Alexander L Shluger

List of Publications by Year
in descending order

276 papers	13,167 citations	24978 57 h-index	31759 101 g-index
277 all docs	277 docs citations	277 times ranked	10195 citing authors

#	Article	IF	Citations
1	Atomistic insight into the formation dynamics of charged point defects: A classical molecular dynamics study of F+ -centers in NaCl. Physical Review Materials, 2022, 6, .	0.9	1
2	Energies and structures of Cu/Nb and Cu/W interfaces from density functional theory and semi-empirical calculations. Materialia, 2022, 21, 101362.	1.3	13
3	Dielectric breakdown in HfO2 dielectrics: Using multiscale modeling to identify the critical physical processes involved in oxide degradation. Journal of Applied Physics, 2022, 131, .	1.1	21
4	Atomistic origin of high-concentration Ce3+ in {100}-faceted Cr-substituted CeO2 nanocrystals. Acta Materialia, 2021, 203, 116473.	3.8	18
5	Modelling the interactions and diffusion of NO in amorphous SiO₂. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 035008.	0.8	4
6	Electron trapping in ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>HfO</mml:mi></mml:mrow><mml:mn>2</m Physical Review Materials, 2021, 5, .	1.9	9
7	Carboxylate Adsorption on Rutile TiO₂(100): Role of Coulomb Repulsion, Relaxation, and Steric Hindrance. Journal of Physical Chemistry C, 2021, 125, 13770-13779.	1.5	8
8	Ultrasensitive hydrogen detection by electrostatically formed silicon nanowire decorated by palladium nanoparticles. Sensors and Actuators B: Chemical, 2021, 346, 130509.	4.0	11
9	Substitutional Tin Acceptor States in Black Phosphorus. Journal of Physical Chemistry C, 2021, 125, 22883-22889.	1.5	5
10	The nature of column boundaries in micro-structured silicon oxide nanolayers. APL Materials, 2021, 9, 121107.	2.2	2
11	Properties of intrinsic point defects and dimers in hexagonal boron nitride. Journal of Physics Condensed Matter, 2020, 32, 055706.	0.7	26
12	Modeling of Intrinsic Electron and Hole Trapping in Crystalline and Amorphous ZnO. Advanced Electronic Materials, 2020, 6, 1900760.	2.6	15
13	Effect of electric field on defect generation and migration in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2020, 102, .	1.1	14
14	Disorder-induced electron and hole trapping in amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml Physical Review B, 2020, 102, .	1.1	15
15	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. Journal of Materials Chemistry A, 2020, 8, 14054-14061.	5.2	8
16	Inverse Perovskite Oxysilicides and Oxygermanides as Candidates for Nontoxic Infrared Semiconductor and Their Chemical Bonding Nature. Inorganic Chemistry, 2020, 59, 18305-18313.	1.9	4
17	Roadmap on multiscale materials modeling. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 043001.	0.8	100
18	Defects in Oxides in Electronic Devices. , 2020, , 1013-1034.		8

#	Article	IF	Citations
19	Role of long-range exact exchange in polaron charge transition levels: The case of MgO. Physical Review Materials, 2020, 4, .	0.9	8
20	Structural, elastic, vibrational and electronic properties of amorphous Sm2O3 from Ab Initio calculations. Computational Materials Science, 2019, 169, 109119.	1.4	10
21	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>b</mml:mi></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>i</mml:mi><mml:mi>n</mml:mi><mml:mi>i</mml:mi></mml:mrow></mml:math> treatment of silicon-hydrogen bond rupture at <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Si</mml:mi></mml:mrow><mml:mo></mml:mo></mml:msub><mml:mi	1.1	29
22	Modeling of Diffusion and Incorporation of Interstitial Oxygen Ions at the TiN/SiO₂ Interface. ACS Applied Materials & Interfaces, 2019, 11, 36232-36243.	4.0	9
23	First principles calculations of optical properties for oxygen vacancies in binary metal oxides. Journal of Chemical Physics, 2019, 150, 044702.	1.2	27
24	Valence change ReRAMs (VCM) - Experiments and modelling: general discussion. Faraday Discussions, 2019, 213, 259-286.	1.6	2
25	Electrochemical metallization ReRAMs (ECM) - Experiments and modelling: general discussion. Faraday Discussions, 2019, 213, 115-150.	1.6	5
26	Phase-change memories (PCM) â€“ Experiments and modelling: general discussion. Faraday Discussions, 2019, 213, 393-420.	1.6	7
27	The role of surface reduction in the formation of Ti interstitials. RSC Advances, 2019, 9, 12182-12188.	1.7	6
28	Defects in Oxides in Electronic Devices. , 2019, , 1-22.		3
29	Mechanisms of Oxygen Vacancy Aggregation in SiO2 and HfO2. Frontiers in Physics, 2019, 7, .	1.0	41
30	Positronium emission from MgO smoke nanocrystals. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 105004.	0.6	6
31	The origin of negative charging in amorphous Al₂O₃ films: the role of native defects. Nanotechnology, 2019, 30, 205201.	1.3	68
32	First Principles Study of the Influence of the Local Steric Environment on the Incorporation and Migration of NO in a-SiO₂. Materials Science Forum, 2019, 963, 194-198.	0.3	2
33	Making amorphous ZnO: Theoretical predictions of its structure and stability. Physical Review B, 2019, 99, .	1.1	22
34	Recommended Methods to Study Resistive Switching Devices. Advanced Electronic Materials, 2019, 5, 1800143.	2.6	452
35	Reorganization takes energy. Nature Nanotechnology, 2018, 13, 360-361.	15.6	4
36	Intrinsic electron trapping in amorphous oxide. Nanotechnology, 2018, 29, 125703.	1.3	31

#	Article	IF	Citations
37	Intrinsic charge trapping in amorphous oxide films: status and challenges. Journal of Physics Condensed Matter, 2018, 30, 233001.	0.7	55
38	Structure and properties of intrinsic and extrinsic defects in black phosphorus. Nanoscale, 2018, 10, 19536-19546.	2.8	38
39	Correlated Defect Creation in HfO2 films. , 2018, , .		0
40	Theoretical Study of Ag Interactions in Amorphous Silica RRAM Devices. , 2018, , .		1
41	Silicon Oxide (SiO_x): A Promising Material for Resistance Switching?. Advanced Materials, 2018, 30, e1801187.	11.1	156
42	Recombination defects at the 4H-SiC/SiO2 interface investigated with electrically detected magnetic resonance and ab initio calculations. Journal of Applied Physics, 2018, 124, .	1.1	17
43	Relation between image charge and potential alignment corrections for charged defects in periodic boundary conditions. Journal of Chemical Physics, 2018, 149, 024103.	1.2	57
44	Effect of electric field on migration of defects in oxides: Vacancies and interstitials in bulk MgO. Physical Review B, 2018, 98, .	1.1	28
45	Role of electron and hole trapping in the degradation and breakdown of SiO<inf>2</inf> and HfO<inf>2</inf> films. , 2018, , .		4
46	Morphology and Growth Mechanisms of Self-Assembled Films on Insulating Substrates: Role of Molecular Flexibility and Entropy. Journal of Physical Chemistry C, 2017, 121, 4393-4403.	1.5	16
47	A microscopic mechanism of dielectric breakdown in SiO2 films: An insight from multi-scale modeling. Journal of Applied Physics, 2017, 121, .	1.1	93
48	Hole trapping in amorphous HfO2 and Al2O3 as a source of positive charging. Microelectronic Engineering, 2017, 178, 235-239.	1.1	16
49	Defect creation in amorphous HfO2 facilitated by hole and electronÂinjection. Microelectronic Engineering, 2017, 178, 279-283.	1.1	11
50	Diffusion and aggregation of oxygen vacancies in amorphous silica. Journal of Physics Condensed Matter, 2017, 29, 245701.	0.7	48
51	Influence of ions on two-dimensional and three-dimensional atomic force microscopy at fluoriteâ€“water interfaces. Nanotechnology, 2017, 28, 245701.	1.3	17
52	Interactions of hydrogen with amorphous hafnium oxide. Physical Review B, 2017, 95, .	1.1	30
53	Intrinsic Resistance Switching in Amorphous Silicon Suboxides: The Role of Columnar Microstructure. Scientific Reports, 2017, 7, 9274.	1.6	41
54	Theoretical modeling of charge trapping in crystalline and amorphous Al₂O₃. Journal of Physics Condensed Matter, 2017, 29, 314005.	0.7	27

#	Article	IF	Citations
55	Calculating free energies of organic molecules on insulating substrates. Beilstein Journal of Nanotechnology, 2017, 8, 667-674.	1.5	1
56	Nanoscale Transformations in Metastable, Amorphous, Siliconâ€Rich Silica. Advanced Materials, 2016, 28, 7486-7493.	11.1	52
57	Role of hydrogen in volatile behaviour of defects in SiO ₂ -based electronic devices. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160009.	1.0	43
58	Intrinsic electron traps in atomic-layer deposited HfO2 insulators. Applied Physics Letters, 2016, 108, .	1.5	44
59	Silica: Nanoscale Transformations in Metastable, Amorphous, Siliconâ€Rich Silica (Adv. Mater. 34/2016). Advanced Materials, 2016, 28, 7549-7549.	11.1	13
60	Deep electron and hole polarons and bipolarons in amorphous oxide. Physical Review B, 2016, 94, .	1.1	44
61	A mechanism for Frenkel defect creation in amorphous SiO₂facilitated by electron injection. Nanotechnology, 2016, 27, 505207.	1.3	50
62	Contribution of electronic excitation to the structural evolution of ultrafast laser-irradiated tungsten nanofilms. Physical Review B, 2016, 93, .	1.1	15
63	Advanced physical modeling of SiO<inf>x</inf> resistive random access memories. , 2016, , .		6
64	Calculating the Entropy Loss on Adsorption of Organic Molecules at Insulating Surfaces. Journal of Physical Chemistry C, 2016, 120, 3913-3921.	1.5	22
65	A relationship between three-dimensional surface hydration structures and force distribution measured by atomic force microscopy. Nanoscale, 2016, 8, 7334-7342.	2.8	59
66	A mechanism of Cu work function reduction in CsBr/Cu photocathodes. Physical Chemistry Chemical Physics, 2016, 18, 7427-7434.	1.3	4
67	Theoretical models of hydrogen-induced defects in amorphous silicon dioxide. Physical Review B, 2015, 92, .	1.1	62
68	Dynamical simulations of an electronically induced solid-solid phase transformation in tungsten. Physical Review B, 2015, 92, .	1.1	44
69	Electron-Injection-Assisted Generation of Oxygen Vacancies in Monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>HfO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Physical Review Applied, 2015, 4, .	1.5	67
70	Photoinduced Br Desorption from CsBr Thin Films Grown on Cu(100). Journal of Physical Chemistry C, 2015, 119, 24036-24045.	1.5	4
71	Hydrogen-Induced Rupture of Strained Siâ”€O Bonds in Amorphous Silicon Dioxide. Physical Review Letters, 2015, 114, 115503.	2.9	82
72	Structure and properties of electronic and hole centers in CsBr from theoretical calculations. Journal of Physics Condensed Matter, 2015, 27, 245501.	0.7	6

#	Article	IF	Citations
73	Structural stability and polarisation of ionic liquid films on silica surfaces. Physical Chemistry Chemical Physics, 2015, 17, 17661-17669.	1.3	20
74	Optical signatures of intrinsic electron localization in amorphous SiO₂. Journal of Physics Condensed Matter, 2015, 27, 265501.	0.7	17
75	Hole trapping at hydrogenic defects in amorphous silicon dioxide. Microelectronic Engineering, 2015, 147, 141-144.	1.1	12
76	Efficient parametrization of complex moleculeâ€“surface force fields. Journal of Computational Chemistry, 2015, 36, 1187-1195.	1.5	9
77	Modelling of oxygen vacancy aggregates in monoclinic HfO₂: can they contribute to conductive filament formation?. Journal of Physics Condensed Matter, 2015, 27, 415401.	0.7	43
78	Imaging Molecules on Bulk Insulators Using Metallic Tips. Nanoscience and Technology, 2015, , 355-378.	1.5	0
79	Nonthermal solid-to-solid phase transitions in tungsten. Physical Review B, 2014, 90, .	1.1	46
80	Nature of intrinsic and extrinsic electron trapping in SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 89, .	1.1	96
81	Enhanced N₂ Dissociation on Ru-Loaded Inorganic Electride. Journal of the American Chemical Society, 2014, 136, 2216-2219.	6.6	52
82	Shear dynamics of nanoconfined ionic liquids. Physical Chemistry Chemical Physics, 2014, 16, 8247-8256.	1.3	60
83	Hydride ions in oxide hosts hidden by hydroxide ions. Nature Communications, 2014, 5, 3515.	5.8	108
84	Using Metallic Noncontact Atomic Force Microscope Tips for Imaging Insulators and Polar Molecules: Tip Characterization and Imaging Mechanisms. ACS Nano, 2014, 8, 5339-5351.	7.3	36
85	Molecular Design and Control Over the Morphology of Selfâ€Assembled Films on Ionic Substrates. Advanced Materials Interfaces, 2014, 1, 1400414.	1.9	19
86	Identification of intrinsic electron trapping sites in bulk amorphous silica from ab initio calculations. Microelectronic Engineering, 2013, 109, 68-71.	1.1	44
87	Structural dynamics of laser-irradiated gold nanofilms. Physical Review B, 2013, 88, .	1.1	56
88	Determining Adsorption Geometry, Bonding, and Translational Pathways of a Metalâ€“Organic Complex on an Oxide Surface: Co-Salen on NiO(001). Journal of Physical Chemistry C, 2013, 117, 1105-1112.	1.5	18
89	Determination of transient atomic structure of laser-excited materials from time-resolved diffraction data. Applied Physics Letters, 2013, 103, .	1.5	36
90	Models of oxygen vacancy defects involved in degradation of gate dielectrics. , 2013, , .		8

#	Article	IF	Citations
91	Effects of atomic scale roughness at metal/insulator interfaces on metal work function. Physical Chemistry Chemical Physics, 2013, 15, 19615.	1.3	19
92	The behaviour of oxygen at metal electrodes in HfO2 based resistive switching devices. Microelectronic Engineering, 2013, 109, 346-350.	1.1	29
93	A computational study of Si–H bonds as precursors for neutral <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si8.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">E</mml:mi></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math> centres in amorphous silica and at the Si/SiO2 interface. Microelectronic Engineering, 2013, 109, 310-313.	1.1	18
94	Mechanisms of Photodesorption of Br Atoms from CsBr Surfaces. Journal of Physical Chemistry C, 2013, 117, 13502-13509.	1.5	6
95	Effects of Oxide Roughness at Metal Oxide Interface: MgO on Ag(001). Journal of Physical Chemistry C, 2013, 117, 5075-5083.	1.5	23
96	Role of applied bias and tip electronic structure in the scanning tunneling microscopy imaging of highly oriented pyrolytic graphite. Physical Review B, 2012, 85, .	1.1	18
97	Nature of oxygen vacancies and associated electron trapping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, HfO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, and HfSiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:msub><mml:mi>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 116403.	1.1	23
98	Two-Dimensional Polaronic Behavior in the Binary Oxides<mml:math	2.9	56
99	Transient Mobility Mechanisms of Deposited Metal Atoms on Insulating Surfaces: Pd on MgO (100). Journal of Physical Chemistry C, 2012, 116, 14471-14479.	1.5	20
100	Hole Trapping at Surfaces of m-ZrO₂ and m-HfO₂ Nanocrystals. Journal of Physical Chemistry C, 2012, 116, 25888-25897.	1.5	26
101	Models of the interaction of metal tips with insulating surfaces. Beilstein Journal of Nanotechnology, 2012, 3, 329-335.	1.5	8
102	Exciton-Driven Highly Hyperthermal O-Atom Desorption from Nanostructured CaO. Journal of Physical Chemistry C, 2011, 115, 692-699.	1.5	5
103	Structure and properties of oxygen centers in CaF<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>crystals fromab initioembedded cluster calculations. Physical Review B, 2011, 84, .	1.1	22
104	Atom-resolved imaging of ordered defect superstructures at individual grain boundaries. Nature, 2011, 479, 380-383.	13.7	219
105	Role of water in atomic resolution AFM in solutions. Physical Chemistry Chemical Physics, 2011, 13, 12584.	1.3	54
106	Electron and hole trapping in polycrystalline metal oxide materials. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 2043-2053.	1.0	36
107	Chemical Resolution at Ionic Crystal Surfaces Using Dynamic Atomic Force Microscopy with Metallic Tips. Physical Review Letters, 2011, 106, 216102.	2.9	56
108	Organic Molecules Reconstruct Nanostructures on Ionic Surfaces. Small, 2011, 7, 1264-1270.	5.2	18

#	Article	IF	Citations
109	Recent Trends in Surface Characterization and Chemistry with Highâ€Resolution Scanning Force Methods. Advanced Materials, 2011, 23, 477-501.	11.1	214
110	Mechanism of laser assisted field evaporation from insulating oxides. Ultramicroscopy, 2011, 111, 567-570.	0.8	45
111	QM/MM method for metalâ€“organic interfaces. Journal of Computational Chemistry, 2010, 31, 2955-2966.	1.5	9
112	The effect of van der Waals interactions on the properties of intrinsic defects in graphite. Carbon, 2010, 48, 4145-4161.	5.4	37
113	Structure and properties of surface and subsurface defects in graphite accounting for van der Waals and spin-polarization effects. Physical Review B, 2010, 82, .	1.1	17
114	Mechanism of Contrast Formation in Atomic Force Microscopy in Water. Physical Review Letters, 2010, 105, 196101.	2.9	47
115	Unambiguous Determination of the Adsorption Geometry of a Metalâ^'Organic Complex on a Bulk Insulator. Nano Letters, 2010, 10, 2965-2971.	4.5	35
116	Functionalized Truxenes: Adsorption and Diffusion of Single Molecules on the KBr(001) Surface. ACS Nano, 2010, 4, 3429-3439.	7.3	58
117	Bonding of Methyl Phosphonate to TiO₂(110). Journal of Physical Chemistry C, 2010, 114, 16983-16988.	1.5	23
118	Controlling electron transfer processes on insulating surfaces with the non-contact atomic force microscope. Nanotechnology, 2009, 20, 264019.	1.3	12
119	Positive and Negative Oxygen Vacancies in Amorphous Silica. ECS Transactions, 2009, 19, 3-17.	0.3	77
120	Oxygen ion conduction in 12CaOÂ·7Al2O3: O2â^' conduction mechanism and possibility of Oâ^' fast conductionâ˜†. Solid State Ionics, 2009, 180, 550-555.	1.3	57
121	Excitation, Ionization, and Desorption: How Sub-Band Gap Photons Modify the Structure of Oxide Nanoparticles. Journal of Physical Chemistry C, 2009, 113, 1274-1279.	1.5	16
122	Doubly positively charged oxygen vacancies in silica glass. Journal of Non-Crystalline Solids, 2009, 355, 1103-1106.	1.5	2
123	Modeling proton transfer and polarons in a molecular crystal diamino-dinitroethylene. Physical Review B, 2009, 80, .	1.1	16
124	Structure and diffusion of intrinsic defects, adsorbed hydrogen, and water molecules at the surface of alkali-earth fluorides calculated using density functional theory. Physical Review B, 2009, 80, .	1.1	32
125	The interaction of oxygen vacancies with grain boundaries in monoclinic HfO2. Applied Physics Letters, 2009, 95, .	1.5	178
126	Siâ€“SiO₂ interface bandâ€gap transition â€“ effects on MOS inversion layer. Physica Status Solidi (A) Applications and Materials Science, 2008, 205, 1290-1295.	0.8	29

#	Article	IF	Citations
127	Intramolecular Dipole Coupling and Depolarization in Selfâ€Assembled Monolayers. Advanced Functional Materials, 2008, 18, 2228-2236.	7.8	57
128	Physics of Nanomechanical Biosensing on Cantilever Arrays. Advanced Materials, 2008, 20, 3848-3853.	11.1	53
129	Energy and site selectivity in O-atom photodesorption from nanostructured MgO. Surface Science, 2008, 602, 1968-1973.	0.8	22
130	Insulatorâ€“conductor transition in 12CaOÂ·7Al2O3 films: On the stability of the crystal lattice under Ar+ bombardment. Thin Solid Films, 2008, 516, 1350-1353.	0.8	4
131	Electron-trapping polycrystalline materials with negative electron affinity. Nature Materials, 2008, 7, 859-862.	13.3	122
132	Modeling of NCâ€AFM Imaging of Alkanethiols on the Au (111) Surface. Israel Journal of Chemistry, 2008, 48, 99-106.	1.0	1
133	Oxygen vacancies in cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> studied by anab initioembedded cluster method. Physical Review B, 2008, 78, .	3.7	37
134	Crystallographic phase transition and high-T_csuperconductivity in LaFeAsO:F. Superconductor Science and Technology, 2008, 21, 125028.	1.8	230
135	F and F⁺ Centers on MgO/Ag(100) or MgO/Mo(100) Ultrathin Films:â€‰ Are They Stable?. Journal of Physical Chemistry C, 2008, 112, 3857-3865.	1.5	31
136	Effect of Molecular and Lattice Structure on Hydrogen Transfer in Molecular Crystals of Diamino-dinitroethylene and Triamino-trinitrobenzene. Journal of Physical Chemistry A, 2008, 112, 4496-4500.	1.1	53
137	Modeling the Diffusive Motion of Large Organic Molecules on Insulating Surfaces. Journal of Physical Chemistry C, 2008, 112, 19577-19583.	1.5	16
138	Designing Molecular Architecture to Control Diffusion and Adsorption on Insulating Surfaces. Journal of Physical Chemistry C, 2008, 112, 4226-4231.	1.5	20
139	Origin of the Asymmetry in the Magnitude of the Statistical Variability of n- and p-Channel Poly-Si Gate Bulk MOSFETs. IEEE Electron Device Letters, 2008, 29, 913-915.	2.2	46
140	AN EFFECT OF CHARGED AND EXCITED STATES ON DECOMPOSITION OF 1,1-DIAMINO-2,2-DINITROETHYLENE. , 2008, , .		0
141	Dynamics of low-coordinated surface atoms on gold nanocrystallites. Journal of Chemical Physics, 2007, 126, 154704.	1.2	10
142	A comparison of dynamic atomic force microscope set-ups for performing atomic scale manipulation experiments. Nanotechnology, 2007, 18, 345503.	1.3	5
143	Controlled Manipulation of Atoms in Insulating Surfaces with the Virtual Atomic Force Microscope. Physical Review Letters, 2007, 98, 028101.	2.9	39
144	Electron Trapping at Point Defects on Hydroxylated Silica Surfaces. Physical Review Letters, 2007, 99, 136801.	2.9	45

#	Article	IF	Citations
145	Effect of Protons on the Optical Properties of Oxide Nanostructures. Journal of the American Chemical Society, 2007, 129, 12491-12496.	6.6	45
146	Dynamical processes at oxide surfaces studied with the virtual atomic force microscope. Physical Review B, 2007, 76, .	1.1	26
147	Multiscale model of the manipulation of single atoms on insulating surfaces using an atomic force microscope tip. Physical Review B, 2007, 76, .	1.1	29
148	Trapping, self-trapping and the polaron family. Journal of Physics Condensed Matter, 2007, 19, 255208.	0.7	182
149	Hydrogen Cycle on CeO₂ (111) Surfaces:â€‰ Density Functional Theory Calculations. Journal of Physical Chemistry C, 2007, 111, 15337-15341.	1.5	131
150	Theoretical Prediction of Intrinsic Self-Trapping of Electrons and Holes in Monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2007, 99, 155504.	2.9	133
151	Shaping the Morphology of Gold Nanoparticles by CO Adsorption. Journal of Physical Chemistry C, 2007, 111, 18848-18852.	1.5	51
152	Inside Powders:Â A Theoretical Model of Interfaces between MgO Nanocrystallites. Journal of the American Chemical Society, 2007, 129, 8600-8608.	6.6	55
153	Nanoporous Crystal 12CaOÂ·7Al2O3:Â A Playground for Studies of Ultraviolet Optical Absorption of Negative Ions. Journal of Physical Chemistry B, 2007, 111, 1946-1956.	1.2	61
154	Dipoleâ^'Dipole Interactions and the Structure of Self-Assembled Monolayers. Journal of Physical Chemistry B, 2007, 111, 4019-4025.	1.2	36
155	Building Blocks for Molecular Devices:â€‰ Organic Molecules on the MgO (001) Surface. Journal of Physical Chemistry C, 2007, 111, 15375-15381.	1.5	20
156	Transient Atomic Configurations of Supported Gold Nanocrystallites at Finite Temperature. Journal of Physical Chemistry C, 2007, 111, 2823-2826.	1.5	11
157	Effect of charged and excited states on the decomposition of 1,1-diamino-2,2-dinitroethylene molecules. Journal of Chemical Physics, 2007, 126, 234711.	1.2	50
158	Spectroscopic properties of oxygen vacancies in monoclinicHfO2calculated with periodic and embedded cluster density functional theory. Physical Review B, 2007, 75, .	1.1	196
159	From Insulator to Electride:Â A Theoretical Model of Nanoporous Oxide 12CaOÂ·7Al2O3. Journal of the American Chemical Society, 2007, 129, 942-951.	6.6	115
160	Optical and EPR properties of point defects at a crystalline silica surface:Ab initioembedded-cluster calculations. Physical Review B, 2007, 75, .	1.1	49
161	The vulnerable nanoscale dielectric. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 653-662.	0.8	5
162	Electronic structure and spectroscopic properties of interstitial anions in the nanoporous complex oxide 12CaOÂ·7Al2O3. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 663-669.	0.8	9

#	Article	IF	Citations
163	Atomic fingerprinting. Nature, 2007, 446, 34-35.	13.7	7
164	Simple Model for DNA Adsorption onto a Mica Surface in 1:1 and 2:1 Electrolyte Solutions. Langmuir, 2006, 22, 7678-7688.	1.6	51
165	Chemisorption of HCl to the MgO(001) surface: A DFT study. Physical Chemistry Chemical Physics, 2006, 8, 4359.	1.3	15
166	Negative oxygen vacancies in HfO2 as charge traps in high-k stacks. Applied Physics Letters, 2006, 89, 082908.	1.5	295
167	Interaction of Organic Molecules with the TiO2(110) Surface:Â Ab Inito Calculations and Classical Force Fields. Journal of Physical Chemistry B, 2006, 110, 4853-4862.	1.2	50
168	Probing Electron Transfer Dynamics at MgO Surfaces by Mg-Atom Desorption. Journal of Physical Chemistry B, 2006, 110, 18093-18096.	1.2	11
169	Ab initio modeling of electron-phonon coupling in high-k dielectrics. Physica Status Solidi C: Current Topics in Solid State Physics, 2006, 3, 3382-3385.	0.8	13
170	Simulation of coherent control of hydroxyl formed due to HCl adsorption on MgO(001). Chemical Physics, 2006, 330, 253-264.	0.9	2
171	Modelling of non-contact atomic force microscopy imaging of individual molecules on oxide surfaces. Nanotechnology, 2006, 17, 2062-2072.	1.3	18
172	Modelling atomic scale manipulation with the non-contact atomic force microscope. Nanotechnology, 2006, 17, 5866-5874.	1.3	26
173	Site-specific laser modification of MgO nanoclusters: Towards atomic-scale surface structuring. Physical Review B, 2006, 74, .	1.1	24
174	Manipulation of defects on oxide surfaces via barrier reduction induced by atomic force microscope tips. Physical Review B, 2006, 73, .	1.1	29
175	Photoluminescence from Au ion-implanted nanoporous single-crystal12CaOâˆ™7Al2O3. Physical Review B, 2006, 73, .	1.1	42
176	Polaron-like Charge Trapping in Oxygen Deficient and Disordered HfO2: Theoretical Insight. ECS Transactions, 2006, 3, 277-290.	0.3	20
177	Localisation assisted by the lattice relaxation and the optical absorption of extra-framework electrons in 12CaOÂ·Al2O3. Materials Science and Engineering C, 2005, 25, 722-726.	3.8	16
178	The effect of the ?-quartz lattice on the optical absorption and stretching frequency of the interstitial O2 molecule. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 503-506.	0.8	4
179	The oxide gate dielectric: do we know all we should?. Journal of Physics Condensed Matter, 2005, 17, S2027-S2049.	0.7	19
180	Measuring Site-Specific Clusterâˆ'Surface Bond Formation. Journal of the American Chemical Society, 2005, 127, 17863-17866.	6.6	29

#	Article	IF	Citations
181	Laser Control of Desorption through Selective Surface Excitation. Journal of Physical Chemistry B, 2005, 109, 19563-19578.	1.2	48
182	Probing Organic Layers on the TiO2(110) Surface. Journal of Physical Chemistry B, 2005, 109, 4554-4560.	1.2	22
183	Hydride Ion as a Two-Electron Donor in a Nanoporous Crystalline Semiconductor 12CaOÂ·7Al2O3. Journal of Physical Chemistry B, 2005, 109, 23836-23842.	1.2	55
184	Spectroscopic features of dimer and dangling bondEâ€² centres in amorphous silica. Journal of Physics Condensed Matter, 2005, 17, 1311-1318.	0.7	15
185	Structure and properties of defects in amorphous silica: new insights from embedded cluster calculations. Journal of Physics Condensed Matter, 2005, 17, S2115-S2140.	0.7	69
186	Realistic model tips in simulations of nc-AFM. Nanotechnology, 2004, 15, S60-S64.	1.3	19
187	Theoretical simulation of non-contact atomic force microscopy imaging of the Â-alumina(0001) surface. Nanotechnology, 2004, 15, S108-S114.	1.3	2
188	Interaction of Silicon Dangling Bonds with Insulating Surfaces. Physical Review Letters, 2004, 92, 036101.	2.9	28
189	Laser control of product electronic state: Desorption from alkali halides. Journal of Chemical Physics, 2004, 120, 2456-2463.	1.2	13
190	Determination of surface exciton energies by velocity resolved atomic desorption. Surface Science, 2004, 564, 62-70.	0.8	30
191	Calibration of embedded-cluster method for defect studies in amorphous silica. Physical Review B, 2004, 69, .	1.1	48
192	Reactivity of (H+)(eâ^') color centers at the MgO surface: formation of O2â^' and N2â^' radical anions. Surface Science, 2003, 542, 293-306.	0.8	30
193	Hopping and optical absorption of electrons in nano-porous crystal 12CaOÂ·7Al2O3. Thin Solid Films, 2003, 445, 161-161.	0.8	4
194	Paramagnetic Defect Centers at the MgO Surface. An Alternative Model to Oxygen Vacancies. Journal of the American Chemical Society, 2003, 125, 738-747.	6.6	134
195	Towards chemical identification in atomic-resolution noncontact AFM imaging with silicon tips. Physical Review B, 2003, 68, .	1.1	32
196	Theories of scanning probe microscopes at the atomic scale. Reviews of Modern Physics, 2003, 75, 1287-1331.	16.4	432
197	Electron Localization and a Confined Electron Gas in Nanoporous Inorganic Electrides. Physical Review Letters, 2003, 91, 126401.	2.9	192
198	Modeling charge self-trapping in wide-gap dielectrics: Localization problem in local density functionals. Physical Review B, 2003, 67, .	1.1	87

#	Article	IF	Citations
199	Mechanism of Interstitial Oxygen Diffusion in Hafnia. Physical Review Letters, 2002, 89, 225901.	2.9	146
200	Role of tip structure and surface relaxation in atomic resolution dynamic force microscopy:CaF2(111)as a reference surface. Physical Review B, 2002, 66, .	1.1	79
201	Control of laser desorption using tunable single pulses and pulse pairs. Journal of Chemical Physics, 2002, 116, 8144-8151.	1.2	16
202	Wavelength selective excitation of surface oxygen anions on highly dispersed MgO. Journal of Chemical Physics, 2002, 116, 1707-1712.	1.2	62
203	Electron trapping at neutral divacancy sites on the MgO surface. Journal of Chemical Physics, 2002, 117, 2844-2851.	1.2	63
204	Solid-state halogen atom source for chemical dynamics and etching. Applied Physics Letters, 2002, 81, 1140-1142.	1.5	8
205	Electronic Properties of Structural Defects at the MgO (001) Surface. Journal of Physical Chemistry B, 2002, 106, 2269-2276.	1.2	140
206	Energies and Dynamics of Photoinduced Electron and Hole Processes on MgO Powders. Journal of Physical Chemistry B, 2002, 106, 12478-12482.	1.2	54
207	Asymmetry and long-range character of lattice deformation by neutral oxygen vacancy in Î±-quartz. Physical Review B, 2002, 66, .	1.1	131
208	Quantitative modelling in scanning force microscopy on insulators. Applied Surface Science, 2002, 188, 306-318.	3.1	20
209	Vacancy and interstitial defects in hafnia. Physical Review B, 2002, 65, .	1.1	560
210	Atomic and ionic processes of silicon oxidation. Physical Review B, 2001, 63, .	1.1	70
211	Contrast formation in atomic resolution scanning force microscopy on CaF2(111): experiment and theory. Journal of Physics Condensed Matter, 2001, 13, 2061-2079.	0.7	93
212	Role of disorder in incorporation energies of oxygen atoms in amorphous silica. Physical Review B, 2001, 63, .	1.1	56
213	Modeling disorder in amorphous silica with embedded clusters:â€ƒThe peroxy bridge defect center. Physical Review B, 2001, 64, .	1.1	39
214	Periodic density functional plane wave calculations of triplet exciton in NaCl. Radiation Effects and Defects in Solids, 2001, 155, 311-315.	0.4	1
215	An effect of thermal disorder on the electronic structure of MgO. Radiation Effects and Defects in Solids, 2001, 154, 217-222.	0.4	1
216	Structure and electrical levels of point defects in monoclinic zirconia. Physical Review B, 2001, 64, .	1.1	307

#	Article	IF	Citations
217	Unambiguous Interpretation of Atomically Resolved Force Microscopy Images of an Insulator. Physical Review Letters, 2001, 86, 2373-2376.	2.9	156
218	Selective laser desorption of ionic surfaces: Resonant surface excitation of KBr. Journal of Chemical Physics, 2001, 115, 9463-9472.	1.2	35
219	Thermal fluctuations, localization, and self-trapping in a polar crystal: Combined shell-model molecular dynamics and quantum chemical approach. Physical Review B, 2001, 64, .	1.1	20
220	Embedded cluster calculations of metal complex impurity defects: properties of the iron cyanide in NaCl. Journal of Physics Condensed Matter, 2000, 12, 8257-8266.	0.7	33
221	Atomically resolved edges and kinks of NaCl islands on Cu(111): Experiment and theory. Physical Review B, 2000, 62, 2074-2084.	1.1	213
222	Structure and Spectroscopy of Surface Defects from Scanning Force Microscopy: Theoretical Predictions. Physical Review Letters, 2000, 85, 3846-3849.	2.9	12
223	Laser-induced reactions in crystals:â€ƒFemtosecond pump-probe spectroscopy andab initiocalculations of self-trapped excitons and holes in KBr. Physical Review B, 2000, 61, 5392-5402.	1.1	31
224	Relative energies of surface and defect states: ab initio calculations for the MgO (001) surface. Surface Science, 2000, 450, 153-170.	0.8	336
225	Models of image contrast in scanning force microscopy on insulators. Journal of Physics Condensed Matter, 1999, 11, R295-R322.	0.7	26
226	Model of noncontact scanning force microscopy on ionic surfaces. Physical Review B, 1999, 59, 2436-2448.	1.1	134
227	Embedded cluster approach: Application to complex defects. Radiation Effects and Defects in Solids, 1999, 151, 215-221.	0.4	4
228	Atomic and chemical resolution in scanning force microscopy on ionic surfaces. Applied Surface Science, 1999, 141, 274-286.	3.1	6
229	Contrast mechanism in non-contact SFM imaging of ionic surfaces. Applied Surface Science, 1999, 140, 327-332.	3.1	29
230	Spectroscopy of low-coordinated surface sites:â€‚Theoretical study of MgO. Physical Review B, 1999, 59, 2417-2430.	1.1	164
231	Mg clusters on MgO surfaces: study of the nucleation mechanism with MIES and ab initio calculations. Faraday Discussions, 1999, 114, 173-194.	1.6	77
232	Electronic structure of excited states at low-coordinated surface sites of MgO. Surface Science, 1999, 421, L157-L165.	0.8	37
233	Dynamics of Silicon Oxidation. Materials Research Society Symposia Proceedings, 1999, 592, 30.	0.1	4
234	Self-lubrication in scanning-force-microscope image formation on ionic surfaces. Physical Review B, 1997, 56, 12482-12489.	1.1	49

#	Article	IF	Citations
235	Ionic and electronic processes at ionic surfaces induced by atomic-force-microscope tips. Physical Review B, 1997, 56, 15332-15344.	1.1	62
236	One-center trapping of the holes in alkali halide crystals. Physical Review B, 1996, 54, 962-969.	1.1	35
237	Atomic and Electronic Structure of the Corundum (0001) Surface. Materials Research Society Symposia Proceedings, 1996, 453, 721.	0.1	2
238	A model of the interaction of ionic tips with ionic surfaces for interpretation of scanning force microscope images. Topics in Catalysis, 1996, 3, 221-247.	1.3	14
239	Polarization of a semi-infinite crystal by a point defect at the surface. Physical Review B, 1996, 53, 136-147.	1.1	5
240	Electron correlation in the self-trapped hole and exciton in the NaCl crystal. Physical Review B, 1995, 52, 6254-6264.	1.1	23
241	Model of scanning force microscopy on ionic surfaces. Physical Review B, 1995, 52, 11398-11411.	1.1	19
242	Optical transitions of theHcenters in alkali halides. Physical Review B, 1995, 52, 4017-4028.	1.1	26
243	Properties of small clusters at ionic surfaces: (NaCl)nclusters (n=1â€“48) at the (100) MgO surface. Physical Review B, 1995, 51, 13631-13644.	1.1	22
244	Topography and dynamics of surface defects on ionic crystals. Radiation Effects and Defects in Solids, 1995, 137, 1-9.	0.4	0
245	Dynamics of lithium ions in lithium oxide. Radiation Effects and Defects in Solids, 1995, 134, 107-110.	0.4	4
246	The excitonic mechanism of Na-atom desorption from the (100)NaCl surface. Journal of Physics Condensed Matter, 1995, 7, L147-L151.	0.7	10
247	Lateral and friction forces originating during force microscope scanning of ionic surfaces. Surface Science, 1995, 343, 273-287.	0.8	32
248	(100) GaP surface charges, potentials, and stoichiometry; a quantum-chemical study. Journal of Physics Condensed Matter, 1994, 6, 4255-4268.	0.7	20
249	Theoretical study of Na-atom emission from NaCl (100) surfaces. Physical Review B, 1994, 49, 11364-11373.	1.1	54
250	Theoretical and experimental investigation of force imaging at the atomic scale on alkali halide crystals. Physical Review B, 1994, 49, 4915-4930.	1.1	70
251	Atomistic theory of the interaction between AFM tips and ionic surfaces. Journal of Physics Condensed Matter, 1994, 6, 1825-1846.	0.7	66
252	Theoretical study of the stabilization of cubic-phaseZrO2by impurities. Physical Review B, 1994, 49, 11560-11571.	1.1	202

#	Article	IF	Citations
253	Small polarons in real crystals: concepts and problems. Journal of Physics Condensed Matter, 1993, 5, 3049-3086.	0.7	151
254	Modelling of the impurity-vacancy interaction in magnesium doped lithium oxide. Journal of Physics Condensed Matter, 1993, 5, 7397-7408.	0.7	7
255	Simulation of defect processes: experiences with the self-trapped exciton. Modelling and Simulation in Materials Science and Engineering, 1993, 1, 673-692.	0.8	34
256	Theoretical studies of atomic emission and defect formation by electronic excitation at the (100) surface of NaCl. Physical Review B, 1993, 47, 10760-10768.	1.1	58
257	Model of self-trapped excitons in alkali halides. Physical Review B, 1993, 47, 6226-6240.	1.1	57
258	Theoretical simulation of VK-centre migration in KCl. I. A quantum-chemical study. Journal of Physics Condensed Matter, 1992, 4, 7417-7428.	0.7	22
259	Theoretical simulation of localized holes in MgO. Journal of Physics Condensed Matter, 1992, 4, 5711-5722.	0.7	33
260	Calculation of adiabatic barriers for cation diffusion in Li2O and LiCl crystals. Modelling and Simulation in Materials Science and Engineering, 1992, 1, 29-38.	0.8	31
261	The calculation of the self-trapping energy in crystals with mixed valence band. Journal of Physics Condensed Matter, 1992, 4, 8311-8320.	0.7	16
262	Self-trapped excitons and interstitial-vacancy pairs in oxides. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1991, 63, 955-964.	0.6	14
263	Structure and interaction of impurity-vacancy (Mg2+-Vc-) dipoles in crystalline LiF. Journal of Physics Condensed Matter, 1991, 3, 2237-2245.	0.7	14
264	A new model for the self-trapped exciton in alkali halides. Journal of Physics Condensed Matter, 1991, 3, 3125-3128.	0.7	20
265	Two types of self-trapped excitons in alkali halide crystals. Physical Review B, 1991, 44, 1499-1508.	1.1	40
266	Self-trapping holes and excitons in the bulk and on the (100) surfaces of MgO. Journal of Physics Condensed Matter, 1991, 3, 8027-8036.	0.7	52
267	The model of a triplet self-trapped exciton in crystalline SiO2. Journal of Physics C: Solid State Physics, 1988, 21, L431-L434.	1.5	62
268	On the nonequivalency of Si-O bonds in silicon dioxide. Journal of Physics and Chemistry of Solids, 1986, 47, 659-664.	1.9	7
269	Quantum-chemical simulation of impurity-induced trapping of a hole: (Li)0centre in MgO. Journal of Physics C: Solid State Physics, 1986, 19, 4183-4199.	1.5	62
270	Application of molecular models to electronic structure calculations of defects in oxide crystals. I. Parametrization of the modified INDO method. Theoretica Chimica Acta, 1985, 66, 355-363.	0.9	85

#	Article	IF	Citations
271	The semiempirical approach to electronic structure of ionic crystal surface. Journal of Physics C: Solid State Physics, 1982, 15, 847-861.	1.5	22
272	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.	0.7	22
273	Semiempirical Calculations of Defect Properties in LiF Crystal. Physica Status Solidi (B): Basic Research, 1981, 108, 673-681.	0.7	22
274	Identifying Performance Limiting Defects in Silicon Carbide pn-Junctions: A Theoretical Study. Materials Science Forum, 0, 858, 257-260.	0.3	2
275	Evidence for an Abrupt Transition between SiO₂ and SiC from EELS and <i>Ab Initio</i> Modelling. Materials Science Forum, 0, 963, 199-203.	0.3	1
276	Optical and EPR properties of point defects at a crystalline silica surface: Ab initio embedded-cluster calculations. , 0, .		1