Instruments & Methods in Physics Research B*, **2018**, 435, 79-82	1.2	12
218	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
217	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
216	Comparative study of [001] surface relaxations of perovskite titanates. *Thin Solid Films*, **1998**, 318, 65-68	2.2	11
215	Quantum chemical calculations of KTN solid solutions. *Solid State Communications*, **1998**, 108, 333-336	1.6	11
214	A comparative study of the atomic and electronic structure of F centers in ferroelectric KNbO3: Ab initio and semi-empirical calculations. *Computational Materials Science*, **1998**, 10, 339-345	3.2	11
213	Size and shape of three-dimensional Cu clusters on a MgO(001) substrate: Combined ab initio and thermodynamic approach. *Physical Review B*, **2006**, 74,	3.3	11
212	First principles slab calculations of the regular Cu/MgO(001) interface. *Surface Science*, **2004**, 566-568, 122-129	1.8	11
211	Ab initio modelling of silver adhesion on the corundum (0001) surface. *Materials Science and Engineering C*, **2003**, 23, 247-252	8.3	11
210	Reaction kinetics beyond rate equations: a correlation-function study of the effects of space dimension and reactant mobilities on the bimolecular annihilation reaction. *Journal of Physics A*, **1994**, 27, 1453-1462		11
209	Quantum-Chemical Calculations of Electronic and Hole Centres and Surface of NaCl Crystals (II). *Physica Status Solidi (B): Basic Research*, **1980**, 98, 427-433	1.3	11
208	Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies. *Journal of Materials Chemistry C*, **2021**, 9, 1693-1700	7.1	11
207	On the Way to Optoionics. *Helvetica Chimica Acta*, **2020**, 103, e2000073	2	11
206	Ab initio simulations on charged interstitial oxygen migration in corundum. *Nuclear Instruments & Methods in Physics Research B*, **2018**, 435, 74-78	1.2	10
205	Static and dynamic screening effects in the electrostatic self-assembly of nano-particles. *Physical Chemistry Chemical Physics*, **2014**, 16, 25449-60	3.6	10
204	Theoretical modeling of antiferrodistortive phase transition for SrTiO3 ultrathin films. *Physical Review B*, **2013**, 88,	3.3	10
203	Electromechanical Properties of BaSrTiO Perovskite Solid Solutions from First-Principles Calculations. *Journal of Physical Chemistry A*, **2017**, 121, 9409-9414	2.8	10

202	Phase competition in (La1 □,Src)CoO3 solid solutions: ab initio thermodynamic study. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 864-869	1.3	10
201	The non-equilibrium charge screening effects in diffusion-driven systems with pattern formation. *Journal of Chemical Physics*, **2011**, 135, 034702	3.9	10
200	First Principles Modeling of Oxygen Mobility in Perovskite SOFC Cathode and Oxygen Permeation Membrane Materials. *ECS Transactions*, **2011**, 35, 823-830	1	10
199	Quantum-chemical simulations of free and bound hole polarons in corundum crystal. *Computational Materials Science*, **1997**, 7, 285-294	3.2	10
198	First-principles calculations of the vibrational properties of H centers in KCl crystals. *Physical Review B*, **1996**, 53, 24-27	3.3	10
197	The kinetics of F-center aggregation under irradiation: many-particle effects in ionic solids. *Physica Scripta*, **1994**, 50, 720-725	2.6	10
196	Molecular cluster approach to magnesium and calcium oxide crystals. I. Perfect crystals. *Physica Status Solidi (B): Basic Research*, **1975**, 72, 787-794	1.3	10
195	Ab initio simulation of (Ba,Sr)TiO3 and (Ba,Ca)TiO3 perovskite solid solutions. *Solid State Ionics*, **2019**, 337, 76-81	3.3	9
194	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
193	First principles simulations of 2D Cu superlattices on the MgO(0 0 1) surface. *Applied Surface Science*, **2004**, 226, 298-305	6.7	9
192	Some nonlinear properties of ferroelectric smart materials. *Physica B: Condensed Matter*, **2001**, 304, 339-347	2.8	9
191	Quantum chemical modelling of polarons and perovskite solid solutions. *Computational Materials Science*, **2001**, 21, 530-534	3.2	9
190	Short-lived luminescence of mixed silver halides. *Journal of Luminescence*, **1993**, 55, 243-252	3.8	9
189	Many-particle effects in kinetics of bimolecular diffusion-controlled reactions. *Chemical Physics Letters*, **1985**, 117, 266-270	2.5	9
188	Influence of defect interaction upon their recombination in ionic crystals. I. *Radiation Effects*, **1980**, 46, 85-90		9
187	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
186	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
185	Microscopic approach to the kinetics of pattern formation of charged molecules on surfaces. *Physical Review E*, **2010**, 82, 021602	2.4	8

184	The Structural Disorder and Lattice Stability of (Ba,Sr)(Co,Fe)O3 Complex Perovskites. *ECS Transactions*, **2011**, 35, 2077-2084	1	8
183	Ab initiocalculations of theFcenters in MgF2bulk and on the (001) surface. *Physica Scripta*, **2012**, 86, 035304	2.8	8
182	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
181	Ab initio simulations on AgCl(111) surface and AgCl(111)/□Al2O3(0001) interface. *Computational Materials Science*, **2005**, 33, 276-281	3.2	8
180	Atomistic modeling of polar LaMnO3 surfaces. *Sensors and Actuators B: Chemical*, **2004**, 100, 81-87	8.5	8
179	Calculations of radiation-induced point defects, polarons and excitons in ferroelectric perovskites. *Nuclear Instruments & Methods in Physics Research B*, **2002**, 191, 22-26	1.2	8
178	Large-scale ab initio modelling of defects in perovskites: Fe impurity in SrTiO3. *Computational Materials Science*, **2002**, 24, 14-20	3.2	8
177	The Dynamics of the Hydride Ion in MgO Single Crystals. *Defect and Diffusion Forum*, **1999**, 169-170, 1-0	0.7	8
176	The kinetics of the bimolecular A+B->0 reaction in condensed matter: Effects of non-equilibrium charge screening. *Journal of Chemical Physics*, **1996**, 105, 9486-9492	3.9	8
175	Kinetics of diffusion-controlled defect accumulation restricted by their recombination. *Solid State Communications*, **1981**, 40, 173-176	1.6	8
174	Radiation-stimulated aggregation of Frenkel defects in solids. *Uspekhi Fizicheskikh Nauk*, **1990**, 160, 1	0.5	8
173	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
172	First principles calculations of oxygen reduction reaction at fuel cell cathodes. *Current Opinion in Electrochemistry*, **2020**, 19, 122-128	7.2	8
171	Manifestation of dipole-induced disorder in self-assembly of ferroelectric and ferromagnetic nanocubes. *Nanoscale*, **2019**, 11, 7293-7303	7.7	7
170	First-principles Study of Perovskite Ultrathin Films: Stability and Confinement Effects. *Israel Journal of Chemistry*, **2017**, 57, 509-521	3.4	7
169	Note: Effective diffusion coefficient in heterogeneous media. *Journal of Chemical Physics*, **2012**, 137, 166101	3.9	7
168	Modeling of yttrium, oxygen atoms and vacancies in □ron lattice. *Journal of Nuclear Materials*, **2011**, 416, 40-44	3.3	7
167	Semi-empirical simulations of F-center diffusion in KCl crystals. *Journal of Physics and Chemistry of Solids*, **1997**, 58, 103-106	3.9	7

166	Structural Phase Transition and Photo-Charge Carrier Transport in SrTiO3. *Ferroelectrics*, **2006**, 337, 179-188	0.8	7
165	Large-scale modelling of the phase transitions in KTa1−xNbxO3 perovskite solid solutions. *Materials Science in Semiconductor Processing*, **2002**, 5, 153-157	4.3	7
164	Modeling of defects and surfaces in perovskite ferroelectrics. *Journal of Crystal Growth*, **2002**, 237-239, 687-693	1.6	7
163	Ab initio modeling of copper adhesion on regular BaTiO3(001) surfaces. *Microelectronic Engineering* , **2005**, 81, 467-471	2.5	7
162	Ab initio calculations of the atomic and electronic structure of layered Ba0.5Sr0.5TiO3 structures. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2005**, 118, 15-18	3.1	7
161	Short-pulse excitation and spectroscopy of KNbO3, LiNbO3 and KTiOPO4. *Radiation Effects and Defects in Solids*, **1999**, 150, 271-276	0.9	7
160	Computer Simulations of I-Center Annealing in KCl and KBr Crystals. Theoretical Interpretation of Thermostimulated Experiments. *Physica Status Solidi (B): Basic Research*, **1995**, 190, 353-362	1.3	7
159	Modelling of point defects in αAL2O3. *Radiation Effects and Defects in Solids*, **1995**, 134, 87-90	0.9	7
158	The decay kinetics of excitonic luminescence in AgCl crystals. *Journal of Physics Condensed Matter*, **1995**, 7, 1483-1491	1.8	7
157	The Kinetics of Correlated Annealing of F, I Centres in KBr Crystals. *Physica Status Solidi (B): Basic Research*, **1993**, 175, K39-K42	1.3	7
156	Temperature and impurity concentration dependences of the efficiency of Frenkel defect accumulation in alkali halide crystals. *Solid State Communications*, **1984**, 51, 225-229	1.6	7
155	Molecular Cluster Approach to Magnesium and Calcium Oxide Crystals. II. F+ and F Centres. *Physica Status Solidi (B): Basic Research*, **1976**, 73, 81-86	1.3	7
154	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
153	Atomic, electronic and magnetic structure of an oxygen interstitial in neutron-irradiated AlO single crystals. *Scientific Reports*, **2020**, 10, 15852	4.9	7
152	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
151	Hybrid DFT calculations of theFcenters in cubic ABO3perovskites. *Journal of Physics: Conference Series*, **2008**, 117, 012019	0.3	6
150	Calculations of the atomic structure of the KNbO3 (110) surface. *Thin Solid Films*, **2000**, 374, 64-69	2.2	6
149	Computer simulations of defects in perovskite KNbO3 crystals. *Ferroelectrics*, **1999**, 229, 69-75	0.6	6

148	Pair and triple correlations in the A+B-->B diffusion-controlled reaction. *Physical Review Letters*, **1994**, 72, 2105-2108	7.4	6
147	Electronic structure of thallous centres and Tl+ - Vk recombination in KCl crystal. *Solid State Communications*, **1983**, 46, 625-629	1.6	6
146	Quantum-chemical simulation of Frenkel pairs separation in a LiF crystal. *Solid State Communications*, **1981**, 40, 669-672	1.6	6
145	Low temperature structural transformations on the (001) surface of SrTiO3 single crystals. *Low Temperature Physics*, **2020**, 46, 740-750	0.7	6
144	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
143	First Principles Simulations on Migration Paths of Oxygen Interstitials in MgAl2O4. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800282	1.3	6
142	Hybrid density functional theoretical study of NASICON-type NaTi(PO) (x = 1-4). *Physical Chemistry Chemical Physics*, **2020**, 22, 11861-11870	3.6	5
141	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
140	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
139	Pattern formation kinetics for charged molecules on surfaces: microscopic correlation function analysis. *Journal of Physical Chemistry B*, **2011**, 115, 14626-33	3.4	5
138	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
137	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
136	Diffusion-controlled annihilation and aggregation of F-centers in thermochemically reduced MgO crystals. *Nuclear Instruments & Methods in Physics Research B*, **2002**, 191, 208-211	1.2	5
135	First-principles calculations of perovskite thin films. *Materials Science in Semiconductor Processing*, **2002**, 5, 129-134	4.3	5
134	Computer modelling of point defects in ABO3 perovskites and MgO. *Computational Materials Science*, **2004**, 30, 376-382	3.2	5
133	Coin metal adsorption on defective MgO(001) surface: ab initio study. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2005**, 2, 347-350		5
132	Effect of electron correlation corrections on phase competition in Ag film on MgO substrate. *Computational Materials Science*, **2002**, 24, 66-71	3.2	5
131	A First-Principles Study of the Ag/a-Al2O3(0001) Interface. *International Journal of Molecular Sciences*, **2001**, 2, 271-280	6.3	5

130	ATOMISTIC CALCULATIONS OF (110) SURFACE RELAXATION FOR PEROVSKITE TITANATES. *Surface Review and Letters*, **1999**, 06, 1215-1219	1.1	5
129	Effect of reactant spatial distribution in the A+B-->0 reaction kinetics in one dimension with Coulomb interaction. *Physical Review E*, **1996**, 54, 6128-6138	2.4	5
128	Optical properties of silver halide fibres: ageing effects. *Journal Physics D: Applied Physics*, **1996**, 29, 578-583	3	5
127	Theoretical simulations of hole centres in corundum crystals. *Modelling and Simulation in Materials Science and Engineering*, **1994**, 2, 109-117	2	5
126	Radiation-induced aggregatization of immobile defects. *Solid State Communications*, **1981**, 39, 351-354	1.6	5
125	First Principles Modeling of Pd-doped (La,Sr)(Co,Fe)O3 Complex Perovskites. *Fuel Cells*, **2016**, 16, 267-271	1.9	5
124	The first principles calculations of CO2 adsorption on (101□0) ZnO surface **2019**,		5
123	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
122	Ab initio modelling of Y□O cluster formation in □Fe lattice. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 2136-2143	1.3	4
121	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
120	Ab initio simulations on Frenkel pairs of radiation defects in corundum. *IOP Conference Series: Materials Science and Engineering*, **2015**, 77, 012001	0.4	4
119	Ab initio calculations of the atomic and electronic structure of MgF2 (011) and (111) surfaces. *Open Physics*, **2011**, 9,	1.3	4
118	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
117	Void superlattice formation in electron irradiated CaF2: Theoretical analysis. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3055-3058	1.2	4
116	Theory of Diffusion and Aggregation of Radiation-Induced Defects in MgO and □Al2O3 Crystals. *Materials Science Forum*, **1997**, 239-241, 391-394	0.4	4
115	Semi-empirical supercell calculations for free- and bound-hole polarons in crystal. *Journal of Physics Condensed Matter*, **1997**, 9, 3559-3573	1.8	4
114	Calculations of F centers in KNbO 3 ferroelectric crystals **1997**, 2967, 150		4
113	A simple analysis of the HA centre destruction temperatures for doped alkali halides. *Solid State Communications*, **1998**, 106, 289-291	1.6	4

112	First-Principles Modeling of LaMnO3 SOFC Cathode Material. *ECS Transactions*, **2008**, 13, 301-306	1	4
111	Large scale computer modelling of point defects in ABO3 perovskites. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2005**, 2, 113-119		4
110	New Polaronic-Type Excitons in Ferroelectric Oxides: INDO-Calculations and Experimental Manifestation. *Materials Research Society Symposia Proceedings*, **2001**, 677, 4151		4
109	The kinetics of colloid formation in solids under irradiation. *Journal of Physics Condensed Matter*, **1995**, 7, L481-L486	1.8	4
108	Self-organization in the A + B -> 0 reaction of charged particles. *Physica A: Statistical Mechanics and Its Applications*, **1992**, 191, 172-176	3.3	4
107	A mesoscopic approach to point-defect clustering in solids during irradiation. *Applied Physics A: Solids and Surfaces*, **1993**, 57, 117-121		4
106	The electronic properties of SrTiO with oxygen vacancies or substitutions. *Scientific Reports*, **2021**, 11, 23341	4.9	4
105	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
104	Statistical characterization of self-assembled charged nanoparticle structures. *Physica Status Solidi (A) Applications and Materials Science*, **2014**, 211, 288-293	1.6	3
103	First-principles phonon calculations of Fe impurity in SrTiO *Journal of Physics Condensed Matter*, **2012**, 24, 104024	1.8	3
102	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
101	A Comparative Hybrid DFT Study of Phonons in Several SrTiO3 Phases. *Integrated Ferroelectrics*, **2011**, 123, 18-25	0.8	3
100	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
99	BacSr1 TiO3 perovskite solid solutions: Thermodynamics from ab initio electronic structure calculations. *Microelectronic Engineering*, **2005**, 81, 478-484	2.5	3
98	Adsorption of atomic and molecular oxygen on the SrTiO3(001) surfaces: Predictions by means of hybrid density functional calculations. *Materials Research Society Symposia Proceedings*, **2005**, 894, 1		3
97	[001] Surface Structure in SrTiO3 Atomistic Study. *Surface Review and Letters*, **1998**, 05, 341-345	1.1	3
96	Semi-empirical indo and shell-model calculations for perovskites. *Radiation Effects and Defects in Solids*, **1999**, 151, 243-247	0.9	3
95	Theory of diffusion-controlled defect aggregation under irradiation: A comparative study of three basic approaches. *Radiation Effects and Defects in Solids*, **1995**, 136, 209-215	0.9	3

94	Theoretical simulation of VK-centre migration in KCl. II. Phenomenological theory. *Journal of Physics Condensed Matter*, **1992**, 4, 7429-7440	1.8	3
93	Temperature dependence of F-centre accumulation efficiency in doped alkali halides. *Journal of Physics C: Solid State Physics*, **1977**, 10, 2903-2915		3
92	Theory of diffusion-controlled tunnelling recombination incorporating Coulomb interaction and annihilation. *Journal of Physics C: Solid State Physics*, **1977**, 10, 4931-4937		3
91	Theoretical and Experimental Studies of Charge Ordering in CaFeO3 and SrFeO3 Crystals. *Physica Status Solidi (B): Basic Research*,2100238	1.3	3
90	Photo de-mixing in mixed halide perovskites: the roles of ions and electrons. *JPhys Energy*,	4.9	3
89	Small radius electron and hole polarons in PbX2 (X = F, Cl, Br) crystals: a computational study. *Journal of Materials Chemistry C*,	7.1	3
88	Evidence for the formation of two types of oxygen interstitials in neutron-irradiated □AlO single crystals. *Scientific Reports*, **2021**, 11, 20909	4.9	3
87	Water Splitting on Multifaceted SrTiO3 Nanocrystals: Computational Study. *Catalysts*, **2021**, 11, 1326	4	3
86	First-Principles Modeling of Oxygen Adsorption on Ag-Doped LaMnO3 (001) Surface. *Journal of Electronic Materials*, **2020**, 49, 1421-1434	1.9	3
85	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
84	BaCoO monoclinic structure and chemical bonding analysis: hybrid DFT calculations. *Physical Chemistry Chemical Physics*, **2021**, 23, 17493-17501	3.6	3
83	(Invited) The Effect of (La,Sr)MnO 3 Cathode Surface Termination on Its Electronic Structure. *ECS Transactions*, **2017**, 77, 67-73	1	2
82	First principles calculations on CeO2 doped with Tb3+ ions. *Optical Materials*, **2019**, 90, 76-83	3.3	2
81	Charged oxygen interstitials in corundum: first principles simulations. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2016**, 13, 932-936		2
80	Quantum chemical simulations of bound hold polarons (V Mg centers) in corundum crystals **1997**,		2
79	Domain wall splitting and creation of the fine domain structure. *Thin Solid Films*, **1998**, 336, 149-152	2.2	2
78	Ab initiostudy of bulk and surface iron defects in SrTiO3. *Journal of Physics: Conference Series*, **2008**, 117, 012001	0.3	2
77	Large-Scale Computer Modelling of Point Defects, Polarons and Perovskite Solid Solutions. *Defect and Diffusion Forum*, **2004**, 226-228, 169-180	0.7	2

76	The kinetic MC modelling of reversible pattern formation in initial stages of thin metallic film growth on crystalline substrates. *Solid State Communications*, **2003**, 125, 463-467	1.6	2
75	Computer modeling of metal colloid formation in tracks of swift heavy ions in ionic solids. *Radiation Effects and Defects in Solids*, **2001**, 155, 145-151	0.9	2
74	Theoretical simulations of I-center annealing in KCl crystals. *Radiation Effects and Defects in Solids*, **1995**, 134, 83-86	0.9	2
73	Atomic and Electronic Structure of the Corundum (0001) Surface. *Materials Research Society Symposia Proceedings*, **1996**, 453, 721		2
72	Aggregation of Frenkel defects under irradiation: a mesoscopic approach. *Nuclear Instruments & Methods in Physics Research B*, **1994**, 91, 87-91	1.2	2
71	Non-steady-state tunnelling recombination in insulating solids, controlled by defect diffusion and rotation. *Radiation Effects and Defects in Solids*, **1989**, 111-112, 191-205	0.9	2
70	Molecular Cluster Approach to Magnesium and Calcium Oxide Crystals III. Charge Distribution Analysis of Some Hole Centres. *Physica Status Solidi (B): Basic Research*, **1976**, 73, 483-486	1.3	2
69	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
68	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
67	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
66	First principles modeling of Ag adsorption on the LaMnO3 (001) surfaces. *Solid State Ionics*, **2015**, 273, 46-50	3.3	1
65	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
64	Radiation defects in complex perovskite solid solutions. *Nuclear Instruments & Methods in Physics Research B*, **2014**, 326, 243-246	1.2	1
63	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
62	Many-particle peculiarities in the bimolecular reaction kinetics. The effect of sink spatial distribution. *Journal of Physics Condensed Matter*, **1996**, 8, 6729-6735	1.8	1
61	Computer modeling of point defects, polarons, excitons, and surfaces in perovskite ferroelectrics **2003**, 5122, 253		1
60	Ab initio thermodynamics for the growth of ultra-thin Cu film on a perfect MgO(001) surface. *Materials Science and Engineering C*, **2005**, 25, 713-717	8.3	1
59	Computer Modeling of Point Defects in Perovskite Crystals. *Ferroelectrics*, **2002**, 268, 59-64	0.6	1

58	Quantum Mechanical Modelling of Pure and Defective KNbO3 Perovskites **2000**, 3-16		1
57	Computer Modeling of Luminescence in ABO3 Perovskites. *Materials Research Society Symposia Proceedings*, **2001**, 667, 1		1
56	Calculations of Surface Structure for SrTiO3 Perovskite. *Materials Research Society Symposia Proceedings*, **2001**, 672, 1		1
55	Kuzovkov and Kotomin reply. *Physical Review Letters*, **1995**, 75, 587	7.4	1
54	A comparison of the effective medium and modified Smoluchowski equations for the reaction rate of the diffusion-controlled reactions. *Journal of Nuclear Materials*, **1996**, 232, 253-255	3.3	1
53	Surface Relaxation in Ferroelectric Perovskites: An Atomistic Study. *Materials Research Society Symposia Proceedings*, **1996**, 459, 219		1
52	Theoretical simulations of the radiation-induced defect processes in insulating materials. *Nuclear Instruments & Methods in Physics Research B*, **1994**, 91, 52-59	1.2	1
51	First-Principles Simulations of Interstitial Atoms in Ionic Solids. *Materials Research Society Symposia Proceedings*, **1995**, 408, 509		1
50	Kinetics of correlated annealing of radiation defects in alkali halide crystals. *Nuclear Instruments & Methods in Physics Research B*, **1992**, 65, 512-515	1.2	1
49	Quantum-chemical approach to defect formation processes in non-metallic crystals. *Radiation Effects and Defects in Solids*, **1989**, 111-112, 177-190	0.9	1
48	Peculiarities of diffusion-controlled recombination kinetics at long time and/or for great initial reagent concentrations. *European Physical Journal D*, **1985**, 35, 541-548		1
47	Influence of defect interaction upon their recombination in ionic crystals. II. *Radiation Effects*, **1980**, 46, 91-96		1
46	Computer Modeling of Point Defects, Impurity Self-Ordering Effects and Surfaces in Advanced Perovskite Ferroelectrics. *Acta Physica Polonica A*, **2000**, 98, 469-481	0.6	1
45	First-Principles Modelling of N-Doped Co3O4. *Latvian Journal of Physics and Technical Sciences*, **2018**, 55, 36-42	0.5	1
44	Semi-Empirical Simulation of Radiation Defects in Oxide Materials **1997**, 51-59		1
43	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
42	Theoretical investigations of nitrogen doping on Co3O4 for water dissociation catalytically activity. *Journal of Physics: Conference Series*, **2018**, 1115, 032032	0.3	1
41	Dopant solubility in ceria: alloy thermodynamics combined with the DFT+U calculations. *Solid State Ionics*, **2018**, 325, 258-264	3.3	1

40	The Two Types of Oxygen Interstitials in Neutron-Irradiated Corundum Single Crystals: Joint Experimental and Theoretical Study. *Physica Status Solidi (B): Basic Research*,2100317	1.3	1
39	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
38	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
37	Formation and interaction of defects in silver halide crystals **1990**, 1228, 140		0
36	Transition levels of acceptor impurities in ZnO crystals by DFT-LCAO calculations. *Journal of Physics: Conference Series*, **2018**, 1115, 042064	0.3	0
35	Defect-Induced Effects in Nanomaterials. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1900181	1.3	
34	Large-Scale Modeling of Defects in Advanced Oxides: Oxygen Vacancies in BaZrO3 Crystals **2016**, 187-198		
33	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	
32	Ab initiomodelling of UN grain boundary interfaces. *IOP Conference Series: Materials Science and Engineering*, **2012**, 38, 012058	0.4	
31	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	
30	Ab initiocalculations of theHcenters in MgF2crystals. *IOP Conference Series: Materials Science and Engineering*, **2012**, 38, 012041	0.4	
29	Atomic Structure of the (0001) Corundum Surface. *Materials Science Forum*, **1997**, 239-241, 633-636	0.4	
28	The Kinetics of Radiation-Induced Defect Accumulation in Ionic Solids. *Materials Science Forum*, **1997**, 239-241, 387-390	0.4	
27	The Diffusion-Controlled Energy Transfer Rate for a Paired Sink Distribution and Donor-Acceptor Interaction. *Physica Status Solidi (B): Basic Research*, **1997**, 201, 339-342	1.3	
26	The effect of the particle generation function on the rate of the diffusion-controlled A + B -> B reaction with a permanent particle source. *Chemical Physics Letters*, **1997**, 270, 229-233	2.5	
25	The microscopic theory of diffusion-controlled defect aggregation. *Computational Materials Science* , **1998**, 10, 22-27	3.2	
24	Atomistic Modeling of a New Storage. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2008**, 634, 2055-2055	1.3	
23	Ab initio Calculations of Copper Nanostructures of MgO Substrate. *Solid State Phenomena*, **2004**, 99-100, 219-222	0.4	

22	Calculations of Atomic and Electronic Structure for (100) Surfaces of SrTiO3 Perovskite. *Materials Research Society Symposia Proceedings*, **2002**, 718, 1	
21	Modeling of primary defect aggregation in tracks of swift heavy ions in alkali halides. *Surface and Coatings Technology*, **2002**, 158-159, 269-272	4.4
20	Calculation of the Effective Diffusion Coefficient in Inhomogeneous Solids. *Defect and Diffusion Forum*, **2001**, 194-199, 163-170	0.7
19	Large- Scale ab initio Simulations of Fe-doped SrTiO3perovskites. *Materials Research Society Symposia Proceedings*, **2002**, 731, 3121	
18	Theoretical Prediction and Experimental Confirmation of Charge Transfer Vibronic Excitons and Their Phase in ABO3 Perovskite Crystals. *Materials Research Society Symposia Proceedings*, **2002**, 718, 1	
17	Primary radiation defect creation and separation in AgBr. *Radiation Effects and Defects in Solids*, **1999**, 150, 185-191	0.9
16	Atomistic Study of Surface Polarization in Superconducting Perovskites. *Materials Research Society Symposia Proceedings*, **1996**, 440, 305	
15	Pattern Formation and Unusual A + B -> 0 Reaction Kinetics between Charged Reactants in Low Dimensions. *Materials Research Society Symposia Proceedings*, **1996**, 463, 275	
14	The Adhesion Nature of Ag/MgO Interface: Hartree-Fock Study. *Materials Research Society Symposia Proceedings*, **1996**, 458, 15	
13	Microscopic theory of colloid formation in solids under irradiation. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1996**, 37, 49-51	3.1
12	The kinetics of diffusion-controlled annealing of Frenkel defects in alkali halide crystals. *Nuclear Instruments & Methods in Physics Research B*, **1994**, 91, 83-86	1.2
11	The Kinetics of Excitonic Luminescence in Mixed Silver Halides. *Materials Research Society Symposia Proceedings*, **1994**, 348, 309	
10	Luminescence of mixed crystals of silver halides at high excitation densities. *Journal of Applied Spectroscopy*, **1991**, 55, 1140-1145	0.7
9	Modification of the indo method for calculating the characteristics of point defects in ionic crystals. *Theoretical and Experimental Chemistry*, **1984**, 19, 363-369	1.3
8	Two approaches to the theory of diffusion-controlled reactions. *Theoretical and Experimental Chemistry*, **1983**, 18, 238-242	1.3
7	Theoretical Simulations of Surface Relaxation for Perovskite Titanates **2000**, 209-220	
6	Calculations of the Electronic and Atomic Structure and Diffusion of Point Defects in KNbO3 Perovskite Crystals and Relevant KTN Solid Solutions. *Materials Research Society Symposia Proceedings*, **2002**, 718, 1	
5	Atomistic Theory of the Growth Mode for a Thin Metallic Film on an Isulating Substrate **2002**, 525-534	

4	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
3	Nanosession: Ionics - Redox Kinetics, Ion Transport, and Interfaces281-289	
2	Low-temperature radiation effects in wide gap materials. *Low Temperature Physics*, **2016**, 42, 537-538	0.7
1	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